Conceptual problems in quantum electrodynamics: a contemporary historical-philosophical approach

Tesis doctoral

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Universidad de Sevilla 2011

Problemas conceptuales en la electrodinámica cuántica: un enfoque histórico-filosófico contemporáneo

Trabajo de investigación para la obtención del Grado de Doctor por la Universidad de Sevilla

Conceptual problems in quantum electrodynamics: a contemporary historical-philosophical approach

Dissertation submitted in fulfillment of the requirements for the Degree of Doctor by the Universidad de Sevilla

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Acknowledgements

I want to express my gratitude to José Ferreirós Domínguéz and Henrik Zinkernagel for making possible this dissertation. I also want to thank Olivier Darrigol with whom I had a productive interchange of views regarding distinct aspects of this work.

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CAPÍTULO 1

INTRODUCCIÓN

De acuerdo con los requisitos del doctorado europeo se presenta una introducción, resumen y conclusiones en español, estado el cuerpo de la tesis presentado en inglés. Se incluye primeramente una brevísima introducción en inglés.

Summary of the introduction

In this work I address what can be called conceptual-mathematical anomalies in quantum electrodynamics. By this I mean conceptual and mathematical problems of the theory that do not affect 'saving the phenomena'. A well-known example is the divergent expressions that appear in the applications of the theory, which can be renormalized without implying any kind of problem in what regards the predictions of the theory.

This work can be seen as following the line of philosophy of physics studies of quantum field theory that started to emerge in a systematic way in the early eighties of last century. One example is Teller's (1995) work on standard quantum electrodynamics.[1] More recently the field has become dominated by scholars that tend to prefer more formal approaches, relying not on the set of theories of the so-called standard model but on tentative formal approaches that promise to give to quantum field theory the solid mathematical foundations that it does not have (see e.g. Fraser 2009). The particular characteristic of these approaches is that they do not deliver testable predictions.

In this work, by following a historical approach, I will return to the standard version of quantum electrodynamics (which is the only one available when we want to get numbers out to compare with experimental results). In this way I will be considering the contributions and discussions by physicists like Einstein, Bohr, Jordan, Pauli, Heisenberg, Fermi, Dirac, Feynman, and others. This does not mean that I will not take into account 'formal' results. That is not the case. Simply, I consider more interesting understanding the physical theories we really have and trying to see how they work so well in the middle of a sea of anomalies. A historical approach enables us to return to the original moments when the concepts were being developed and the problems faced for the first time; it also enables to take advantage of the insights of the physicists that created the theory. However I must call attention to the fact that I am not doing history.

[1] What makes Teeler's work to be not simply a work on foundations of physics but a philosophical account of quantum field theory is, in particular, his exploration of an interpretation of quantum fields in terms of propensity (instead of substance). This has implicit worries of an ontological nature; in simple terms it relates to the philosophical question of what is the ontological implication of a physical description in terms of quantum fields.

What I am doing is using history as a guide to a tentative clarification of some unclear aspects of the theory.

Since I am not taking into account more recent contributions, a work that goes back to the early fifties of last century and before might seem dated. Here I must distinguish between the above mentioned 'formal' approaches and technical developments made in quantum electrodynamics. Two good examples of these are the use of renormalization group technics and lattice regularization. To the best of my knowledge these more recent developments do not affect the views being presented here. They might complement them, but it was never my intention to present a full study of all the facets of quantum electrodynamics. My objective is less ambitious; it is to show that a historical approach can deliver interesting and 'new' insights regarding current philosophical issues related to quantum field theory in general and quantum electrodynamics in particular.

This work spins around two main vectors. One is the divergence of the S-matrix series expansion; the other is the spatio-temporal description of physical processes in the theory. Regarding the first vector, I will be presenting an interpretation that for some will seem a bit strange (my interpretation resembles views by Bohr from the early thirties of last century); also (independently of my particular interpretation) I will explore the consequences of having just an asymptotic series to describe the interaction of radiation and matter. In a nutshell I defend that having an asymptotic series implies that the theory is intrinsically approximate, i.e. it can only describe the interaction of radiation and matter in an approximate way with just a few terms of a series expansion and not give an exact solution corresponding to treating radiation and matter as one closed system.[2] Here I am not simply accepting pragmatically a fact. The use of only a few terms of an infinite series expansion must be philosophically made acceptable by clarifying the concepts of radiation and matter and their interaction as implemented in the mathematical structure of the theory; that is, I want to provide a 'philosophical' justification for disregarding the large-order terms of the series expansion (by addressing 'gently' the question of the relation of the mathematical structure to the physical concepts this structure gives 'flesh' to).

Philosophically the typical justification of saying that the computational time would make impossible, in practice, to calculate large-order terms is not enough; neither saying that the possible contribution of these terms is irrelevant since at a high-energy new physics is coming in. This is the usual position of the believers in string theory or whatever theory of everything that might be 'underneath' the standard model. For these, quantum electrodynamics is just an effective field theory that works well in a particular energy range, being only a 'valid' approximation (even if just delivering asymptotic results) to an underlining level of description of reality. On this view the divergence of the S-matrix series expansion is considered unproblematic. I have no reason to believe in this traditional Nagel type of intertheoretical reduction. In fact the second vector of my work leads me to consider that quantum electrodynamics cannot be seen as more fundamental than classical electrodynamics, i.e. the relation of classical and quantum electrodynamics is not one of theory reduction but more complex.

[2] The readers even if not agreeing with my view that quantum electrodynamics consists in an intrinsically perturbative approach should at least not too easily rely on so-called non-perturbative 'results' and take the time for a critical analysis of these. For example it is usually considered that the lattice regularization is non-perturbative because from the start the space-time lattice implies an energy-momentum cutoff to all orders of the perturbative calculation. However in lattice quantum electrodynamics we still have a divergent S-matrix, and it is this that makes the theory intrinsically approximate.

The study of the spatio-temporal description of physical processes in quantum electrodynamics is the other main vector of my work. Again I present a controversial view. Quantum electrodynamics is not able to describe physical processes in time in a way similar to classical theory. In fact it *relies on* the classical temporality (as time goes by…) to construct an asymptotic temporal description, in the sense of going from $-\infty$ to $+\infty$, of physical processes (we will see for example that it is this characteristic that enables the charge renormalization procedure). This, in Feynman's words, global space-time approach has severe limitations in what regards the possibility of describing such a simple thing as a delayed interaction between charged particles, and I do not see how we can from the quantum electrodynamical level of description arrive at the temporal description of classical electrodynamics.

Here is how I delelop my views. To warm up for the discussion of the Dirac equation and its interpretation being given in chapter 3, I will consider in chapter 2 the simpler case of the Schrödinger equation and (part of) its interpretations. In chapter 3, by trying to fit together the different interpretations of the Dirac equation, analyzing in particular the two-body problem, I will arrive at the well-known description of interactions in terms of quanta exchange. In chapter 4 I will consider the other cornerstone of quantum electrodynamics, the quantized electromagnetic field, and try a clarification of the concept (or better, notion) of quantum vacuum. The description of interactions in quantum electrodynamics is addressed in chapter 5. Here I will consider the problem of the divergence of the series expansion of the S-matrix and the relevance or not of the Haag theorem to the consistency of the theory. Chapter 6 is dedicated to an excursion into the history of renormalization and to recover views by Bohr and Dirac that I consider to present renormalization in a 'new' light. In chapter 7 I analyze the spatio-temporal description of physical processes in quantum electrodynamics and the status of the so-called virtual quanta (that are a crucial element in the description of interactions in terms of quanta exchange). Finally the results of chapter 7 are used in chapter 8 to defend the idea that quantum electrodynamics is an upgrade of classical electrodynamics and the theory of relativity (i.e. that classical electrodynamics does not reduces to quantum electrodynamics). In the appendix I make a digression and present an analysis of Bohr's views on space and time in quantum mechanics in relation to his quantum postulate (this will enable to address the Bohrian interpretation of the wave function followed in this work).

Comentarios iniciales

Un interés sistemático desde una perspectiva más filosófica respecto a la teoría cuántica de campos es algo reciente, de la década de los 80. Esto no significa que temas que se han tornado tópicos del debate filosófico no se hayan mencionado antes. Un ejemplo es el tratamiento por M. Bunge del estatus de las llamadas partículas virtuales en la electrodinámica cuántica (Bunge, 1970). Pero un tratamiento sistemático - una especie de programa de investigación filosófica de la teoría cuántica de campos – ganó 'momentum' en los 80 en particular con los trabajos de M. Redhead y P. Telller.

Centrándome en la aportación de Teller y en particular en su libro "An interpretive introduction to quantum field theory" del 95, Teller, enfocando la electrodinámica cuántica, analiza una serie de aspectos de la teoría: trata de interpretar la teoría. ¿Qué es según Teller, en la práctica, interpretar la teoría? Por lo menos en parte es claramente un análisis conceptual de la teoría. Teller propone interpretar el concepto de partícula, específicamente de cuanto, que se tiene en la teoría tratando de distinguirlo de la concepción clásica; también el concepto de campo cuántico; la descripción de interacciones, y la cuestión de la renormalización. ¿Qué hace que este análisis conceptual sea algo filosófico y no simplemente algo hecho por un físico? Simplemente que el enfoque parta de una actitud filosófica. Así en este caso particular, asistimos, por ejemplo, a la propuesta por Teller de sustitución de la idea de sustancia por la de propensión (propensity) para hablar de los campos cuánticos (pues un campo cuántico se tiene que ver como 'estando' en un determinado estado cuántico al cual se pueden asociar distintas probabilidades para observar un número distinto de cuantos). En términos sencillos lo que hace el análisis conceptual-filosófico y no simplemente físico es la presencia implícita o explícita de preocupaciones filosóficas en particular de carácter ontológico (o 'anti-ontológico') y algunas veces de carácter epistemológico.

La línea de trabajo desarrollada por Teller (y otros) se basa como antes he mencionado en el estudio de una teoría física: la electrodinámica cuántica. Este no es el único enfoque que encontramos en la filosofía de la física respecto a las teorías cuánticas de campo. A finales de los 90 empezó a ganar 'momentum' otro enfoque basado en versiones axiomáticas de teorías cuánticas de campo, en particular la teoría cuántica de campos algebraica (algebraic quantum field theory). En años recientes incluso empezó un debate respecto a que formulación de la teoría cuántica de campos es más meritoria para servir de base para la discusión filosófica. Un ejemplo reciente es un artículo de D. Fraser (2009), defendiendo que el trabajo filosófico de interpretación de las teorías de campos se debe basar en exclusiva en la versión algebráica. Me resulta extraña esta visión; el que se tenga que optar por un determinado enfoque, más aun cuando la opción es por las versiones axiomáticas que no tienen en palabras de Fraser ningún modelo físico realista (i.e. son versiones matemáticas sin aplicación empírica). Me resulta paradójico que en la filosofía de una ciencia empírica como la física se quiera utilizar como punto de partida del estudio filosófico no las teorías físicas que de hecho tenemos (como la electrodinámica cuántica) y sí formulaciones matemáticas que aún no han dado prueba de que puedan ser realmente teorías físicas (aunque eventualmente fallidas), pues estas versiones axiomáticas no están al nivel de presentar previsiones que se puedan contrastar con resultados experimentales.

Aquí voy a tratar de la electrodinámica cuántica centrándome por lo tanto en una teoría física, pero tendré también en cuenta resultados formales que pueden ayudar a la

interpretación de la teoría. No se trata entonces de escoger una entre dos opciones excluyentes.

Este trabajo se debe ver entonces dentro de la línea 'iniciada' por Redhead y Teller. Pero hay un aspecto en que se diferencia claramente de la filosofía de la física especializada en la teoría cuántica de campos que se ha desarrollado hasta la actualidad. Es en la opción, que se puede ver como metodológica, de usar la historia de la física como elemento esencial en el desarrollo del trabajo. Es por lo tanto un trabajo histórico-filosófico. Aquí también existe un debate, en este caso respecto al papel de la historia en la filosofía de la ciencia (ver por ejemplo Schickore, 2009). No voy entrar en ello. Considero que se puede hacer un buen (o mal) trabajo en filosofía de la física con o sin aportación explícita de la historia de la física. Como referí, mi opción por la historia es metodológica, o sea, no tiene por qué conllevar una particular visión filosófica del papel de la historia en la filosofía de la ciencia. La opción por desarrollar un análisis conceptual de la electrodinámica cuántica desde una perspectiva histórica resulta del hecho personal e 'intransmisible' de que sólo a través del estudio histórico me es posible intentar comprender las teorías físicas. Es más bien una necesidad que una elección. Lo que resulta importante es que por lo menos parte de las ideas que voy a defender surgen precisamente de haber seguido un enfoque histórico. Así en este caso particular el enfoque histórico resultó 'productivo'. No trato de sacar conclusiones más generales respecto al papel de la historia en la filosofía de la física.

El papel de la historia en el trabajo

Es importante referir que este no es un trabajo de historia y si un trabajo que parte de la historia interna de la electrodinámica cuántica[3] para hacer un análisis conceptual de la teoría, enfocando en particular lo que se pueden llamar anomalías conceptuales-matemáticas (i.e. anomalías que no conllevan problemas en lo que respecta a 'salvar los fenómenos').

Debido al tema elegido, es posible reducir el ámbito del enfoque histórico a una historia conceptual. En particular considero solamente la evolución teórica sin tratar con detalle aspectos de la historia de la experimentación y su relevancia en el desarrollo conceptual de la teoría cuántica. Así no considero aspectos de historia cultural o material entre otras.[4]

El objetivo aquí es hacer una presentación sintética y coherente del desarrollo conceptual de la electrodinámica cuántica centrándome en aspectos esenciales de la teoría y enfocando en particular aquellos relacionados con los problemas tratados en este trabajo. De este modo evito repeticiones y el tratamiento de líneas 'secundarias' que incluso han influido en el desarrollo conceptual. Por ejemplo en lo que respecta al cambio conceptual que llevó a la dualidad onda-partícula me centro solamente en la contribución teórico-conceptual de Einstein y no trato la importante contribución de los físicos experimentales (que influirán directamente en las ideas de de Broglie).[5] Eso porqué para tratar los desarrollos técnicos y conceptuales de la electrodinámica cuántica resulta más directa la conexión teórica entre el trabajo de Einstein y Jordan que el

[3] Algunas de las principales referencias usadas en este trabajo son las siguientes: Jammer (1966), Mehra & Rechenberg (1982, 1987, 2000, 2001), Kuhn (1978), Kragh (1984, 1990, 1992), Darrigol (1984, 1986, 1992), Schweber (1994), Sánchez Ron (2001), Roqué (1992).

[4] Algunos ejemplos en que se enfocan algunos aspectos que se pueden considerar de historia cultural o material de la teoría cuántica son, e.g., Kragh (1999), McCormmach y Jungnickel (1986), Galison (1987).

[5] Una historia detallada de este tema se puede encontrar en Wheaton (1983).

origen de las ideas de de Broglie (ver capítulo 4). Tampoco considero la relevancia de este tema respecto a la interpretación de la teoría cuántica por ejemplo en la idea de complementariedad de Bohr. Hago siempre una presentación de los temas siguiendo solamente la 'línea' histórica que conecta el trabajo de los principales físicos teóricos que han hecho trabajos de primera importancia para el desarrollo de la teoría y en la medida que resulta necesario para la comprensión de aspectos conceptuales de la teoría tratados en este trabajo. Con este fin sigo una línea similar a la de Darrigol (2009).

En su trabajo Darrigol busca presentar una historia coherente y simplificada de la teoría cuántica que por ejemplo sea útil a los filósofos:

> The present paper is an attempt at simplifying this history so as to make it more helpful to physicists and philosophers. (Darrigol, 2009, p. 151)

Este objetivo lleva a la adopción de una metodología específica:

> The simplification I have in mind implies the selection of significant events and processes, as well as the occasional substitution of more direct reasoning for unnecessarily complicated reasoning. It does not imply any arbitrary invention, and it avoids common misconceptions
>
> I have selected a few important steps, in such a manner that any given step can be seen as a consequence of the anterior steps in a given situation. (Darrigol, 2009, p. 151)

En este trabajo también busco una simplificación de la historia conceptual de la electrodinámica cuántica, en particular en la elección de etapas secuenciadas de forma lineal y presentadas de forma simplificada. Teniendo en cuenta el desarrollo simultáneo de dos de los elementos básicos de la teoría – la cuantización de la materia y del campo electromagnético – que comparten en gran parte la misma historia conceptual, busqué evitar, en los distintos capítulos, presentaciones históricas que fueran redundantes. Así hay elementos históricos que se mencionan de manera general en distintos capítulos por una cuestión de claridad y 'secuencia histórica' pero que solo se tratan en detalle cada uno una vez en distintas capítulos del trabajo.[6]

Este enfoque histórico limitado cumple el objetivo específico de este trabajo, y es relativo a este que se debe analizar. Esto no significa que si el objetivo fuera por ejemplo el estudio de la interacción entre aspectos teóricos y experimentales en el cambio conceptual este enfoque sea suficiente. En este caso sería necesaria otro tipo de historia en que aspectos de instrumentación y experimentación (y más en general de historia material) sean considerados. Otro ejemplo sería un tratamiento simultáneo de los cambios conceptuales y la 'retórica' de la comunidad científica que les acompaña. En este caso sería esencial un enfoque teniendo en cuenta la historia cultural.

El trabajo

El trabajo se encuentra por supuesto dividido en capítulos perfectamente acotados que podrían dar la sensación de una progresión lineal en que exista una problemática central y algunos desarrollos derivados. No es así aunque lo presente así. De este modo, se podría ver el segundo capitulo (la ecuación de Schrödinger y su interpretación) y el tercero (la ecuación de Dirac y su interpretación) como la presentación de uno de los pilares de la electrodinámica cuántica, siendo el otro pilar la cuantización del campo

[6] Por ejemplos en los capítulos 2 y 3 se hace referencia a trabajos de Einstein y Dirac publicados respectivamente en 1909 y 1927 que se analizan con más detalle en el capítulo 4.

electromagnético presentada en el capítulo 4 (donde también se trata la cuestión del concepto de vacío). Ya el capitulo 5 se podría ver como el central donde se trata la interacción del campo cuántico de Dirac (definido por la ecuación de Dirac) y del campo cuántico electromagnético. Aquí se tratan cuestiones claves para entender la teoría: la divergencia de la serie de expansión de la matriz-S y las posibles consecuencias del teorema de Haag en lo que respecta a la consistencia de todas las aplicaciones de la teoría. Partiendo de este punto central se explorarían algunas implicaciones y temas relacionados. En el capitulo 6 se trata la cuestión de la interpretación de la renormalización (en que se sigue una línea Bohriana también presente en el capítulo anterior) y, como preparación para el 7, aspectos de la renormalización de la carga eléctrica relacionadas con la descripción en el ámbito temporal de procesos físicos, tema tratado de forma más amplia en el capitulo 7. Aquí los resultados del capitulo central, el 5, serán útiles para el análisis de la descripción que la teoría nos da a nivel espacio-temporal de procesos físicos (resultados estos que también están presentes en parte en el tratamiento del vacío en el capitulo 4). En particular propongo una lectura del concepto de partícula virtual contra-corriente respecto a lo que es la comúnmente aceptada. Finalmente en el capitulo 8 desarrollo las consecuencias del anterior para la cuestión filosóficamente importante de la relación de la electrodinámica clásica y la cuántica.

Al contrario de lo que esta presentación lineal y progresiva de la teoría (en la que la descripción de interacciones tiene un papel central) pueda dar que pensar, lo que me llevó a este trabajo es la comprensión de los conceptos de espacio y tiempo al nivel de la teoría cuántica de campos (así en realidad lo central sería el capítulo 7 y una serie de cosas que no elaboro aquí). Escogí la electrodinámica cuántica por ser la más sencilla de las teorías pertenecientes al llamado modelo standard, y por ser la versión cuántica de la mejor teoría clásica de que disponemos: la electrodinámica clásica. Con esto no quiero quitarle importancia a otras teorías clásicas, pero la electrodinámica es probablemente la teoría que tenemos mejor testada y mejor testable (tanto a nivel clásico como cuántico), o por lo menos así lo veo. Este estudio ('in progress') de los conceptos de espacio y tiempo va más allá de lo que presento aquí. En este trabajo analizaré solamente algunos aspectos de la descripción de procesos físicos en la electrodinámica cuántica.

Esta parte más especifica del programa más general me llevó al estudio del concepto de intercambio de cuantos (quanta exchange) que aparece en la descripción perturbativa de la interacción de la radiación con la materia. Esto me obligó a considerar una serie de cuestiones: la cuestión del estatus de los llamados cuantos virtuales; la divergencia de la matriz-S (que me resultó 'útil' para las ideas que defiendo); un modelo, que resulta ser semi-clásico de interacción entre electrones de átomos (bounded electrons); el teorema de Haag que aparentemente hacía peligrar todo el edificio de la electrodinámica cuántica; la reinterpretación de la descripción hecha por la ecuación de Dirac del átomo de hidrógeno en términos de intercambio de cuantos entre el núcleo y el electrón; e incluso aspectos 'no-temporales' en el procedimiento de renormalización.

Todo esto ha sido reelaborado y 'linealizado' en la presentación que sigue según el esquema presentado antes. En este proceso incorporé algunos temas relacionados como un estudio más detallado del vacío en la teoría y la relación entre la teoría cuántica y la clásica. Otro tema incluido es el de la interpretación de las funciones de onda en la teoría cuántica, que es un aspecto básico de cualquier análisis conceptual que se quiera hacer en la electrodinámica cuántica. Siguiendo a B. Falkenburg (2007) creo que la interpretación como colectividades (ensemble interpretation) es la que de modo más inmediato 'conecta' con el tipo de experimentos que se hacen en la física de altas energías. Esto me llevó a N. Bohr (al cual ya había llegado por el enfoque histórico

encontrando su crítica a la electrodinámica cuántica) y debido al programa más general que me interesa pronto llegué a la conclusión que los conceptos (clásicos) de espacio y tiempo que Bohr maneja en su interpretación de la cuántica son un marco fundamental para comprender esa interpretación. No exploro aquí las posibles conexiones que esa concepción del espacio y tiempo pueda tener con el caso de la electrodinámica cuántica ya que eso implicaría un tratamiento del espacio y tiempo en la teoría de la relatividad (especial). Eso pertenece al programa más 'general' de estudio de los conceptos de espacio y tiempo. Aquí me limito a algunos aspectos conceptuales de la electrodinámica cuántica.

Paso ahora a un resumen 'alargado' en español de la versión linealizada y ordenada del trabajo en los aspectos que conciernen a la electrodinámica cuántica (habiendo dejado el tema de la interpretación Bohriana de la cuántica para un apéndice, que me permite especificar de forma más precisa la interpretación de la función de onda adoptada en este trabajo).

El capítulo 2

Este capítulo es una preparación del siguiente. En el capítulo 3 enfocaré la cuestión de la interpretación de la ecuación de Dirac. Hay aspectos de esa historia que se pueden ver también en el caso 'más sencillo' de la mecánica cuántica no-relativista en la ecuación de Schrödinger. Así el capítulo 2 está dedicado a una presentación histórica del surgimiento de la ecuación de Schrödinger y de las tentativas iniciales para su interpretación.

En 1926 apareció un artículo en *Annalen der Physik* en el cual su autor E. Schrödinger presentaba una nueva teoría atómica siguiendo las ideas de L. de Broglie en que este asociaba un fenómeno ondulatorio al electrón (la onda de de Broglie). Schrödinger obtuvo una ecuación de onda (no relativista) que permitía obtener los niveles de energía para el átomo de hidrógeno tal como Bohr había hecho en la llamada vieja teoría atómica (old quantum theory), pero desde un enfoque más fundamental.

Se puede obtener una solución analítica de la ecuación en el caso del átomo de hidrógeno tratado como un electrón en un potencial central tipo coulombiano. Aprovechando la simetría del problema y usando coordenadas esféricas la función de onda (solución de la ecuación) tiene la forma $\psi = \psi_\theta \psi_\phi \psi_r$. La parte radial de la ecuación tiene la forma

$$\frac{\partial^2 \psi_r}{\partial r^2} + \frac{2}{r}\frac{\partial \psi_r}{\partial r} + \left(\frac{2mE}{K^2} + \frac{2me^2}{K^2 r} - \frac{n(n-1)}{r^2} \right) \psi_r = 0 ,$$

donde n tiene que ser un entero. La imposición de que n sea un entero resulta de que la parte de la función de onda ψ_ϕ cuando ϕ aumenta de un múltiplo 2π permanece igual. Esto implica que ψ_ϕ es dado por $2\pi^{-1/2} e^{im\phi}$, donde m es un entero positivo, negativo, o cero. Para que la ecuación de la función ψ_θ tenga soluciones es necesario que n sea un entero positivo de modo que $|m| \leq n$.

Un aspecto importante de la ecuación radial es que tiene puntos singulares en r = 0 y r = ∞. Teniendo en cuenta estos dos puntos singulares y las condiciones de frontera

(boundary conditions) que imponen a la ecuación de onda, esta sólo tiene solución cuando tenemos:

$$\frac{2me^2}{K\sqrt{-2mE}} = l = n'+n+1 .$$

De aquí sigue que la energía de un electrón 'dentro' del átomo de hidrogeno sólo puede tener valores discontinuos:

$$E_\lambda = \frac{2\pi^2 me^4}{h^2 l^2}$$, donde l es el llamado número cuántico principal

.

Esta solución corresponde al típico problema de valor propio en el cual tenemos una ecuación dependiente de un parámetro, en este caso la energía E, y las soluciones tienen que satisfacer condiciones de frontera particulares (en este caso la función de onda tiene que ser finita en r = 0 y aproximarse a cero para $r \rightarrow \infty$). Encontramos un problema similar en el caso clásico de una cuerda en vibración. Las extremidades están fijas y esto implica que la cuerda sólo puede tener una determinada frecuencia y sus harmónicos.

Schrödinger consideró que de este modo la ecuación tenía en sí misma implícitas las condiciones cuánticas, que no resultarían de ninguna discontinuidad cuántica en la física y sí de tratarse de un fenómeno ondulatorio. Sea como sea, en sus primeros artículos Schrödinger no desarrolló demasiado la interpretación de la función de onda; se limitó a unos pocos comentarios, asociando la función de onda a algún tipo de proceso ondulatorio en el interior del átomo.

Una limitación importante con la que Schrödinger se debatió en esta fase del desarrollo de su mecánica ondulatoria fue la imposibilidad de describir la intensidad y polarización de la radiación emitida por un átomo. En particular Schrödinger sólo pudo obtener la expresión $h\nu = E' - E''$ (donde ν es la frecuencia de la radiación emitida cuando un electrón pasa de un estado estacionario con energía E′ a otro con energía E′′) del modelo atómico de Bohr de forma aproximada.

En un artículo posterior Schrödinger relacionó la función de onda que llamó de campo mecánico escalar (mechanical field scalar) con una distribución de electricidad en el espacio, que se podría ver como el término de 'fuente' (source) en las ecuaciones de Maxwell-Lorentz. Con este fin Schrödinger consideró que la densidad de electricidad ρ_{el} sería dada por la parte real de

$$\psi \frac{\partial \overline{\psi}}{\partial t},$$

en que $\overline{\psi}$ es el conjugado complejo de la función de onda ψ. Usando esta hipótesis en el tratamiento del efecto Stark, Schrödinger pudo obtener la 'regla de frecuencias' de Bohr de forma exacta, además de poder calcular la intensidad y polarización de la radiación emitida. Desarrollando más esta interpretación electromagnética de la función de onda Schrödinger extendió su formalismo para el caso de sistemas con un estado variable en el tiempo (time-dependent systems). Esto llevó a Schrödinger a adoptar una función de onda compleja y por lo tanto a redefinir su anterior expresión para la densidad de carga ahora dada por $e\psi\overline{\psi}$, donde e es la carga eléctrica del electrón.

Schrödinger pronto reconoció las limitaciones de esta interpretación de la función de onda (describiendo una distribución de electricidad en el espacio) ya que incluso en el caso más sencillo de un único electrón es también necesario tener en cuenta la evolución espacio-temporal de la función de onda. Por una parte, la interpretación electromagnética permitía calcular intensidades y polarizaciones, pero por otra parte la interpretación como una onda propagándose en el espacio era necesaria para determinar sucesivas densidades de carga (y por lo tanto mediciones de intensidades), o sea, para conectar sucesivas observaciones. Así, en realidad la interpretación de la función de onda por Schrödinger tenía un aspecto doble.

Pronto las tentativas iniciales de Schrödinger dieron paso a la interpretación probabilística (statistical interpretation), pero esto no lo voy a considerar. Aquí lo que me interesa es la ambigüedad que encontramos en la interpretación de Schrödinger que por lo menos en parte usa su ecuación de onda como una ecuación clásica describiendo la propagación de un campo mecánico escalar en el espacio. Es un punto interesante ya que en el caso de la ecuación de Dirac se va encontrar también una ambigüedad en lo que respecta a la interpretación de la ecuación, siendo incluso posible 'escoger' (como ha hecho P. Jordan) ver la ecuación como una ecuación de un campo clásico posteriormente cuantizado.

Podemos imaginar una situación hipotética en la que no teniendo aún el concepto de electrón como partícula, un experimento como el de C. J. Davisson y L. H. Germen nos lleva a aceptar la idea de que existen unas ondas de materia que resultan tener las características propuestas por de Broglie (esto es doblemente imaginario ya que de Broglie claramente manejaba expresiones que implicaban al mismo tiempo una característica ondulatoria y corpuscular). ¿Podemos ver la ecuación de Schrödinger como la ecuación de una onda de materia 'clásica'? Y en caso afirmativo ¿cómo se obtienen los aspectos corpusculares?

Mirando el caso más sencillo de un átomo de hidrógeno queda claro hasta qué punto se puede usar la ecuación de Schrödinger como una ecuación describiendo un campo material 'clásico'. Volviendo al enfoque inicial de Schrödinger, considerando una onda de de Broglie en un potencial central tenemos

$$\Delta\phi + 8\pi^2 \mathrm{m}\left(\nu + \frac{\mathrm{e}^2}{\mathrm{h}}\frac{1}{\mathrm{r}}\right)\phi = 0\,.$$

De aquí resulta, en un tratamiento totalmente clásico, que las frecuencias posibles de la onda de de Broglie son dadas por

$$\nu = -\frac{2\pi^2 \mathrm{m e}^4}{\mathrm{h}^3}\frac{1}{(\mathrm{n_r} + \mathrm{l} + 1)^2}\,,\ \text{donde } \mathrm{n_r},\ \mathrm{l} = 0,\ 1,\ 2,\ \ldots.$$

Por analogía con el caso del cuanto de luz, consideramos que la energía de una onda de de Broglie (en el interior de átomo) con una frecuencia ν es dada por $E = h\nu$. De esta 'regla cuántica' resulta que los niveles de energía en el átomo son dados por

$$\mathrm{E} = -\frac{2\pi^2 \mathrm{m e}^4}{\mathrm{h}^2}\frac{1}{(\mathrm{n_r} + \mathrm{l} + 1)^2}\,,$$

un resultado de acuerdo con la derivación de la teoría atómica de Bohr. La diferencia con la derivación original de Schrödinger es que en ésta Schrödinger usó desde el inicio la relación entre energía y frecuencia adoptada en este caso al final. Así Schrödinger presentó realmente una ecuación 'cuántica' que se asemeja (en el caso de sistemas con un solo electrón) a una ecuación de onda clásica.

Aquí tenemos un resultado que vamos a volver a encontrar en el capitulo 3. Cuando adoptamos como punto de partida una ecuación que interpretamos como clásica necesitamos una regla de cuantización de las variables físicas de la onda de manera que se pueda también describir el aspecto corpuscular asociado a los electrones.

El capítulo 3

La primera tentativa de Schrödinger de obtener una ecuación de onda fue una ecuación relativista y no su conocida ecuación no-relativista. No resultó. La ecuación obtenida dio una descripción equivocada de los niveles de energía. Eso llevó Schrödinger a optar por un proyecto menos ambicioso pero que resultó más exitoso.

La derivación de una ecuación de onda relativista para el electrón siguió desafiando a los físicos. Después del descubrimiento de que se podía asociar un momento angular interno al electrón – al cual se asoció un número cuántico específico, el spin – W. Pauli intentó incorporar el spin a la mecánica ondulatoria. Para eso consideró una función de onda de Schrödinger dependiente también del spin que resulta tener sólo los valores $\pm \hbar/2$. Así Pauli definió una función de onda con dos componentes, una correspondiendo a un electrón con el spin hacia arriba (spin up) $\psi(\mathbf{x}, +1/2)$ y otra a un electrón con el spin hacia abajo (spin down) $\psi(\mathbf{x}, -1/2)$. Esta función de onda de dos componentes será solución de dos ecuaciones acopladas (coupled equations) con la forma

$$H\left(\frac{\hbar}{i}\frac{\partial}{\partial q}, s\right)\psi = E\psi$$

La cuestión es ahora cómo definir en la ecuación de onda los operadores de spin **s**. Pauli los definió como $s_x = 1/2\ \sigma_x$, $s_y = 1/2\ \sigma_y$, $s_z = 1/2\ \sigma_z$, donde σ_x, σ_y, σ_z son las llamadas matrices de Pauli:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Pauli tuvo que incorporar elementos en su ecuación de forma ad hoc para obtener un acuerdo con los resultados disponibles, pero sólo ha podido hacer correcciones relativistas de primer orden, o sea, no pudo llegar a una ecuación realmente relativista.

A finales de 1927 P. A. M. Dirac llegó a una ecuación de onda relativista del electrón. Su primera tentativa de formular una ecuación relativista fue lo que se conoce como la ecuación de Klein-Gordon (obtenida por distintos físicos y que coincide con la ecuación relativista que Schrödinger exploró). En términos de un hamiltoniano relativista podemos ver la ecuación como una sustitución directa del momento y energía por los operadores cuánticos correspondientes:

$$\{p_x^2 + p_y^2 + p_z^2 - E/c^2 + m^2c^2\}\psi = 0$$

$$\left\{\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\frac{m^2c^2}{h^2}\right\}\psi=0\,.$$

P. Ehrenfest hizo a Dirac interrogarse por la opción adoptada para el hamiltoniano, preguntándole si había diferencia entre el que Dirac había escogido y el siguiente:

$$mc^2\sqrt{1-(p_1^2+p_2^2+p_3^2)/m^2c^2}=E$$

Dirac consideraba que ninguna de las dos opciones servía como base para el desarrollo de una ecuación relativista. Necesitaba una ecuación lineal en la derivada temporal y que, para estar de acuerdo con la relatividad, las derivadas respecto a las variables espaciales fueran también lineales.

Parece que lo que permitió a Dirac salir del bloqueo provocado por la expresión matemática del hamiltoniano fue constatar la siguiente identidad:

$$|\vec{p}|=\sqrt{p_1^2+p_2^2+p_3^2}=\sigma_1p_1+\sigma_2p_2+\sigma_3p_3\,,$$

donde σ_1, σ_2, σ_3 son las matrices de Pauli. Eso llevó a Dirac a buscar una expresión relativista análoga en que apareciera el término correspondiente a la masa de electrón:

$$|\vec{p}|=\sqrt{p_1^2+p_2^2+p_3^2+m^2c^2}=\alpha_1p_1+\alpha_2p_2+\alpha_3p_3+\alpha_4mc\,.$$

Dirac consideró que de la ecuación obtenida usando la expresión anterior $\{p_0-(m^2c^2+p_1{}^2+p_2{}^2+p_3{}^2)^{1/2}\}\psi=0$ debería ser posible obtener la expresión relativista $\{p_0{}^2-m^2c^2-p_1{}^2-p_2{}^2-p_3{}^2\}\psi=0$. Esto implica un conjunto de relaciones matemáticas entre los coeficientes aún por determinar:

$$\alpha_\mu\alpha_\nu+\alpha_\nu\alpha_\mu=0\ (\mu\neq\nu);\ \mu,\nu=1,2,3,4,$$

$$\alpha_\mu{}^2=1.$$

No hay ningún conjunto de matrices 2 × 2 que satisfagan las condiciones anteriores. Esto llevó a Dirac a considerar la siguiente posibilidad más simple, la de matrices 4 × 4. De este modo los coeficientes propuestos por Dirac son:

$$\sigma_1=\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}\qquad\sigma_2=\begin{pmatrix}0&-i&0&0\\i&0&0&0\\0&0&0&-i\\0&0&i&0\end{pmatrix}\qquad\sigma_3=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}$$

$$\rho_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \qquad \rho_2 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix} \qquad \rho_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

con $\alpha_1 = \rho_1\sigma_1$, $\alpha_2 = \rho_1\sigma_2$, $\alpha_3 = \rho_1\sigma_3$, $\alpha_4 = \sigma_3$. Así tenemos de inmediato la ecuación de Dirac:

$$[p_0 - \rho_1(\sigma, p) - \rho_3 mc]\psi = 0\,,$$

donde $p_0 = i\hbar\,\partial/(c\partial t)$ y $\mathbf{p} = (p_1, p_2, p_3)$, con $p_r = -i\hbar\,\partial/(c\partial x_r)$ y r = 1, 2, 3; $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ es un vector formado por las anteriormente indicadas matrices 4 × 4. Dirac generalizó su resultado para el caso de un electrón en un campo externo. Siguiendo una prescripción de la electrodinámica clásica Dirac hizo la sustitución $p_0 \rightarrow p_0 + e/c.A_0$ y $\mathbf{p} \rightarrow \mathbf{p} + e/c.\mathbf{A}$, donde A_0 y $\mathbf{A}$ son el potencial escalar y vector. Esto resulta en la ecuación

$$[p_0 + \frac{e}{c}A_0 - \rho_1(\sigma, p + \frac{e}{c}A) - \rho_3 mc]\psi = 0\,.$$

Dirac desarrolló su ecuación partiendo del hamiltoniano para una partícula puntual sin tener en cuenta el spin. Pero resulta que el spin del electrón aparecía naturalmente en la descripción hecha usando esta ecuación. Dirac trató de explorar la relación entre su ecuación y la ecuación de Klein-Gordon que es la 'esperada' de acuerdo con el hamiltoniano clásico relativista. Tomando el cuadrado de su ecuación Dirac obtuvo una que incluye los términos de la ecuación de Klein-Gordon y dos adicionales

$$\left\{\left(p_0 + \frac{e}{c}A_0\right)^2 - \left(p + \frac{e}{c}A\right)^2 - m^2c^2 - \frac{\hbar e}{c}(\sigma, H) + i\rho_1\frac{\hbar e}{c}(\sigma, E)\right\}\psi = 0\,.$$

Dirac concluyo que el electrón en un campo externo se comportaba como teniendo un momento magnético $eh/4\pi mc \cdot \boldsymbol{\sigma}$ que es lo esperado para un electrón con un momento angular interno (spin). Así su ecuación implicaba que el electrón tenía un momento angular interno dado por $\hbar/2 \cdot \boldsymbol{\sigma}$.

Como Dirac usó matrices 4 × 4 en su ecuación, la función de onda tenia 4 componentes. Inicialmente Dirac pensó que podía retener sólo dos de los componentes que corresponderían a un electrón con carga negativa, energía positiva y dos posibles estados para el spin, siendo posible descartar los componentes correspondientes a energías negativas. Pronto Dirac reconoció que en el caso de un campo electromagnético externo intenso no era posible hacer una separación clara de soluciones correspondientes a energías positivas y negativas. En particular, O. Klein demostró que para el caso sencillo de una onda con energía positiva incidente en una barrera de potencial, podía además de una onda reflectada (correspondiente a una energía positiva) haber también una onda transmitida a través de la barrera (con energía negativa). Este resultado conocido como la paradoja de Klein será importante como analogía en la comprensión de dificultades matemáticas con las que se enfrenta la electrodinámica cuántica.

A finales de 1929 partiendo de una idea de H. Weyl, Dirac propuso una solución para la dificultad de las energías negativas. La idea era tomar los dos componentes extras de la función de onda como describiendo el protón y no el electrón. Con ese fin Dirac propuso una nueva interpretación de su ecuación. Supuso que casi todos los estados con energía negativa estaban ocupados y que los agujeros (holes) en ese mar (sea) de electrones de energía negativa eran los protones. Dirac expuso estas ideas en una carta a Bohr. En la respuesta Bohr comentó que no comprendía como se podría evitar en ese caso una energía eléctrica infinita (debido al número infinito de electrones con energía negativa). Bohr se mostro inclinado a ver en la dificultad con las soluciones de energía negativa una limitación en la aplicación de los conceptos fundamentales sobre los cuales se basa la teoría atómica ("In the difficulties of your old theory I still feel inclined to see a limit of the fundamental concepts on which atomic theory hitherto rests"). Así Bohr se propuso reinterpretar el significado de la paradoja de Klein considerando que uno se enfrentaba por una parte con dificultades que resultan de un uso (en el ámbito matemático) ilimitado del concepto de potencial ("difficulties involved in an unlimited use of the concept of potentials") y por otra parte con un ejemplo de un límite en la aplicación del concepto de potencial cuando se tienen en cuenta posibles situaciones experimentales concretas ("an example of the actual limit of applying the idea of potentials in connection with possible experimental arrangements"). Bohr llamó la atención al hecho de que en la teoría se está considerando electrones con una carga elemental. Esto impide la construcción de una barrera de potencial 'real' comparable a lo que matemáticamente se puede considerar. La paradoja de Klein surge para barreras de potencial definidas matemáticamente que no se consiguen realizar en la práctica experimental debido a la existencia de una carga eléctrica elemental. Dicha carga es un parámetro básico de la teoría ("due to the existence of an elementary unit of electrical charge we cannot build up a potential barrier of any height and steepness desired without facing a definite atomic problem"). Así Bohr consideraba que dentro del límite real de aplicación de la teoría esta era consistente. En este caso la paradoja resultaba de ir más allá de lo permitido realmente por la teoría. Bohr esperaba que los problemas de una posible transición desde estados con energía positiva a estados con energía negativa no ocurrirían en aplicaciones consistentes, y así no sería necesaria la 'hole theory' (teoría de los agujeros) de Dirac.

Dirac no aceptó la visión de Bohr y dio un ejemplo donde era necesario tener en cuenta estados con energía negativa sin que ello conllevara ningún tipo de dificultadas. En el caso de un proceso de dispersión (scattering) de radiación por un electrón, este puede pasar por un estado intermedio con energía negativa. Dirac mostró que teniendo en cuenta su 'hole theory' se podía, sin permitir esa transición, tener otra en que un electrón (en un estado negativo) 'salta' primero para el estado positivo final (y el electrón inicial ocupa ese estado negativo) de modo que el resultado final es el mismo que el anterior y permite obtener las formulas de dispersión correctas. Dirac también consideró que no había ningún problema de energía eléctrica infinita debido al 'mar' de electrones negativos. Eso es así porque lo que se observa no es el valor absoluto de la energía y sí variaciones en relación al estado 'normal' de un mar 'lleno' de electrones con energía negativa. Es evidente por la descripción que Dirac hace de los procesos de dispersión en su teoría que ésta ya no consiste en la descripción de un solo electrón y sí de un sistema con muchos electrones (en realidad con un número infinito de ellos).

Las ideas de Dirac no fueron bien recibidas. Más importante que todas las demás críticas fue tal vez el cálculo de J. R. Oppenheimer en 1930 que demostró que la probabilidad de un electrón de aniquilarse con un protón (correspondiendo esto a que el electrón ocupe un 'agujero' del 'mar') era absurdamente elevada y totalmente

incompatible con la estabilidad de la materia. Esto echó por tierra la 'hole theory' de Dirac en este formato. Oppenheimer propuso volver a considerar el electrón y el protón como dos partículas independientes cada una con su propio mar de partículas con energía negativa. De este modo no habría ningún problema de una posible aniquilación entre electrones y protones. Dirac pronto adoptó esta idea y propuso que el 'agujero' fuera una nueva partícula, un anti-electrón aún no 'descubierto'.

En 1932 se observó un fenómeno que se ha podido encuadrar en la teoría de Dirac como el anti-electrón que él propuso. Pero esto no significó que los físicos aceptaran su 'hole theory'. En realidad un enfoque distinto del de Dirac era posible sin que fuera necesario un 'mar' con un número infinito de partículas con energía negativa. Se puede ver el origen de este nuevo enfoque, basado en el concepto de campo, en un trabajo de Dirac de 1927 presentando un tratamiento no relativista de la interacción de radiación electromagnética con un átomo. Dirac presentó en este artículo dos maneras de considerar un campo electromagnético cuántico. En uno, Dirac consideró un conjunto de cuantos de luz descrito por una ecuación de Schrödinger. En este caso se tienen que retener solamente las soluciones simétricas de la función de onda describiendo los cuantos de luz para que ésta esté de acuerdo con la llamada estadística de Bose-Einstein. Dirac optó por un método enrevesado que físicamente correspondía a imponer la simetría de la función de onda, que posteriormente se denominó de segunda cuantización. La otra manera adoptada por Dirac para llegar a una descripción cuántica del campo electromagnético consistió en hacer la expansión en serie de Fourier del campo y tratar los coeficientes de expansión no como números y sí como operadores satisfaciendo relaciones de conmutación. Dirac encontró que los dos procedimientos permitían llegar a la misma descripción al nivel cuántico del campo electromagnético.

Contrariamente a la lectura de Dirac que veía la 'segunda cuantización' como un procedimiento para imponer la estadística de Bose-Einstein a la función de onda del campo electromagnético, Jordan interpretó el esquema de la 'segunda cuantización' de una manera bien distinta. Para él consistía en la cuantización de una onda clásica descrita por una ecuación clásica, que podían ser las ecuaciones de Maxwell-Lorentz en el caso del campo electromagnético o la ecuación de Schrödinger (como si fuera una ecuación de un campo clásico) en el caso de electrones tratados no como partículas y sí como ondas de de Broglie 'clásicas'. Este enfoque de Jordan tenía la ventaja de permitir tratar las ondas cuantizadas en el espacio físico y no en un espacio de configuración abstracto (que es lo que ocurre cuando se considera un sistema con varias partículas usando la ecuación Schrödinger como una 'ecuación cuántica'). Aplicando este enfoque en el caso de electrones, Jordan debido a que a estos se aplica el principio de exclusión de Pauli tuvo que usar unas relaciones de conmutación distintas de las adoptadas para el caso del campo electromagnético. Después de algunas dificultades de orden técnico en la implementación de las llamadas relaciones de anti-conmutación, Jordan pudo demostrar que partiendo de una descripción de los electrones como un campo clásico (descrito por una 'ecuación clásica' de Schrödinger) se podía por un procedimiento de cuantización llegar a una descripción cuántica de los electrones equivalente a la que se tiene considerando de partida los electrones como partículas cuánticas (descriptas por una 'ecuación cuántica' de Schrödinger). Aquí encontramos de nuevo la posibilidad de jugar con la ambigüedad de interpretar la ecuación de Schrödinger a la que hago referencia en el capitulo anterior. Con este resultado Jordan concluyó que sería posible una formulación de la teoría cuántica en que la materia y la radiación se puedan concebir como ondas (cuantizadas) en interacción en el espacio-tiempo.

Esta visión fue adoptada por W. Heisenberg y Pauli en el desarrollo de una teoría cuántica de campos describiendo la interacción entre radiación y materia. En su caso

usaron como punto de partida la ecuación de Dirac como una ecuación de onda clásica. La solución de de Broglie de la ecuación es cuantizada de acuerdo con el procedimiento de Jordan. En el desarrollo de este enfoque se llegó a una formulación en que se trataba de forma totalmente simétrica los electrones y los positrones (anti-electrones). Así, partiendo de la ecuación de Dirac y su ecuación adjunta (adjoint equation) como ecuaciones clásicas derivadas de un lagrangiano clásico, un campo arbitrario se puede escribir en términos de soluciones correspondientes a partículas libres:

$$\psi(\mathbf{x}) = \int \frac{d^3p}{(2\pi)^{3/2}} \left(\frac{m}{E_{\mathbf{p}}}\right)^{1/2} \left\{ \sum_{r=1}^{2} b_r(\mathbf{p}) w^r(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} + \sum_{r=3}^{4} b_r(-\mathbf{p}) w^r(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{x}} \right\}.$$

La cuantización consiste en sustituir los coeficientes de expansión por operadores que satisfacen las relaciones de anti-conmutación $[b_n, b_m]_+ = [b_n^*, b_m^*]_+ = 0$ y $[b_n, b_m^*]_+ = \delta_{nm}$. Con este procedimiento $\psi(\mathbf{x})$ y el campo adjunto (adjoint spinor field) $\psi^*(\mathbf{x})$ se convierten en operadores que actúan en vectores de estado (state vectors) de un espacio de Fock; y $b_r(\mathbf{p})$ y $b_r^*(\mathbf{p})$ se interpretan como operadores de aniquilación (annihilation operators) y creación (creation operators) de un electrón en el estado ($\mathbf{p}$, r). Haciendo la redefinición de los operadores para estados con energía negativa como $b_{r+2}(-\mathbf{p}) = d_r^*(\mathbf{p})$ y $b_{r+2}^*(-\mathbf{p}) = d_r(\mathbf{p})$ con r = 1, 2, estos operadores se pueden interpretar como los operadores de creación y aniquilación de un positrón con energía positiva. Después de este cambio, la expansión del operador $\psi(\mathbf{x})$ es ahora

$$\psi(\mathbf{x}) = \int \frac{d^3p}{(2\pi)^{3/2}} \left(\frac{m}{E_{\mathbf{p}}}\right)^{1/2} \sum_{r=1}^{2} \left\{ b_r(\mathbf{p}) w^r(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} + d_r^*(\mathbf{p}) \upsilon^r(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{x}} \right\}.$$

Con esta formulación no hay estados con energía negativa que son ahora interpretados como positrones con energía positiva. Así ya no es necesario suponer un 'mar' con un número infinito de electrones con energía negativa. También en los operadores de campo $\psi(\mathbf{x})$ y $\psi^*(\mathbf{x})$ tenemos en simultaneo componentes relacionados con los electrones y con los positrones.

Consideremos ahora el operador de energía y momento (energy-momentum operator)

$$P^\mu = \sum_r \int d^3p\, p^\mu [a_r^*(\mathbf{p}) a_r(\mathbf{p}) + b_r^*(\mathbf{p}) b_r(\mathbf{p})] = \int d^3p\, p^\mu [n^-(\mathbf{p}) + n^+(\mathbf{p})],$$

y el operador de carga (total charge operator)

$$Q = \sum_r \int d^3p [-a_r^*(\mathbf{p}) a_r(\mathbf{p}) + b_r^*(\mathbf{p}) b_r(\mathbf{p})] = \int d^3p [n^+(\mathbf{p}) - n^-(\mathbf{p})],$$

donde $n^-(p)$ es el número de electrones y $n^+(p)$ es el número de positrones. Como Jordan había propuesto, se puede ver que el hecho de que la carga eléctrica tenga valores discretos resulta de la cuantización de un campo clásico.

El capítulo 4

Como es bien sabido en 1905 A. Einstein propuso que determinados aspectos de la radiación electromagnética se podían explicar mejor haciendo referencia a una concepción corpuscular de la luz. Esto no significaba volver a una especie de teoría Newtoniana de la luz. Einstein sólo propuso que en el límite de frecuencias elevadas en que la ley de Wien es válida, la luz debe, desde un punto de vista termodinámico, comportarse como si fuera constituida por partículas independientes de energía (light quanta). En 1909 Einstein presentó más resultados en esta línea, estudiando las fluctuaciones energéticas de radiación en equilibrio termodinámico en el interior de una cavidad. Einstein obtuvo una expresión con dos términos, uno que se explica haciendo referencia a propiedades ondulatorias de la radiación y el otro a propiedades corpusculares. Einstein consideró que el desarrollo futuro de la física pasaría por una teoría en la que existiera una especie de fusión de estos dos aspectos: una teoría que explicara el aspecto dual de la luz.

Después del desarrollo de la mecánica de matrices por Heisenberg y de su reformulación matemática por M. Born (con Jordan y Heisenberg) en lo que ahora llamamos de mecánica cuántica, ha sido posible tratar la cuestión de la cuantización de la radiación. Esto empezó ya en los momentos iniciales del desarrollo del formalismo matemático de la mecánica cuántica. Un momento importante fue el estudio por Jordan de un campo electromagnético libre dentro de una cavidad. De una manera no muy rigurosa Jordan pudo deducir los resultados de Einstein de 1909 respecto a la dualidad onda-partícula en la radiación. Jordan trató la radiación electromagnética libre como un conjunto infinito de osciladores harmónicos, cuantizando de forma independiente cada oscilador. El aspecto más importante de este procedimiento directo es la interpretación que Jordan le dio. Jordan vio que podía relacionar los cuantos de luz con las oscilaciones cuantizadas del campo. Así la discontinuidad de energía surge como una propiedad del campo cuántico. Considerando que a cada oscilador k con energía ν_k está asociado un número cuántico n_k, la energía del campo es dada por $E_n = h\sum_k \nu_k n_k$. Según Jordan se tiene que ver también n_k como el número de cuantos de luz con frecuencia ν_k existentes en el interior de la cavidad.

Nuevos e importantes desarrollos ocurrieron con Dirac. Como ya referí, en un artículo de 1927, Dirac presentó un tratamiento de la interacción del campo electromagnético con un átomo desde dos perspectivas iniciales distintas. En uno de los enfoques basado en la cuantización del campo electromagnético clásico Dirac siguiendo a Jordan hizo una expansión de Fourier del campo en términos de sus modos normales (matemáticamente equivalentes a osciladores harmónicos) tratando los coeficientes como operadores. Otra aportación importante fue, en 1928, el desarrollo conjunto por Jordan y Pauli de un procedimiento de cuantización relativista del campo electromagnético libre. Por esas fechas, como mencioné en el capitulo 2, Pauli y Heisenberg empezaron a intentar desarrollar una electrodinámica cuántica relativista partiendo de la idea de Jordan de tratar la radiación y la materia como campos cuánticos. Después de diversos problemas de orden técnico, Pauli y Heisenberg pudieron desarrollar un método de cuantización del campo electromagnético partiendo del lagrangiano clásico del campo (que resultaba equivalente al método anterior de Jordan y Pauli en el caso de un campo libre). Su (primer) trabajo publicado en 1929

presentaba una falta clara de aplicaciones y no trataba la cuestión de la energía (self-energy) infinita de las partículas cargadas.

De forma independiente de Pauli y Heisenberg, E. Fermi desarrolló un método más directo en el cual, al contrario del trabajo de Dirac de 1927, no sólo el campo de radiación era cuantizado sino todo el campo electromagnético descrito por el potencial vector y el potencial escalar. Con ese fin Fermi usó la ecuación de d'Alembert para el potencial vector y el potencial escalar: $\Box A_\mu = j_\mu$. Para hacer esta ecuación equivalente a las de Maxwell, Fermi tenía que tener en cuenta la llamada condición de Lorentz $\partial_\mu A^\mu = 0$, que él vio como una condición que tienen que satisfacer los operadores de campo (definidos haciendo la expansión de Fourier del potencial vector y potencial escalar).

En los meses siguientes a la publicación de su primer artículo sobre la electrodinámica cuántica, Pauli y Heisenberg mejoraron su método evitando trucos formales que habían usado. La clave para esto fue la invariancia de gauge. En este trabajo implementaron el esquema de Fermi desde el suyo basado en el formalismo lagrangiano. Al hacerlo notaron que la manera en que Fermi aplicaba la condición de Lorentz no era correcta y que sólo se podía aplicar como una condición suplementaria sobre los vectores de estado: $(\partial_\mu A^\mu)\Psi = 0$.

Fermi clarificó en parte el significado físico de la condición subsidiaria en una nota posterior. Al contrario del trabajo de Dirac de 1927, en su primer artículo Pauli y Heisenberg no consideraron solamente el campo de radiación (descrito por un potencial vector transversal con dos grados de libertad, correspondiendo a dos polarizaciones perpendiculares a la dirección de propagación de la onda), y si tal como Fermi consideraron los cuatro grados de libertad asociados al potencial vector y potencial escalar más generales. Pero no llegaron a discutir la relación existente entre los potenciales más generales y el potencial vector transversal del campo de radiación.

Alguna clarificación de este punto lo dio L. Rosenfeld también en 1929 mostrando (en un sistema de referencia particular) que las cuatro polarizaciones de un modo normal del campo se relacionan de una forma sencilla con el vector de campo (wave vector): dos componentes correspondiendo a la luz transversalmente polarizada, uno a una polarización longitudinal, y otro a una polarización de tipo escalar o temporal (time-like polarization).

Adoptando la idea de Pauli y Heisenberg respecto a la condición subsidiaria, Fermi mostró que los componentes longitudinales y escalares del campo – que por la condición subsidiaria no se pueden ver como grados de libertad independientes del campo – correspondían a la interacción de Coulomb entre partículas cargadas.

En este momento el desarrollo de la cuantización del campo electromagnético en interacción con cargas quedó básicamente concluido. En términos más generales la electrodinámica cuántica era aún muy imperfecta; por ejemplo, el problema de la energía propia infinita (self-energy) de las partículas cargadas aún estaba por resolver. En la practica sólo se podían hacer unos cuantos cálculos de segundo orden en teoría de perturbaciones sin que los resultados fueran divergentes.

La cuantización del campo electromagnético de forma totalmente relativista implementada por Fermi, Pauli y Heisenberg, usando la condición de Lorentz, resultó no llevar a ninguna incongruencia en la práctica. Pero al estudiar con detenimiento las consecuencias de la condición subsidiaria este método no es consistente. Una solución para este problema surgió a inicios de los 50 con el desarrollo de un formalismo basado en una métrica indefinida del espacio de Hilbert (el método de Gupta-Bleuler). Pero en la manera en que normalmente se hacen los cálculos el operador de métrica no aparece. Esto da una justificación *a posteriori* para la manera en que se venían haciendo los

cálculos. Ahora, hasta el final de este capítulo me concentraré en lo que debería ser el más sencillo de los estados del campo electromagnético cuántico: el vacío.

El estado fundamental (el vacío) del campo electromagnético es el estado en que este tiene la menor energía posible. Esto corresponde a no haber ningún fotón (cuanto de luz) transversal presente. Lo que corresponde en el ámbito clásico a esta situación es que haya una región del espacio sin campo electromagnético. Contrariamente a la situación clásica, al estado fundamental del campo electromagnético cuantizado se asocian efecto físicos, los llamados efectos del vacío (vacuum effects), siendo el efecto Casimir tomado como un ejemplo claro de esto.

En el efecto Casimir se supone que al colocarse dos placas metálicas frente a frente en el espacio vacío, el estado fundamental del campo electromagnético cuantizado provoca una fuerza entre las placas (eso se explica teniendo en cuenta que las placas van a influir en las condiciones de frontera que definen el número de modos del campo incluso en su estado fundamental).

En realidad, como H. Zinkernagel señalo, una interpretación física es posible sin que sea necesario considerar el campo electromagnético cuántico en su estado fundamental. Por ejemplo en el caso del efecto Casimir eso se consigue teniendo en cuenta que las placas metálicas no son condiciones matemáticas de frontera y si son constituidas por materia cargada.

Que los llamados efectos del vacío se expliquen de otro modo no significa que el estado fundamental sea equivalente a la situación clásica de un vacío espacial. En realidad considerando el caso sencillo de un oscilador dipolar en el espacio vacío, se verifica que es necesario tenerse en cuenta el estado fundamental del campo electromagnético para que las relaciones de conmutación de los operadores de posición y momento del oscilador estén de acuerdo con lo esperado en el formalismo cuántico. Pero aquí se trata solamente de un aspecto formal sin conllevar aspectos que se puedan observar. Donde podemos encontrar resultados experimentales relacionados con el vacío del campo electromagnético es en las llamadas fluctuaciones del campo.

Así en el estado fundamental del campo electromagnético cuantizado el valor medio (expectation value) de los campos eléctricos y magnéticos es nulo: $\langle 0|\mathbf{E}|0\rangle = \langle 0|\mathbf{B}|0\rangle = 0$. Pero lo mismo no ocurre con la variancia (variance). Esto es porque $\langle 0|\mathbf{E}^2|0\rangle$ y $\langle 0|\mathbf{B}^2|0\rangle$ son distintos de cero incluso para el estado fundamental. De acuerdo con la interpretación del formalismo cuántico adoptada aquí, tenemos que considerar un contexto experimental particular en el que se hacen mediciones del campo electromagnético, y hacer mediciones repetidas en las mismas condiciones. Así se obtiene una distribución de resultados de estas mediciones independientes de acuerdo con una desviación estándar (standard deviation) $\sqrt{\langle 0|\mathbf{E}^2|0\rangle}$ de una medición correspondiendo a un campo nulo. Así se espera que midamos algunas veces un campo eléctrico distinto de cero incluso para un campo en su estado fundamental.

En experimentos hechos usando una técnica llamada de 'balanced homodyne detection' es posible obtener lo que se pueden interpretar como fluctuaciones de cuadratura (quadrature fluctuations) del vacío que corresponden a la desviación estándar que predice la teoría. Así parece que siempre se pueden obtener 'efectos del vacío' en experimentos pero solamente al nivel de las llamadas fluctuaciones cuánticas presentes también en cualquier estado con un número definido de fotones.

Los elementos más básicos de la electrodinámica cuántica ya están presentes en el artículo de Dirac de 1927. En este trabajo el campo electromagnético y la materia son descritos por hamiltonianos clásicos. Un tercer término describe la interacción entre el campo y la materia: $H = H_{mat} + H_{elect} + H_{int}$. A través del procedimiento de cuantización el hamiltoniano total se convierte en un operador. Pero es importante notar que la radiación y la materia son cuantizados por separado. Por razones (aparentemente) prácticas Dirac usa un método perturbativo para desarrollar las aplicaciones de la teoría.

Como ya comenté el enfoque de Dirac fue desarrollado, en particular, por Jordan, Pauli, Heisenberg, y Fermi. Mirando ahora a la electrodinámica cuántica desde el método lagrangiano establecido, tenemos dos campos clásicos descritos, uno por las ecuaciones de Maxwell-Lorentz y otro por la ecuación de Dirac. Como ya mencioné la ecuación de Dirac se puede ver como una ecuación describiendo un campo clásico. Usando el esquema habitual de la expansión en serie de Fourier de la función de onda, el campo se puede ver como un conjunto infinito de modos propios en que después de la cuantización los coeficientes se convierten en operadores. En el caso del campo electromagnético se usa un procedimiento equivalente. Hasta este momento se está considerando dos campos cuantizados independientes. La electrodinámica cuántica es una teoría que nos describe la interacción entre la radiación y materia representados por estos campos cuánticos.

El lagrangiano de la electrodinámica cuántica se puede definir partiendo de los lagrangianos para el campo de Dirac libre, el campo electromagnético libre, y un término describiendo la interacción entre ellos:

$$L = L_m + L_{em} + e\overline{\psi}\gamma^\mu \cdot \psi A_\mu .$$

De partida la cuantización se hace para los campos libres, no para el caso (que resulta imposible de tratar) de un sistema cerrado de campos en interacción. Se tiene en cuenta el término de interacción $e\overline{\psi}\gamma^\mu \cdot \psi A_\mu$ por un procedimiento perturbativo que parte de los campos libres para describir procesos físicos.

En las aplicaciones de la teoría se considera (siempre) un estado inicial (en $t = -\infty$) correspondiendo a campos libres y un estado final (en $t = +\infty$) que también corresponde a campos libres. La amplitud de transición desde el estado inicial ϕ_A al estado final ϕ_B es dada por $S_{AB} = (\phi^*_B S \phi_A)$, donde S es la llamada matriz-S. La matriz-S es dada por

$$S = \sum_{n=0}^{\infty} \left(\frac{e}{\hbar c} \right)^n \frac{1}{n!} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dx_1 \dots dx_n P\{\overline{\psi} \not{A} \psi(x_1), \dots, \overline{\psi} \not{A} \psi(x_n)\} .$$

Vemos que la matriz-S que depende solamente del término de interacción se escribe como una serie de potencias de *e*, donde *e* es la carga eléctrica: $S = 1 + eS^{(1)} + e^2 S^{(2)} + \dots$. Un elemento esencial de este método es el llamado 'switching on' y 'switching off' (conexión y desconexión) adiabática de la interacción entre los campos para poder calcular integrales que van de $-\infty$ a $+\infty$.

Consideremos por ejemplo la aplicación de la electrodinámica cuántica a la descripción de la aniquilación en dos fotones de un par electrón-positrón: $e^+ + e^- \rightarrow 2\gamma$. El estado inicial corresponde a un campo de Dirac con dos cuantos, uno correspondiente al electrón y otro al positrón (el campo electromagnético se supone en el estado

fundamental). Después de la aniquilación entre el electrón y el positrón, el campo de Dirac se encuentra en su estado fundamental (i.e., sin que haya ningún cuanto) y el campo electromagnético se queda ahora en un estado con dos fotones. En segundo orden la amplitud de transición es dada por

$$\begin{aligned} S_{fi} = (-e)^2 \int d^4x_1 \int d^4x_2 \langle 2\gamma | A_\mu(x_1) A_\nu(x_2) | 0 \rangle (\gamma_\mu)_{\alpha\beta} (\gamma_\nu)_{\gamma\delta} \\ \times \Big[\langle 0 | \Psi^{(+)}_\beta(x_1) \overline{\Psi}^{(-)}_\gamma(x_2) \overline{\Psi}^{(+)}_\alpha(x_1) \overline{\Psi}^{(+)}_\delta(x_2) | e^- e^+ \rangle \theta(t_1 - t_2) \\ - \langle 0 | \Psi^{(+)}_\gamma(x_2) \overline{\Psi}^{(-)}_\beta(x_1) \overline{\Psi}^{(+)}_\alpha(x_1) \overline{\Psi}^{(+)}_\delta(x_2) | e^- e^+ \rangle \theta(t_2 - t_1) \Big]. \end{aligned}$$

No entraré en los detalles de esta expresión, sólo comentaré algunos aspectos más relevantes. En está expresión encontramos términos que corresponden a la 'propagación' de un cuanto (virtual) entre los puntos del espacio-tiempo x_1 y x_2, y componentes relacionadas con los estados libres de cada campo (estados de Fock): $|e^- e^+\rangle$, $|2\gamma\rangle$, y los estados de vacío de cada campo $|0\rangle$. Así, sólo entran en el cálculo de interacciones estados pertenecientes al espacio de Fock de cada campo. Parece entonces que se tiene un procedimiento sencillo, basado en la matriz-S, para describir cualquier proceso físico que corresponda a una interacción entre el campo de Dirac y el campo electromagnético.

El problema es que la conexión adiabática de la interacción (adiabatic switching) se supone que permite pasar de la situación descrita por los hamiltonianos (o lagrangianos) de los campos libres H a la situación de interacción descrita por el hamiltoniano (o lagrangiano) de los campos en interacción H_I. Ahora, de acuerdo con el llamado teorema de Haag, en términos informales, los vectores de estado para los campos libres y los vectores de estado de los campos en interacción están en espacios distintos y no se pueden 'conectar'. Por el teorema de Haag se puede concluir que si partimos de un campo libre en $t = -\infty$ tendremos siempre un campo libre para todo t. Así resulta necesario desde el inicio considerar vectores de estado de campos en interacción. Ahora bien, como hemos visto, esto no es lo que se hace en la electrodinámica cuántica. Dicho en pocas palabras, el teorema de Haag implica que el método perturbativo usado en la teoría para describir la interacción entre la radiación y la materia es desde un punto de vista matemático inconsistente. Así tenemos el problema de comprender cómo es posible que un método matemáticamente inconsistente permita la obtención de resultados excelentes cuando los comparamos con datos experimentales. Trataré de mostrar que los buenos resultados de la teoría pese al teorema de Haag se pueden explicar si se tiene en cuenta la base física de la teoría y no solamente su estructura matemática.

Como ya referí antes, la teoría se desarrolla partiendo de la cuantización independiente de dos campos clásicos. Describimos siempre su interacción como una pequeña perturbación a sus estados libres. En realidad no tratamos los campos como un sistema único cerrado. Pero desde un punto de vista matemático si consideramos todos los términos de la serie de expansión de la matriz-S, eso corresponde a describir un sistema cerrado. La cuestión es que la serie de expansión de la matriz-S es divergente. ¿Qué implicaciones tiene esto? Parece entonces que la situación es aún peor que la amenaza de inconsistencia matemática debido al teorema de Haag. Si la serie es divergente eso significa que si no calculamos sólo unos cuantos términos y tratamos de hacer un cálculo lo más exacto posible, a partir de un determinado orden, en vez de tenerse resultados cada vez más ajustados a los datos experimentales tendremos resultados cada vez peores. Así parece que la teoría sólo 'funciona bien' porque

hacemos unos cálculos limitados. Tal no es el caso. Si es cierto que desde un punto de vista matemático el que se tenga en cuenta sólo unos cuantos términos de la serie no tiene aparente justificación, cuando tenemos en cuenta la base física de la teoría sí se puede justificar el no considerar los términos de orden elevado que 'estropean' los cálculos.

Como referí la teoría ha sido estructurada alrededor de la idea de que la interacción entre radiación y materia es débil (weak). Esto está relacionado con lo siguiente: (1) el término de interacción en el Lagrangiano es pequeño; (2) debido a esto cuantizamos los campos en separado como campos libres; (3) tomamos el término de interacción como un término perturbativo. Ahora, como ya mencioné, si intentamos calcular toda la matriz-S, correspondiendo a tratar la radiación y materia como un sistema cerrado, se obtiene un resultado divergente. Se puede concluir así que, en la práctica, la noción de que la interacción es débil implica que es imposible pasar de la descripción de campos libres (y su interacción) a la situación de campos (totalmente) en interacción.

Desde una perspectiva formal se puede mostrar que un posible sistema de campos en interacción no se puede describir usando la representación de Fock para campos libres. Esto significa que desde un punto de vista formal para un sistema cerrado de campos en interacción no se puede usar la base física constitutiva de la electrodinámica cuántica que es la idea de interacción débil y su implementación en la teoría. Así, podemos ver que no se consideran los términos de orden elevado de la serie de expansión de la matriz-S debido a que su inclusión correspondería a un uso impropio de la estructura matemática más allá de la base física que se supone que ésta representa. Por tanto en la electrodinámica cuántica tenemos los conceptos de radiación y materia, y de una interacción débil entre ellos, pero no de campos en interacción (que corresponde a un sistema cerrado de radiación y materia). Así, hago una correspondencia entre la obtención de resultados matemáticos con significado (no divergentes) y la manera como se implementa la base física de la teoría. En este caso tenemos cálculos intrínsecamente aproximados de la interacción débil entre dos sistemas físicos distintos (radiación y materia).

Creo que esta situación tiene semejanzas con las ideas de Bohr respecto a la paradoja de Klein. Como ya referí antes, para Bohr la paradoja de Klein resultaba de considerarse potenciales 'matemáticos' sin tenerse en cuenta la estructura atómica de la materia (parte constituyente de la base física de la teoría). La paradoja resultaba de usarse la matemática más allá de lo que los conceptos físicos de la teoría realmente permitían. Como en el caso de la paradoja de Klein la divergencia de la serie de expansión de la matriz-S resulta de aplicarse la estructura matemática de la teoría más allá de su contenido físico provocando un colapso de los cálculos

Volviendo a la cuestión del teorema de Haag, resulta que en la electrodinámica cuántica evitamos las consecuencias del teorema porque ni siquiera intentamos describir un sistema cerrado de campos en interacción, solamente la interacción entre radiación y materia como sistemas distintos. Así no hay ningún conflicto de la teoría con el teorema de Haag.

El capítulo 6

Cuando en 1929-30, Heisenberg y Pauli presentaron en dos artículos una teoría de campos relativista de la interacción entre un campo electromagnético cuantizado y un campo de Dirac cuantizado, cambiaron de una primera opinión en que la energía propia infinita del electrón no constituía un problema mayor a una postura más circunspecta en

que reconocían que este problema podía incluso hacer inaplicable la teoría. La situación de la electrodinámica cuántica en los años treinta no mejoró.

Como hemos visto, para tratar de resolver inconsistencias en su teoría del electrón relacionadas con la existencia de soluciones con energía negativa, Dirac propuso su teoría de los agujeros (hole theory). De aquí surgió un nuevo problema con infinitos. En esta teoría/interpretación de la ecuación de Dirac se considera que todos los estados correspondientes a energías negativas están en su mayoría ocupados por electrones. Esto llevó a Dirac a considerar que el campo electromagnético es generado por la diferencia entre la densidad eléctrica actual y la que corresponde a tener todos los estados de energía negativa ocupados (el estado normal). Así la ecuación para el campo eléctrico es dada por Div $\mathbf{E} = -4\pi (\rho - \langle\rho\rangle_{vacío})$. Explorando las consecuencias de esta definición Dirac estudió cómo un campo externo podría influir en la definición del estado normal, esto es, trató de calcular cúal era la distribución de electrones con energías negativas que se puede considerar como la normal en el caso en que estén sujetos a un campo externo. Considerando el caso sencillo de un campo eléctrico externo estático, Dirac concluyó que este cambiaba la distribución de electrones con energía negativa de una manera que correspondía a una neutralización parcial de la carga que producía el campo estático. Si se asumía que su ecuación era exacta eso llevaba a una cancelación total de la carga externa – un resultado sin sentido. Eso llevó a Dirac a suponer que la ecuación no se puede aplicar para energías ultra-relativistas del orden de $137mc^2$. Así no teniendo en cuenta el efecto del campo en electrones con energía más negativa que $-137mc^2$, tenemos que la neutralización de la carga (que origina el campo externo) debido a los restantes electrones es pequeña, del orden de 1/137. Así Dirac concluye que todas las partículas cargadas tienen una carga efectiva menor que su carga real (del orden 136/137).

Esta definición de un valor máximo de energía resulta fundamental para obtener un resultado finito. Así en un calculo posterior usando la llamada aproximación de Hartree-Fock Dirac obtiene un resultado infinito que sólo puede reducir a uno finito imponiendo una energía de corte (cut-off energy). Esto no es simplemente un truco matemático. Dirac presenta una justificación física para usarse este procedimiento. De acuerdo con Dirac (siguiendo ideas de Bohr) la teoría cuántica sólo se aplica a fenómenos en que las distancias son mayores que el diámetro clásico del electrón, esto es del orden de e^2/mc^2. Esto corresponde a energías del orden $(\hbar c/e^2)(mc^2) \cong 137mc^2$, que es el valor adoptado por Dirac como límite para la energía. Esta aplicación está de acuerdo con la idea de Bohr de que no se pueden hacer integraciones tomando la energía con cualquier valor debido a que la teoría trata el electrón como una partícula puntual (point-charge). Así sería inconsistente en las aplicaciones de la teoría considerar energías que corresponderían a distancias menores que el 'diámetro' del electrón. Esta importante idea se va a quedar soterrada en el posterior desarrollo de técnicas para enfrentar los problemas de infinitos en la teoría. No voy a entrar aquí en los detalles de esta técnica provisoria aplicada por Dirac a la que se le dio el nombre un poco despectivo de física de substracción (subtraction physics); sólo refiero que durante los años treinta no ha sido posible resolver los distintos problemas de energía-propia que tenía la teoría. El único 'desarrollo' importante ha sido la comprobación por V. F. Weisskopf de que la energía-propia del electrón divergía 'sólo' de forma logarítmica. En la práctica sólo se podían hacer unas cuantas aplicaciones de la teoría en el orden más bajo de perturbaciones y nada más.

En 1947 los resultados experimentales de W. Lamb respecto a un desvío del nivel de energía del estado $2^2S_{1/2}$ respecto al $2^2P_{1/2}$ en el átomo de hidrogeno llevó a una serie de físicos (incluyendo los más brillantes de una nueva generación) a enfrentar de nuevo la

cuestión de los infinitos en la teoría (la guerra había dejado estas cuestiones teóricas en segundo plano). El primer momento de esta nueva fase en la historia de la electrodinámica cuántica lo encontramos en un cálculo no-relativista realizado por H. A. Bethe que le permitió obtener de forma aproximada el desvío observado experimentalmente. Para eso Bethe hizo uso del método de 'substracción' de Dirac en el sentido en que impuso un limite de energía en las integrales (un 'cut-off' de energía). El otro aspecto fue tomar la parte que sería infinita como una corrección de la masa del electrón y considerar que la masa observable está constituida por una masa 'mecánica' y el efecto de la interacción del electrón con su propio campo (la parte que resulta infinita). Adoptó básicamente un procedimiento ya necesario en la electrodinámica clásica debido al mismo tipo de problema (una energía-propia infinita) que se denomina renormalización. Es importante notar que, al contrario de Dirac, Bethe no dio ninguna motivación física para el 'cut-off'.

Unos pocos meses después del cálculo de Bethe, un físico de la nueva generación J. Schwinger desarrolló un método relativista pero no-covariante para calcular el desvío de Lamb (Lamb shift), usando para ello la renormalización de la masa y de la carga. La visión de Schwinger respecto a la renormalización es que ésta indicaba que la teoría necesitaba cambios para energías ultra-relativistas. Schwinger esperaba que una futura teoría mejorada debería imponer límites a la energía que permitiera la existencia de un 'cut-off' natural. Pero, al contrario de Dirac, Schwinger pensaba en términos de una mejora más bien matemática y no vio el problema como una incompatibilidad entre los conceptos físicos de la teoría (e.g. el concepto de electrón puntual) y la inexistencia de un límite natural asociado en las aplicaciones matemáticas de la teoría. Otro aspecto del trabajo de Schwinger es que, como los cálculos fueron realizados de forma no-covariante, había muchas ambigüedades en el procedimiento adoptado para identificar los términos divergentes.

Otro físico de la nueva generación que dio una contribución fundamental a la teoría fue R. P. Feynman. Partiendo de la propuesta de Bethe de buscar una modificación para frecuencias elevadas de forma claramente relativista (que permitiera evitar los infinitos por un procedimiento sin ambigüedades), Feynman buscó una modificación consistente de la electrodinámica. Feynman empezó con el caso de la electrodinámica clásica desarrollando un método llamado regularización, en que el uso de un término extra en las expresiones matemáticas permitía que todos los resultados fueran finitos. Feynman aplicó después este procedimiento para el caso en que los electrones (y positrones) se describen con la ecuación de Dirac.

El método de regularización de Feynman resulta ser inconsistente desde el punto de vista de la interpretación física de la teoría. Eso significaba que en la práctica después de hacer la regularización de los términos que en otro caso serían infinitos, estos se tenían que 'absorber' en la masa y carga del electrón correspondiendo a hacerse una renormalización. Para que los resultados no dependieran del término de regularización, se tenía que considerar el límite en que este dejaba de aparecer en las expresiones. Como ya se había hecho la renormalización de los términos infinitos esto ya no causaba problemas. El método de Feynman era entonces un procedimiento equivalente al de Schwinger, su ventaja era ser un método covariante y por lo tanto sin ambigüedades en la manera como se manejaban los términos infinitos. Así el procedimiento de Feynman no fue una nueva teoría mejorada y fue solamente un procedimiento para manejar de forma clara integrales que resultan ser divergentes.

Resulta claro que la nueva generación de físicos tenía una actitud mucho más pragmática que la anterior, tratando de poner la teoría en funcionamiento sin detenerse demasiado en los posibles problemas conceptuales asociados a la regularización y

renormalización. Una excepción es la visón de F. Dyson respecto a este tema. La concepción de Dyson resulta tener alguna semejanza con la de Dirac y Bohr, entonces ya olvidada. Dyson imagina dos tipos de observadores, el 'ideal' y el 'real'. En el caso del observador 'ideal' este tendría instrumentos de medición sin estructura atómica pudiendo 'medir' la interacción puntual de los campos cuánticos (y así obtendría resultados infinitos); el observador 'real' tiene instrumentos de medida constituidos por átomos y por lo tanto se tiene que tener en cuenta la estructura atómica de la materia. Así las mediciones del observador 'real' están limitadas y eso le impide hacer observaciones submicroscopicas. De este modo solo obtiene resultados finitos.

El capítulo 7

La descripción en orden más bajo de teoría de perturbaciones de los procesos físicos en la electrodinámica cuántica está libre del problema de infinitos. Esto puede permitir un análisis más claro de la descripción espacio-temporal de los procesos físicos que se tiene en la teoría. Me concentraré en la descripción de la dispersión entre electrones (electron-electron scattering).

En 1948 Dyson demostró la equivalencia entre los métodos de Schwinger (y Tomonaga) y Feynman. Lo hizo usando la llamada matriz-S. Como ya mencioné la matriz-S se aplica por un procedimiento perturbativo y es divergente. Los términos de orden superior de la matriz-S no cambian la descripción espacio-temporal (cualquiera que sea) que se puede tener con este método, por eso consideraré sólo la expansión de la matriz-S hasta segundo orden. En este caso la interacción entre los electrones resulta de un intercambio (exchange) de fotones virtuales (ver figura 1).

En la descripción espacio-temporal global (overall space-time approach)[7] de Feynman consideramos la propagación de un fotón virtual entre todos los puntos del espacio-tiempo de Minkowski. El propagador de Feynman es dado por

$$\langle 0|T\{A^{\mu}(x)A^{\nu}(x`)\}|0\rangle = i\hbar c D_F^{\mu\nu}(x-x')$$

Esta expresión significa que estamos considerando un fotón 'creado' en un punto del espacio-tiempo y 'aniquilado' en otro punto. El uso de T{ } significa que en esta expresión covariante incluimos, dependiendo del orden temporal, la propagación de un electrón a otro y viceversa, pues $T\{A^{\mu}(x)A^{\nu}(x')\} = A^{\mu}(x)A^{\nu}(x')$ si $t > t'$, y $T\{A^{\mu}(x)A^{\nu}(x')\} = A^{\nu}(x')A^{\mu}(x)$ si $t' > t$. La amplitud de transición en segundo orden resulta de la contribución de todas las posibles interacciones entre los campos de Dirac y Maxwell 'conectados' por un propagador de fotónes:

$$S^{(2)}(2e^- \to 2e^-) = \frac{-e^2}{2!}\int d^4x_1 d^4x_2 N\left[(\overline{\psi}^- \gamma^{\alpha}\psi^+)_{x_1}(\overline{\psi}^- \gamma^{\beta}\psi^+)_{x_2}\right] iD_{F\alpha\beta}(x_1 - x_2).$$

Los fotones se denomina virtuales por dos motivos. Uno es que la relación de energía y momento (energy-momentum relation) para el fotón virtual no es $k^2 = (k^0)^2 -$

[7] En este trabajo se va usar esta terminología pese a que teniendo en cuenta sus implicaciones respecto a la descripción temporal de los fenómenos físicos no parece la más adecuada.

$\mathbf{k}^2 = 0$. Esto se debe a que en la expresión del propagador $\mathbf{k}$ y k^0 son independientes el uno del otro; también resulta que el propagador no es nulo para separaciones del tipo espacial (space-like separations) lo que corresponde a una 'propagación' con una velocidad superior a la de la luz. El segundo punto es que este fotón virtual no se puede en principio observar.

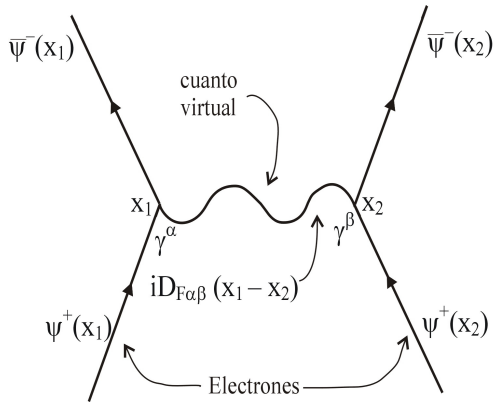

Figura 1: La interacción entre electrones en segundo orden, que resulta del intercambio de un fotón virtual (Este es un ejemplo de un diagrama de Feynman).

Una cuestión bastante debatida en la filosofía de la física es el estatus de las partículas virtuales. Por lo general la idea es que las partículas virtuales se tienen que ver como un artefacto de la expansión perturbativa sin aportar ninguna 'imagen' física de las interacciones. El argumento principal usado en la defensa de esta visión es el llamado argumento de la superposición. De acuerdo con este argumento la descripción por la matriz-S de las interacciones resulta en una serie infinita de términos de orden cada vez mayor, lo que corresponde a tener un número infinito de combinaciones de cuantos virtuales. Así los cuantos virtuales se tendrán que ver como descripciones pictóricas de términos matemáticos (pues se pueden asociar a distintos diagramas de Feynman).

El problema es que este argumento no es válido en la electrodinámica cuántica. Como ya mencioné la serie de expansión de la matriz-S es divergente y tenemos argumentos físicos para sólo considerar los primeros términos. Así no tenemos un número infinito de cuantos virtuales en la descripción de las interacciones. En este caso el intercambio de fotónes virtuales es más que algo meramente matemático, es la manera en que la teoría nos describe (a nivel físico) las interacciones. Pero hay que tratar de comprender lo que es realmente la descripción global de las interacciones. El aspecto crucial es que la teoría no nos da una descripción en el tiempo de las interacciones. En el método de la matriz-S consideramos siempre límites de integración entre $t = -\infty$ y $t = +\infty$; no hay manera de evitarlo. Esto es consistente con las posibilidades experimentales. El caso es que no hay acceso experimental al 'mecanismo' de la interacción. Lo que sí se puede hacer es determinar (en el ámbito teórico y experimental) la llamada sección transversal (cross-section) que permite calcular/verificar la probabilidad de observar un determinado resultado final de la interacción.

Se presenta la cuestión inmediata de saber si esta es una limitación de un método en particular o una característica de la teoría. En cuanto al método, la matriz-S es bastante general y otros métodos también perturbativos tienen el mismo tipo de problema. Lo que tal vez fuera posible es considerar otro tipo de situaciones que aún se puedan ver

como descritas por la teoría en las cuales se tenga una descripción temporal más en acuerdo con lo que se espera desde la física clásica: una interacción retardada debido a la velocidad finita de la luz. Dejaré esta cuestión para el siguiente capítulo.

El capítulo 8

Aquí trataré la cuestión de la relación entre la electrodinámica clásica y la cuántica. Del capítulo anterior quedó por analizar una cuestión que trae implícita la que acabo de mencionar. En la electrodinámica clásica tenemos la posibilidad de considerar que la interacción electromagnética (dependiente del tiempo) resulta de la emisión y absorción de ondas electromagnéticas que se propagan a la velocidad de la luz. En el caso de la electrodinámica cuántica hasta el momento sólo se ha podido describir las interacciones a nivel temporal de forma global (entre $t = -\infty$ y $t = +\infty$). La cuestión está en saber si hay un término medio entre estos dos extremos y qué implicaciones tiene para nuestra visión de la relación entre las dos teorías.

En un primer momento podría parecer que un modelo sencillo de la interacción entre dos electrones atómicos podría darnos este término medio que se busca. Aparentemente este modelo se desarrolla dentro de la electrodinámica cuántica. Así cuando un átomo inicialmente en un estado excitado emite un fotón, éste solo será absorbido por otro átomo después aproximadamente de un intervalo de tiempo r/c, donde r es la distancia entre los átomos y c la velocidad de la luz. Un aspecto fundamental de este modelo es la forma específica dada a la densidad bilineal (bilinear density) $\overline{\psi}\gamma^{\mu}\psi$ que aparece en el término de segundo orden de la matriz-S usado en este modelo:

$$\text{const} \int_{V_x} d^4x \int_{V_y} d^4y (\overline{\psi}(x)\gamma^{\mu}\psi(x)) D_c(x-y) (\overline{\psi}(y)\gamma^{\mu}\psi(y)) ,$$

con $\overline{\psi}\gamma^{\mu}\psi \sim a_1 a_2^{*} \rho_{\mu}(x) \exp [i\omega_0 t - t^2/T^2]$, donde $\omega_0 > 0$. Sin entrar en detalles se puede verificar que la expresión adoptada es la misma que se obtiene por consideraciones clásicas. Esto es importante pues significa que el modelo se está aplicando no en un 'régimen cuántico' sino en el límite de correspondencia entre las dos teorías donde por construcción la teoría cuántica tiene que dar resultados equivalentes a la teoría clásica. Así se trata más bien de un modelo semi-clásico.

Vemos que no se consigue dentro de la electrodinámica cuántica tener una descripción en el tiempo de las interacciones. Si suponemos la electrodinámica cuántica como una teoría más fundamental a la cual se reduce la teoría clásica tenemos un problema. La teoría clásica nos permite asociar intervalos de tiempo (duraciones) a los procesos físicos. Se supone que 'por debajo' existe un mundo cuántico descrito por una teoría cuántica. Estos procesos cuánticos deberían estar en el 'interior' de los procesos macroscópicos a los cuales se asocian duraciones claras. El problema es que según la electrodinámica cuántica no podemos asociar ningún intervalo de tiempo, por más cualitativo que sea, a los procesos cuánticos. Tenemos así el problema de justificar la emergencia de los intervalos de tiempo asociados a procesos descritos por la física clásica desde una descripción cuántica. Así un elemento clave de la emergencia de lo clásico (classicality) se nos escapa.

Por este motivo me resulta difícil aceptar la visión tradicional de la teoría cuántica como más fundamental y a la cual se reduce la teoría clásica. Teniendo en cuenta que la

electrodinámica cuántica se construye, en parte, por un proceso de cuantización de la electrodinámica clásica, resulta más aceptable la idea de que la electrodinámica cuántica depende de la clásica y no se puede considerar por separado de la versión clásica. Son las dos en conjunto lo que nos permite describir los fenómenos que 'catalogamos' como de interacción electromagnética entre radiación y materia.

Esta visión está de acuerdo con la idea de O. Darrigol de una estructura modular de las teorías físicas. De acuerdo con Darrigol la práctica y la historia de la física revelan que las teorías no son un todo homogéneo y separado; por el contrario las teorías se aplican en conjunción unas con otras. Así una teoría se debe ver más bien como constituida por componentes o módulos que pueden ser ellos mismos teorías con distintos dominios de aplicación.

CHAPTER 2

THE SCHRÖDINGER EQUATION AND ITS INTERPRETATION

1 Introduction

To set the 'stage' for the study of quantum electrodynamics, in particular of Dirac's relativistic quantum-mechanical equation and its different interpretations, I will consider in this chapter the non-relativistic and quantum-mechanical Schrödinger equation. In section 2 I will consider some of the historical developments of the quantum theory previous to Schrödinger's contribution. I will focus in particular on Albert Einstein's work on light quanta (which as we will see in chapter 4 is a fundamental aspect of the quantized electromagnetic field) and Louis de Broglie's work on wave aspects of electrons (which is an immediate precursor of Schrödinger's approach). In section 3 I consider the early 'stages' of the development of the Schrödinger equation not addressing the interpretation problem, i.e. the physical meaning of the equation. Section 4 will be dedicated to this problem. I will focus on Schrödinger's 'electrodynamic' interpretation. We will see that this interpretation has a two-fold aspect. On one side Schrödinger uses his electrodynamic interpretation of the wave function as giving rise to a charge density distribution in space. But on the other side Schrödinger also takes the wave function as a 'real' wave propagating in space. In fact, that there can be an ambiguity in the interpretation of the Schrödinger equation can be made clear by considering the simple case of the hydrogen atom. We will see that it is possible to consider the Schrödinger equation as the equation of a 'classical' de Broglie wave that is afterwards quantized. We will encounter similar ambiguities in the next chapter when looking into the details of the Dirac equation.

2 The 'pre-history' of the Schrödinger equation

In 1900 Max Planck presented a derivation of the energy distribution law of the normal spectrum, which he had previously proposed with no rigorous theoretical justification but with a good agreement with observational data. In his derivation Planck considered a system of resonators (Hertzian oscillating dipoles) in thermodynamic equilibrium with electromagnetic radiation at a constant temperature (Klein, 1975, pp. 461-462). There are two main separate parts in Planck's derivation. One consists in deriving the relation between the average energy of a resonator (having frequency ν) and the density of the (blackbody) electromagnetic energy at the same frequency. This Planck achieved by thermodynamics and classical electrodynamics. The other part of Planck's derivation

consisted in using Ludwig Boltzmann's combinatorics in the determination of how the total energy of resonators with a particular frequency is distributed at a particular instant over the resonators, taken to be independent of one another (Jammer, 1966, pp. 10-22; Kuhn, 1978, pp. 97-110).

Boltzmann had developed his combinatorics as a procedure (without physical meaning in itself) to determine the most probable distribution of molecular velocities in a perfect gas. For that he considered a fiction wherein molecules can take only discrete energy values. Each particular microstate of the gas corresponds to a particular distribution of discrete elements of energy by the molecules (what Boltzmann called a complexion). Then, by determining the maximum number of complexions (under particular constraints) the equilibrium distribution was obtained. That is, the equilibrium macrostate of the gas (with N molecules and a total energy E) is the one for which there are more microstates available. In the end of the calculation the continuous limit was taken. Boltzmann then obtained the Maxwell distribution law of molecular velocities in a perfect gas (Darrigol, 1992, pp. 62-63).

Planck had already obtained, in part by ad hoc means, an energy distribution law that was in excellent agreement with experimental data. In the search for theoretical foundations to his law Planck found it necessary to make use of Boltzmann's ideas. Planck, when applying Boltzmann's combinatorics to the case of resonators in thermodynamic equilibrium with electromagnetic radiation at a constant temperature, considered that the total energy of N resonators consisted in an integer number P of energy elements distributed over the resonators. However, to arrive at his law Planck had to keep the energy elements to the end of the calculation. He could not take the continuous limit (Darrigol, 1992, pp. 67-73). In this way, the essential point that enables the derivation of Planck's distribution law is to consider that the total energy E of N resonators with frequency ν is composed of an integer number of energy elements ε. This has been seen as "Planck's introduction of the quantum of action" (Jammer, 1966, p. 19), or the moment "at which discontinuity entered physics" (Klein & Shimony & Pinch, 1979, p. 431).

This view was challenged in 1978 when Thomas S. Kuhn put forward the idea that Planck did not consider the quantization of the energy of each individual resonator in his derivation (Kuhn, 1978). This apparently heterodox view has been corroborated (Darrigol, 1992), and without going into the complexities of Planck's approach to statistical mechanics, we find evidence of this in Planck's own writing in his 1900 article:

> We consider, however – this is the most essential point of the whole calculation – E to be composed of a very definite number of equal parts and use thereto the constant of nature $h = 6.55 \times 10^{-27}$ erg sec. This constant multiplied by the common frequency ν of the resonators gives us the energy element ε in erg, and dividing E by ε we get the number P of energy elements which must be divided over the N resonators. If the ratio is not an integer, we take for P an integer in the neighborhood. (Planck, 1900, p. 84)

The last sentence clearly indicates by itself that "the energy of N independent resonators, and *a fortiori* the energy of a single resonator, was not thought to be restricted to multiples of [ε]" (Darrigol, 1992, p. 74), as would be the case if each individual resonator had its energy quantized.

According to Kuhn the discontinuity in the energy of the resonators entered physics in Albert Einstein's 1906 article about Planck's theory. Einstein considered that:

We must, therefore, recognize the following position as fundamental to the Planck theory of radiation: The energy of an elementary resonator can take only values which are integral multiples of (R/N)βν [where R is the gas constant, N Avogadro's number, and β a constant]. During absorption and emission the energy of a resonator changes discontinuously by an integral multiple of (R/N) βν. (Quoted in Kuhn, 1978, p. 170)

Already in his previous article of 1905, about creation and conversion of light, Einstein mentioned the 'elementary quanta' (associating it with Planck's theory), but in this work what Einstein was considering was an atomistic view of light in analogy with the atomic theory of matter. Like in the case of matter, where we have to consider a quantity of energy associated with the atoms or electrons that "can not be split into arbitrarily many, arbitrarily small parts" (Einstein, 1905, p. 91) – in contrast to the continuous distribution of energy of the electromagnetic field –, in the case of light (in the limit of short wavelengths) we can consider, at least from a thermodynamical point of view, that its energy is discontinuously (atomistically) distributed in space.

In the 1905 work Einstein considered the thermodynamical properties of light. In particular it was found that the volume dependence of the entropy of monochromatic radiation with energy E and frequency ν, in the limit where Wien's law is valid, is the same as the volume dependence of the entropy of a gas of mutually independent particles with energy hν. Einstein considered that "when a light ray starting from a point is propagated, the energy is not continuously distributed over an increasing volume, but it consists of a finite number of energy quanta localized in space, which move without being divided and which can be absorbed or emitted as a whole" (Einstein, 1905, p. 92). Einstein proposed his heuristic argument on the nature of light considering not Planck's distribution law, but what can be seen as the limit of Planck's law for short wavelengths: Wien's law. In this way, Einstein's argument about the atomicity of light was not applicable to radiation of all wavelengths, as he remarked: "Monochromatic radiation of low density behaves – as long as Wien's radiation formula is valid – in a thermodynamic sense, as if it consisted of mutually independent energy quanta" (Einstein 1905, p. 102; for details on Einstein's derivation of his result see e.g. Sánchez Ron, 2001, pp. 170-172).

What might have led Einstein to this work is certainly a combination of factors. One factor seams to be the "profound formal difference between the theoretical ideas that physicists have formed concerning gases, and other ponderable bodies, and Maxwell's theory of electromagnetic processes in so-called empty space" (quoted in Klein, 1963, p. 62). At a conference in September 1909, Einstein gave a further argument along these lines, based on general characteristics of the theories, for the light-quanta hypothesis (Klein, 1964, p. 7). Concerning the emission and absorption of light, Einstein considered more appealing a corpuscular theory due to the symmetrical treatment of the two processes. In the case of the classical theory there is not an elementary process that is the opposite to the process of emission of an outwardly propagated spherical wave (Einstein, 1909b, p. 387). But possibly the most important motivation for the work (at least according to Einstein's autobiographical notes; see Einstein, 1979) was Einstein's intention of applying his own statistical methods in deriving Planck's distribution. It turns out that Einstein found a problem in the theoretical foundations he was using. He did not arrive at Planck's distribution law but to what would become known as the Rayleigh-Jeans distribution law, noticing for the first time what would be called the ultraviolet divergence: the infinite energy of the radiation field due to the high frequencies of the field. In trying to understand the origin of the problem Einstein took Planck's distribution law as an empirically confirmed law and set to study its low and high frequency behavior. In this way Einstein explored the frequency range in which his

classical derivation was problematic. Einstein studied the thermodynamical behavior of radiation of high frequency (low wavelength), in which Wien's law can be seen as a limiting case of Planck's law, arriving at his breakthrough idea of light quanta.

At this stage it was clear to Einstein that classical electrodynamics was at stake (remember also the other probable motivations for this work concerning the structure of radiation). In the introduction of the article Einstein stated his view on the theory:

> The wave theory of light, which operates with continuous spatial functions, has proved itself splendidly in describing purely optical phenomena and will probably never be replaced by another theory. One should keep in mind, however, that optical observations apply to time averages and not to momentary values, and it is conceivable that despite the complete confirmation of the theories of diffraction, reflection, refraction, dispersion, etc., by experiment, the theory of light, which operates with continuous spatial functions, may lead to contradictions with experiment when it is applied to the phenomena of production and transformation of light. (Einstein 1905, p. 86)

Einstein did not developed in this work an analysis of the detailed theoretical motives that made his classical derivation different from Planck's, i.e. the failure of classical electrodynamics, and neither did he conduct a critical study of Planck's own derivation. He was content to indicate where the problem might be and to explore more of the experimental evidence for his light quanta hypothesis. Besides the 'blackbody' radiation described by Planck's distribution law and whose study in the limit of high frequencies led Einstein to the light quanta hypothesis, Einstein focused on situations where radiation was created or transformed and where he expected the corpuscular structure of light to show up: the phenomenon of fluorescence, the photoelectric effect, and the ionization of gases by ultraviolet radiation. All these three cases were easily explained by taking into account the light quanta hypothesis.

Einstein took a closer look on Planck's distribution law in the article from 1906 mentioned previously, where he presented his view on Planck's theory taking into account his idea of the light quanta (ter Haar, 1967, pp. 17-18). Einstein concluded that "Planck's theory makes implicit use of the … light-quantum hypothesis" (quoted in Pais, 1979, p. 875). This is due, according to Einstein, to the fact that to deduce Planck's distribution law the resonators can not have any arbitrary value of energy but only integer multiples of $h\nu$ (Einstein, 1906, p 195). Einstein gave a general deduction in which depending on the assumption made on the energy range of a resonator the Rayleigh-Jeans law or Planck's law was obtained. In the second case Einstein took the energy of a resonator to have a discrete energy spectrum.

A pause is needed at this point. It is important to remember (as mentioned above) that Planck did not consider in his derivation that the energy of each resonator could take only discrete values. This is where Kuhn's interpretation is coming in. Also Einstein did not stop here. He made a connection between the discontinuous energy spectrum of the resonators and the light quanta hypothesis. The (implicit) connection in Einstein's argumentation to the light quanta idea can be made recalling that in his 1905 article Einstein considered that "a light quantum transfers all of its energy to a single electron" (Einstein, 1905, p 104). With this 'simplest picture' of the absorption (or emission) of light by matter, Einstein considered that "by emission and absorption, the energy of a resonator changes by jumps of integral multiples of [$h\nu$]" (Einstein, 1906, p. 195). This makes a connection between the existence of discontinuous energy levels in the resonators (that for Einstein is necessary to make a proper derivation of Planck's distribution law) and the existence of light quanta. But there is still the problem that in the derivation of Planck's distribution law by Einstein (as it was the case also with Planck), use is being made of results from classical electrodynamics whose foundation

is at stake due to the light quanta hypothesis. We must recall Einstein's doubts about classical electrodynamics. In particular, as we have seen, he explicitly mentions the possibility of the theory to have meaning only when considering time averages. In this way it turned out that the necessary adoption (at this point) of results from classical electrodynamics was paradoxical as Einstein recognizes:

Although Maxwell's theory is not applicable to elementary resonators, nevertheless the mean energy of an elementary resonator in a radiation space is equal to the energy calculated by means of Maxwell's theory of electricity. This proposition would be immediately plausible if, in all those parts of the spectrum that are relevant for observation, $\varepsilon = (R/N)\beta\nu$ were small compared with the mean energy $\overline{E}_\upsilon$ of a resonator; however, this is not at all the case, for within the range of validity of Wein's radiation formula, $e^{\beta\upsilon/T}$ is large compared with 1. It is easy to prove that according to Planck's theory of radiation, within the range of validity of Wien's radiation formula, $\overline{E}_\upsilon / \varepsilon$ has the value $e^{-\beta\upsilon/T}$, thus, $\overline{E}_\upsilon$ is much smaller than ε. Therefore only a few resonators have energies different from zero. (Einstein, 1906, p. 196)

Einstein's view relating the discontinuous change in the number of energy elements of a resonator to the emission or absorption of light quanta was later critically analyzed by Paul Ehrenfest and others. The reason was that Einstein was identifying the quanta of energy (energy elements) that an oscillator may take, which, being indistinguishable, are not particles (in the classical sense), with light-quanta taken (implicitly) to be classical distinguishable particles (Jammer, 1966, pp. 51-52). To be rigorous Planck's law cannot be 'deduced' from the light quanta hypothesis within Einstein's procedure without a further hypothesis (regarding the statistics of light quanta), as is implicit in Einstein's deduction of Planck's distribution law in a 1907 paper (ter Harr, 1967, p. 18). But this was only clarified after the work of Satyendra Nath Bose (see below).

Toward the end of 1908 there was a further development in the light-quanta hypothesis. Einstein made a calculation of the energy fluctuations in blackbody radiation and obtained an expression with two terms. One term results from the interference of waves as expected from Maxwell-Lorentz electrodynamics, and, according to Einstein, the other term is expected by taking the radiation to be "independent moving point quanta of energy $h\nu$" (quoted in Hermann, 1971, p. 58).

Einstein extended his approach and considered also the fluctuations of the radiation pressure. For that he took the radiation to be in a cavity in which one of the walls is a mirror that can move freely in the direction perpendicular to its normal. Again an expression with two terms was obtained with the same physical explanation as in the energy fluctuation case. According to Einstein "if the first term alone were present, the fluctuation of the radiation pressure could be completely explained by the assumption that the radiation consists of independently moving, not too extended complexes of energy $h\nu$" (Einstein, 1909a, p. 369).

This result, published in 1909, at the same time that it confirmed the significance of the light quanta hypothesis, gave to Einstein further evidence on the limitations of considering radiation as composed by independent particles (already in his 1905 work, Einstein knew that this hypothesis was only applicable to electromagnetic waves of high frequency):

I am not at all of the opinion that one should think of light as being composed of mutually independent quanta. This would be the most convenient explanation of the Wien end of the radiation formula. But already the division of a light ray at the surface of refractive media absolutely prohibits this view. A light ray divides, but a light quantum indeed cannot divide without change of frequency. (Letter from Einstein to Lorentz, 23 May 1909, quoted in Howard, 2005, p. 6)

Until 1916 after the completion of his gravitation theory Einstein did little further work on the quantum theory. But in that year a breakthrough occurred regarding the light quanta hypothesis (Klein, 1964, p. 16). In September of that year Einstein wrote in a letter to Michele Besso that "in each energy transfer from radiation to matter the momentum $h\nu/c$ is also transferred to the molecule. Hence we conclude that every such elementary process is a completely directed event. With that the light-quanta must be considered as good as being substantiated" (quoted in Mehra & Rechenberg, 1982, p. 515). This view came about due to Einstein's development of a simple statistical approach to the emission and absorption of radiation by matter. Einstein developed his approach by taking into consideration very simple assumptions. He took into account the general result from quantum theory that the molecules in interaction with radiation can only have a discrete set of energy states (an idea first proposed by him in 1906). As in the classical case where there is emission of radiation by a dipole oscillator independently of any external field, Einstein proposed that a molecule would emit radiation when by spontaneous emission, that is, without any external influence, a transition between a state Z_m and a state Z_n occurred. By analogy with the probabilistic description of the radiative decay, Einstein assigned a constant coefficient to this transition: $A^n_m = dW / dt$, where dW is the probability of the spontaneous process taking place in the time interval dt. Also, there would be, as in the classical case, an induced emission or absorption of energy due to the presence of electromagnetic radiation (Einstein, 1917, pp. 170-171).

According to classical theory a radiation beam will transfer energy and momentum to a molecule in accordance with the law of conservation of energy and momentum. But in what regards the emission of radiation, "according to classical theory the emission is in the form of a spherical wave" (Einstein, 1917, p. 172). In this case there would be no transfer of momentum to the molecule. To make compatible his derivation of Planck's law with general results regarding the thermal equilibrium between molecules and radiation, Einstein found it necessary to consider that the emission or absorption of radiation results from an elementary process in which there is a transfer of energy $h\nu$ and momentum $h\nu/c$, in such a way that "the momentum is directed along the direction of propagation of the ray [of light] if the energy is absorbed, and directed in the opposite direction, if the energy is emitted" (Einstein, 1917, p. 182). In the case where the transition in the molecule is induced by an external field the change in the momentum of the molecule will be in the direction of the radiation beam. In the case where there is no external field present and the emission of radiation is spontaneous, Einstein considered that

> If a molecule undergoes a loss of energy of magnitude $h\nu$ without external influence, by emitting this energy in the form of radiation (spontaneous emission), this process is also a directed one. There is no emission of spherical waves. The molecule suffers in the spontaneous elementary process a recoil of magnitude $h\nu/c$ in a direction which is in the present state of the theory determined by 'chance'. (Einstein, 1917, p. 182)

In this way Einstein found it necessary, for the consistency of his approach regarding the elementary interaction of radiation and matter, to associate with the light-quanta with energy $h\nu$ also a momentum $h\nu/c$, which according to relativity theory corresponds to a particle with zero rest mass (Pais, 1979, pp. 886-887).

In the derivation of his results concerning the momentum of the light-quanta, Einstein considered the motion of molecules under the influence of the radiation. As we have seen, already in 1909 Einstein had made a similar calculation, in this case to determine the (perpendicular) motion of a movable flat plate that closes a vessel

containing an ideal gas and radiation in thermodynamical equilibrium. The expression obtained for the radiation pressure contained two terms, exactly like the corresponding expression for the energy fluctuations, which could be given the same interpretation. The first term of the formula is related to a corpuscular feature and the other to a wave feature. Einstein did not make any strong claims relating the radiation pressure and a possible momentum of the light-quanta even if he remarked that "if the radiation were to consist of very few extended complexes with energy hν which move independently … then as a consequence of fluctuations in the radiation pressure such momenta would act on our plate as are represented by the first term only of our formula" (quoted in Pais, 1979, p. 887). Contrary to his 1916 work, in this work Einstein was not considering the elementary interaction of radiation and matter and making a derivation of Planck's formula by taking into account this interaction, only making more general statistical calculations that did not provide any insight into the 'mechanism' of an elementary interaction.

This development of the light-quanta hypothesis still did not deal with the limitation of considering the light-quanta as independent, which according to Einstein was "a picture which represents the roughest visualization of the light-quantum hypothesis" (quoted in Pais, 1979, p. 887). Also, in his derivation Einstein had to take into account results from Maxwell-Lorentz electrodynamics. A derivation of Planck's law taking into account the light-quanta hypothesis and without any reference to classical electrodynamics arrived in Einstein's hands in 1924 in a letter from a physicist from India. Bose found a way to derive Planck's law without using classical electrodynamics and by making an explicit use of the concept of light-quanta with an energy hν and a momentum hν/c (Bose, 1924). In his derivation, Bose used for the particles the same counting method applied (in his book) by Planck to the distribution of energy elements over the oscillators (Darrigol, 1986, p. 212).

Einstein applied Bose's methods to the development of a quantum theory of a monoatomic ideal gas. In his third paper on the theory of an ideal gas Einstein mentioned what seems to be his initial motivation for this work: "this theory appears to be justified in case one starts from the conviction that a light-quantum is distinguished (apart from its polarization property) from a monoatomic molecule basically by the fact that its rest mass is arbitrary small" (quoted in Mehra & Rechenberg, 1982, p. 573). The basic difference in Einstein's approach is that he uses the energy-momentum relation for nonrelativistic particles with mass m, and that he imposes the constraint of a fixed number of molecules in the gas.

Following criticism by Ehrenfest, in his second paper on gas theory Einstein recognized that Bose's counting method implied that "the quanta or molecules are not treated as being independent of one another" (quoted in Howard, 2005, p. 9). This is the crucial point that had prevented Einstein to approach a full derivation of Planck's law using his light-quanta hypothesis. In his 1905 work Einstein took the light-quanta to be independent classical-like particles, thus being able only to justify Wien's law. In this paper Einstein stressed that the difference between the Boltzmann counting procedure (applied to classical particles) and the Bose counting was that the gas molecules (or the light quanta) could not be taken to be statistically independent. According to Einstein the entropy formula for an ideal monoatomic gas derived using Bose statistics "expresses indirectly a certain hypothesis of a mutual influence between molecules" (quoted in Darrigol, 1986, p. 211). Besides his important conclusions regarding the behavior of the gas at a low temperature (the condensation effect), Einstein derived an expression for the energy fluctuation of an ideal monoatomic gas that was analogous to the formula for the radiation fluctuation he had obtained in 1909. Again he had an

expression with two terms. According to Einstein "only the first of these would be present if the molecules were independent of each other" (quoted Mehra & Rechenberg, 1982, p. 618). Regarding the second term Einstein wrote that "one can interpret it, also in the case of gases, by associating with the gas a radiation phenomenon in a suitable manner and computing its interference fluctuations" (quoted in Mehra & Rechenberg, 1982, p. 618). That is, like in the case of blackbody radiation Einstein interpreted the second term as resulting from an undulatory behavior, now associated with the monoatomic gas molecules. Following Louis de Broglie's ideas (as presented in his 1924 thesis) Einstein associated a scalar wave field with the monoatomic gas and took the second term of the fluctuation formula as resulting from the "square fluctuation of this wave field" (quoted in Mehra & Rechenberg, 1987, p. 413).

From his Brother, the experimental physicist Maurice de Broglie, it was clear to de Broglie, around 1920, that there is a need "of always connecting together the points of view of waves and corpuscles" (quoted in Mehra & Rechenberg, 1982, p. 584) in the interpretation of experimental results regarding different forms of radiation.[8] In a series of notes published between 1922 and 1923, de Broglie developed his undulatory mechanics, where he tried to explain the dual character of radiation, extending also this duality to the description of matter. It seems that the first step in de Broglie's theoretical work came when he took the mass of the light-quanta to be very small but different from zero. This move made it possible to relate Einstein's formulas $E = m_0c^2$ and $E = h\nu$, where m_0 is the light quanta rest mass. The expression $m_0c^2 = h\nu_0$, suggested to de Broglie the existence of an internal periodic phenomenon with a frequency ν_0 associated with any massive particle not only the light quanta. An apparent paradox occurred when considering a particle moving with a uniform velocity v with regard to a stationary observer. The observer would take the energy of the moving particle to be $E = m_0c^2 (1-\beta)^{-1/2}$, and the internal frequency to be $\nu_1 = \nu_0(1-\beta)^{1/2}$. In this way for a moving particle the internal frequency would not be related with the frequency given by $E = h\nu$. This 'second' wave appeared to be unrelated to the particle because it had a wave velocity superior to c. However, de Broglie noticed that this fictitious wave would remain in phase with the internal periodic phenomenon and took this 'phase wave' as guiding the motion of the particles. He considered that "any moving body may be accompanied by a wave and that it is impossible to disjoin motion of body and propagation of wave" (quoted in Jammer, 1966, p. 244). In the case of 'matter waves' (the phase waves associated with matter) de Broglie found an important result in the case of orbiting electrons. de Broglie considered that "the rays of the phase waves coincide with the trajectories [of the particles]" (quoted in Mehra & Rechenberg, 1982, p. 593). In simple terms we can say that a particle and its associated wave follow the same trajectory. In the case of an electron in a close circular trajectory, by taking the electron and the (fastest) wave to start motion at a particular point of the trajectory at an initial time t = 0, they will meet on the orbit again at a later time $\tau = T\beta^2 / (1-\beta^2)$, where T is the period of revolution of the electron. At this moment the internal phase of the electron is $2\pi\nu_1\tau = m_0c^2\ T\beta^2 / h(1-\beta^2)^{\frac{1}{2}}$. By requiring the phases of the phase wave and the internal periodic motion to be equal at this point, de Broglie obtained the expression $m_0\nu^2(1-\beta)^{-1/2}T = nh$, where n is an integer. This expression corresponds to the Bohr-Sommerfeld quantum condition. In this way the quantization could be seen as a resonance condition on the phase wave associated with the electron when considering closed trajectories.

[8] See Wheaton (1991) for an account of the importance of experimental work in conceptual developments in the quantum theory and in particular on de Broglie's ideas.

3 The coming to be of the Schrödinger equation

After reading Einstein's remarks on de Broglie's ideas, Erwin Schrödinger got hold of a copy of de Broglie's thesis (where his ideas were developed in detail) and set to work on what would become known as wave mechanics. In a first moment Schrödinger tried to "visualize the phase wave of an electron on Kepler orbits. The 'rays' certainly correspond to neighbouring Kepler ellipses having the same energy. This, however, leads to horrible 'caustics' or the like, for the wave front" (quoted in Mehra & Rechenberg, 1987, p. 416). Having difficulties in exploring a 'direct' geometrical picture of the phase wave, Schrödinger turned to finding a wave equation that described the phase wave associated with the electron. The first attempt was the derivation of a relativistic wave equation that later would become known as the Klein-Gordon equation. Schrödinger used the equation to determine the eigenvibrations of the hydrogen atom, but got the wrong results (when compared with Arnold Sommerfeld's 1924 results on the hydrogen atom obtained within the so-called old quantum theory). Only in the non-relativistic limit was Bohr's original result recovered. This put in danger the whole program of a wave-theoretical approach since de Broglie's phase wave was developed taking into account relativistic considerations. Schrödinger finally settled for the development of a non-relativistic wave equation as we can see from a letter to Wilhelm Wien in late December 1925:

> At the moment I am plagued by a new atomic theory … I believe that I can write down a vibrating system – constructed in a comparatively natural manner and not by *ad hoc* assumptions – which has as its eigenfrequencies the term frequencies of the hydrogen atom … at the moment I still have to learn the mathematics to handle the vibration problem fully – a linear differential equation, similar to Bessel's, however less known and exhibiting strange boundary conditions; these are connected with it and not imposed from outside. (Quoted in Mehra & Rechenberg, 1987, 460 & 461)

Within a few weeks the results of his ongoing research started to appear in *Annalen der Physik*. In his notebooks, besides the derivation of his relativistic equation, Schrödinger made a derivation of a non-relativistic wave equation by considering de Broglie's results. Schrödinger considered a generalized de Broglie's phase wave frequency relation, for an electron with mass m, charge e, and velocity υ, in a Coulomb potential (i.e. the electron of the hydrogen atom):

$$h\nu = mc^2 + \frac{m\upsilon^2}{2} - \frac{e^2}{r}.$$

Using this result, Schrödinger took the non-relativistic momentum of the electron ($m\upsilon^2$) into de Broglie's relation for the phase velocity (in the non-relativistic limit)

$$u = \frac{h\nu}{m\upsilon}.$$

Inserting the non-relativistic result for u into the relativistic equation for the phase wave he had previously put forward, Schrödinger obtained a non-relativistic wave equation for the hydrogen atom:

$$\Delta\psi + \frac{4\pi^2}{h^2} 2m\left(h\nu - mc^2 + \frac{e^2}{r} \right)\psi = 0 ,$$

or

$$\Delta\psi + \frac{2m}{K^2}\left(E + \frac{e^2}{r} \right)\psi = 0 , \text{ with } K^2 = \frac{h^2}{4\pi^2} \text{ and } E = h\nu - mc^2 ,$$

as it appears in the first *Annalen* paper, where Schrödinger presented the wave equation as resulting from a variational approach without giving much insight into the physical considerations that led him to the wave equation (Schrödinger, 1926a). Schrödinger presented some considerations regarding the adoption of a second-order differential equation as the basis for the development of his wave mechanics in his second paper on the subject (Schrödinger, 1926b). This type of equation had traditionally been used to describe wave phenomena. By 'striving for simplicity' Schrödinger settled for a second-order differential equation:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)\psi - \frac{1}{u^2}\frac{\partial^2}{\partial t^2}\psi = 0 .$$

Then by assuming the wave to have a simple time dependency (i.e. a periodic behavior in time with frequency ν): $\psi \sim \exp(2\pi i\nu\tau)$, Schrödinger obtained a time-independent relativistic wave equation:

$$\Delta\psi = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)\psi = -\frac{4\pi^2\nu^2}{u^2} .$$

This was the equation that by taking into account de Broglie's results led him to his wave equation for the hydrogen atom, as we have seen above.

In the 'derivation' of the wave equation, Schrödinger considered, as we have just seen, the time-independent case corresponding to a situation where the parameter E (which in the case of a bound electron is the energy of the hydrogen atom) has a time-independent value, i.e. E does not change in time.

In the application of this wave equation to the hydrogen atom, an analytic solution can be found, by taking into account the spherical symmetry of the Coulomb potential, and making a separation of the wave equation in spherical coordinates: $\psi = \psi_\theta\psi_\phi\psi_r$. It is in the radial equation that interesting things happen:

$$\frac{\partial^2\psi_r}{\partial r^2} + \frac{2}{r}\frac{\partial\psi_r}{\partial r} + \left(\frac{2mE}{K^2} + \frac{2me^2}{K^2 r} - \frac{n(n-1)}{r^2} \right)\psi_r = 0 ,$$

where n takes up only integer values. The limitation of n to integers comes about because in the solution of the angular equations the part of the wave function ψ_ϕ dependent on the azimuthal angle ϕ must be single-valued (i.e. when ϕ is increased by

2π or a multiple of 2π, ψ_ϕ must be unchanged). This implies that ψ_ϕ is given by $2\pi^{-1/2}e^{im\phi}$, where m is a positive or negative integer or zero. Also to have finite solutions in the equation for ψ_θ it is necessary that n be a positive integer or zero so that $|m| \leq n$. An important aspect of the radial equation is that it has singular points at r = 0 and r = ∞.

We will consider here the case of bound states for which E takes negative values. Taking into account that the Coulomb potential goes to zero more strongly than 1/r as r $\rightarrow \infty$ the asymptotic solution of the radial equation can be obtained by disregarding the Coulomb potential in the radial equation, and by taking into account that the wave function must approach zero as r $\rightarrow \infty$. This boundary condition implies that, in the asymptotic limit, $\psi_r \sim e^{-r}$. The other singular point r = 0 is taken care of by considering $\psi_r \sim U_r e^{-r}$, where U_r can be expressed as a power series. By considering the two boundary conditions it turns out that the power series must terminate, and, being n' the highest power of U_r in the finite order power series, there is a solution to the radial equation only when we have:

$$\frac{2me^2}{K\sqrt{-2mE}} = l = n' + n + 1 .$$

From this it follows that the energy for the bound states of the hydrogen atom can take only discrete values:

$$E_\lambda = \frac{2\pi^2 me^4}{h^2 l^2}$$, where l is the so-called principal quantum number.

This type of solution to a wave equation can be seen as a proper value problem, i.e. there is a differential equation with a numerical parameter (in this case the energy E), and the solutions must satisfy particular boundary conditions (in this case the wave function has to be finite at r = 0 and approach zero as r $\rightarrow \infty$). The values of the parameter (E) for which there are non-trivial solutions are called proper values (eigenvalues), and the corresponding solutions of the equation are called proper functions (eigenfunctions). In the case of Schrödinger's wave equation further 'physical' conditions are imposed on the wave function to obtain the non-trivial or physical solutions (one example of such a condition is the assumption of the single-valuedness of the wave function). We have a similar situation in the classical case of a vibrating string. The end points of the string are held fixed, and this entails that the string can only take a discrete set of wavelengths (Mandl, 1957, pp. 5-8).

In a work previous to the publications on wave mechanics, Schrödinger addressed Einstein's work on a quantum gas theory by applying an idea inspired on, but different from, de Broglie's phase wave. Contrary to de Broglie who considered phase waves propagating in the field-free space, Schrödinger considered standing waves enclosed in a cavity (which provides natural boundary conditions exactly like in the classical case of a vibrating spring). In his first paper on wave mechanics Schrödinger called attention to this difference:

I was led to these deliberations in the first place by the suggestive papers of M. Louis de Broglie, and by reflecting over the space distribution of those 'phase waves', of which he has shown that there is always a *whole number*, measured along the path, present on each period or quasi-period of the electron. The main difference is that de Broglie thinks of progressive waves, while we are led to stationary proper vibrations

if we interpret our formulae as representing vibrations. I have lately shown that the Einstein gas theory can be based on the consideration of such stationary proper vibrations, to which the dispersion law of de Broglie's phase waves has been applied. (Schrödinger, 1926a, p. 9)

Another essential difference with de Broglie is that, while de Broglie had a dualistic perspective associating a phase wave with a material particle, Schrödinger simply replaced the molecules by phase waves. According to Schrödinger "a molecule of rest-mass m, moving with velocity $v = \beta c$, constitutes nothing but a 'signal' – one might say, 'the wave crest' – of a wave system" (quoted in Mehra & Rechenberg, 1987, p. 439). Schrödinger's interpretation based solely on wave characteristics is something that was new in Schrödinger's work on wave mechanics (as can be seen in another earlier work on Einstein's gas theory, where Schrödinger only makes some considerations related to the statistics of the molecules), it emerged with the developments of the work. We have then already at the early stages of the development of wave mechanics a turn towards an (apparently) more classical approach to the description of quantum systems using some sort of a yet very provisional wave interpretation. This is clear from the fact that also in the case of the energy levels of the hydrogen atom, Schrödinger sees it as a proper value problem. That is, in this case we consider also standing waves where the natural boundary conditions (due to the singular points) can be seen as resulting from the fact that the equation "carries within itself the quantum conditions" (quoted Mehra & Rechenberg, 1987, p. 575). We would be in a situation no different from that of a vibrating spring. This is for Schrödinger the most important aspect of his work. Schrödinger was able to "show that the customary quantum conditions can be replaced by another postulate, in which the notion of 'whole numbers', merely as such, is not introduced. Rather when integralness does appear, it arises in the same natural way as it does in the case of the node-numbers of a vibrating string" (Schrödinger, 1926a, p. 1). In this way the discrete energy levels of the hydrogen atom has its origin "in the finiteness and single-valuedness of a certain space function" (Schrödinger, 1926a, p. 9).

4 The interpretation and later developments of the Schrödinger equation

In his first articles on wave mechanics Schrödinger did not develop much a physical interpretation of the wave function. Schrödinger had the idea that "the waves in the phase space are something real in a sense" (quoted in Mehra & Rechenberg, 1987, p. 536), but to make this 'sense' precise turned out to be a difficult task. Schrödinger's initial idea was to "connect the [wave] function ψ with some *vibration process* in the atom" (Schrödinger, 1926a, p. 9), but he recognized that "it is only in the one electron problem that the interpretation [of the wave function] as a vibration in the real three-dimensional space is immediately suggested" (Schrödinger, 1926b, p. 28). This situation had come out in Schrödinger's correspondence with several physicists. In a letter to Sommerfeld, Schrödinger recognized this point: "since ψ in general depends on many more than three variables, the immediate interpretation as vibrations in the three-dimensional space is made difficult in any desirable manner" (quoted in Mehra & Rechenberg, 1987, p. 542). Also his simple view of particles as 'wave crests' brought the sharp criticism of Hendrik Lorentz who called Schrödinger's attention to the fact that a wave packet, which might according to Schrödinger represent a particle, "can never stay together and remain confined to a small volume in the long run … because of this unavoidable blurring a wave packet does not seem … to be very suitable for representing things to which we want to ascribe a rather permanent individual existence" (quoted in Jammer, 1966, p. 31; see also Bohm, 1951, pp. 60-66).

An even greater problem was that at this point Schrödinger was unable to account for the intensities and polarizations of the emitted radiation in an atomic transition. To be exact not even a clear relation between the emission frequency and the energies of the atomic levels involved in the emission process was available. Bohr had developed in 1912-1913 a model of the atom based on the idea of stationary states – not submitted to the consequences of the classical theory of radiation –, where the electron can jump from one stationary state to another by emission or absorption of radiation with a frequency ν given by the relation $h\nu = E' - E''$, where E' and E'' are the energies of each stationary state (Bohr, 1913). A first attempt to address this line of problems was presented in the first paper on wave mechanics. In here Schrödinger tried to obtain Bohr's frequency relation within his wave mechanics approach. For this Schrödinger considered a constant parameter C that would appear in an expression relating the proper frequency with the proper energy of a stationary proper vibration (representing in Schrödinger's approach Bohr's stationary states). By considering C "very great compared with all the admissible negative E-values" (Schrödinger, 1926a, p. 10), an expansion in terms of E of the expression was possible:

$$\nu = C'\sqrt{C + E} = C'\sqrt{C} + \frac{C'}{2\sqrt{C}}E + \ldots$$

According to Schrödinger this expression "permits an understanding of the Bohr frequency condition. According to the latter the emission frequencies are proportional to the E-differences, and therefore from [the previous expression] also to the differences of the proper frequencies ν of those hypothetical vibration processes" (Schrödinger, 1926a, p. 10). In this way Schrödinger considered that "the emission frequencies appear therefore as deep 'difference tones' of the proper vibrations themselves. It is quite conceivable that on the transition of energy from one to another of the normal vibrations, something – I mean the light wave – with a frequency allied to each frequency difference, should make its appearance" (Schrödinger, 1926a, p. 10).

Schrödinger recognized that in this way he could only obtain Bohr's relation in an approximate form, but expected that the development of a relativistic wave theory would solve this problem. An improvement over this situation was published in a subsequent paper where Schrödinger again addressed the problem of the coupling between the dynamic processes in the atom and the electromagnetic field. According to a letter to Sommerfeld, Schrödinger expected that a relation might be obtained between the matter wave functions and the Maxwell-Lorentz electromagnetic current: "The ψ-vibrations must then correspond to the four-current, i.e., the [Maxwell-Lorentz] four-current must be replaced by something derived from the function ψ, say the four-dimensional gradient of ψ. But this is all pure fantasy; in reality I have still not thought about it at all" (quoted in Mehra & Rechenberg, 1987, p. 779). In the paper, a first approach to this idea was presented. According to Schrödinger "the mechanical field scalar (which I denote by ψ) is perfectly capable of entering into the unchanged Maxwell-Lorentz equations between the electromagnetic field vectors as the 'source' of the latter; just as, conversely, the electromagnetic potentials enter into the coefficients of the wave function, which defines the scalar field" (Schrödinger, 1926c, p. 60). In this work Schrödinger considered the case of an electron in a central field (the hydrogen atom) and made the fundamental assumption that the space density of electricity ρ_{el} is given by the real part of

$$\psi \frac{\partial \overline{\psi}}{\partial t},$$

where $\overline{\psi}$ is the complex conjugate of the wave function ψ. This implies that "the charge of the electron is not concentrated in a point, but is spread out through the whole space" (Schrödinger, 1926e, p. 1066). The fluctuation of the charge is given by the previous expression. From this it was simple to determine "the radiation, that by ordinary electrodynamics will originate from these fluctuating charges" (Schrödinger, 1926a, p. 1066). This was done by calculating the electrical dipole moment, using the above expression for ρ_{el}. For example the dipole moment in the Cartesian z direction is given by

$$\iiint z \psi \frac{\partial \overline{\psi}}{\partial t} dxdydz.$$

Despite Schrödinger's recognition that this approach "is far from completely satisfactory and is in no way final" (Schrödinger, 1926c, p. 61), it was clear that a progress had been made as can be seen by his treatment of an atom in a constant electric field (the Stark effect). By applying the above mentioned hypothesis to the physical meaning of ψ, Schrödinger was able not only to obtain, exactly and not as an approximation, Bohr's 'frequency-rule' that gives the frequency of the electromagnetic radiation as the difference between the (term) frequencies of two stationary wave functions, but also to calculate the intensities and polarizations of the emitted radiation, which were in agreement with experiments.

A further development of this electrodynamic interpretation occurred due to Schrödinger's extension of his wave mechanics to the case of time-dependent systems, which was necessary for example to treat the case of dispersion of radiation by atoms. The development of a general time-dependent wave equation (which Schrödinger referred to as the real wave equation) made it necessary to consider the wave function complex. This led Schrödinger to re-work his expression for the space density of electricity ρ_{el}, which now was written as $e\psi\overline{\psi}$, where e is the total electric charge of the electron and $\psi\overline{\psi}$ can be seen as a weight function. With this new expression Schrödinger was able to give a more clear 'electromagnetic meaning' to the 'mechanical field scalar': when integrating the space density of electrical charge ρ_{el} over the whole of space Schrödinger obtained a time-independent finite value (while the previous expression yields zero). This implied the conservation of charge.

Schrödinger extended this interpretation to the case of a system with several electrons:

> $\psi\overline{\psi}$ is a kind of weight-function in the system's configuration space. The wave-mechanics configuration of the system is a superposition of many, strictly speaking of all, point-mechanical configurations kinematically possible. Thus, each point-mechanical configuration contributes to the true wave-mechanics configuration with a certain weight, which is given precisely by $\psi\overline{\psi}$. (Schrödinger, 1926d, p. 120)

Schrödinger recognized the loose character of this provisory interpretation, as we can read in the final part of a set of lectures delivered in March 1928:

> We have hitherto avoided putting forward any definite assumption as to the physical interpretation of the function $\psi(q_1, q_2, \ldots, q_n, t)$ relating to a system whose configuration in terms of ordinary mechanics is

described by the generalized co-ordinates $q_1, q_2, \ldots, q_n$. This interpretation is a very delicate question. As an obvious generalization of the procedure of spreading out the electronic charge according to a relative density function $\psi\overline{\psi}$ (which furnished satisfactory results in the one-electron problem; see section 5), the following view would present itself in the case of a general mechanical system: the real natural system does not behave like the picture which ordinary mechanics forms of it (e.g. a system of point-charges in a definite configuration), but rather behaves like what would be the result of spreading out the system, described by $q_1, q_2, \ldots, q_n$, *throughout its configuration-space* in accordance with a relative density function $\psi\overline{\psi}$. This would mean that, if the ordinary mechanical picture is to be made use of at all, the actual system behaves like the ordinary mechanical picture, present in all its possible configurations at the same time, though "stronger" in some of them than in others.

I maintained this view for some time. The fact that it proves very useful can be seen from the one-electron problem (see section 5). No other interpretation of the ψ-function is capable of making us *understand* the large amount of information which the constants a_{kl} [(related to the electric moment)] furnish about the intensity and polarization of the radiation. Yet this way of putting the matter is surely not quite satisfactory. For what does the expression "to behave like" mean in the preceding sentences? The "behaviour " of the ψ-function, i.e. its development in time, is governed by nothing like the laws of classical mechanics; it is governed by the wave-equation. (Schrödinger, 1928, p. 205-206)

We see that Schrödinger recognizes his view as not quite satisfactory.[9] This came about from his recognition that even in the case of one electron it is not enough to see the wave function as meaning a continuous distribution of electricity in actual space. As Schrödinger mentions, it is necessary also to take into account the space-time behavior of the wave function as described by the wave equation. Michel Bitbol has stressed this point:

Schrödinger became fully aware that [the electrodynamic interpretation] could not work alone, that somehow it had to be combined with the original wave interpretation. Whereas the electrodynamic interpretation enables one to make sense of the line intensities and polarizations, the wave representation was still needed to calculate the relevant charge distributions as well as the evolution between two measurements of line intensities. The problem Schrödinger had to face was the following: we need not one but two representations of the atomic phenomena. One of them, namely the electrodynamic representation, is directly related with the 'observed facts', but it does not provide the link between subsequent observed facts; in a word, it is 'factual' but not 'effective'. The second one, namely, the wave representation, is perfectly able to provide a link between the observed facts, but not to account for all the aspects of the facts themselves; it is 'effective' but not 'factual'. As long as Schrödinger wanted to merge the 'effective' and the 'factual' into a single representation, according to the classical ideal, the persistent duality of the models had to be considered as a symptom of failure. (Bitbol in Schrödinger, 1995, p. 3)

The two-fold aspect of Schrödinger's tentative interpretation is clearly present in Schrödinger's article on the Compton effect[10] published in 1927. In this work Schrödinger explained the Compton effect as resulting from the scattering of a light wave and a matter wave (a de Broglie wave). Even if Schrödinger uses his interpretation of the wave function as giving rise to a charge density distribution in space, the crucial aspect of his calculations is to consider a wave function as a 'real' wave propagating in space (Schrödinger even makes the analogy to a sound wave). A very interesting aspect

[9] Following these statements showing the difficulty Schrödinger was having in giving a solid and clear meaning to his interpretation, Schrödinger mentioned that "an obvious statistical interpretation of the ψ-function has been put forward, viz. that it does not relate to a single system at all but to an assemblage of systems, $\psi\overline{\psi}$ determining the fraction of the systems which happen to be in a definite configuration" (Schrödinger, 1926c, p. 206). I will not look into Born's well-known statistical interpretation or Schrödinger's criticism of this interpretation (which like his own reformulation of his interpretation extended for several decades. For details on early interpretation issues see e.g. Jammer (1974). For an account of the adoption of Born's statistical interpretation see e.g. Mehra & Rechenberg (2000), Mara Beller (1990), Pais (1982). For details on Schrödinger's views see Bitbol (1996).

[10] Regarding the Compton effect see e.g. Sánchez Ron (2001, pp. 382-392).

of this two-fold use of the wave function is that, the de Broglie or matter wave (associated with an electron with rest mass m_0) is described by Schrödinger's (relativisitc) wave equation, which in the context of its use, is, in practice, taken to be an equation for a 'classical' wave function of a matter wave (Schrödinger, 1927).

Later workers on quantum mechanics have explored and clarified this possibility of giving very different meanings to the wave equation, i.e. as an equation describing a probability wave in a configurational space or an equation describing a matter wave in actual space. In the next chapter we will look in particular into Pascual Jordan's approach, fundamental in the development of a quantum theory of fields. In this chapter I shall follow Schrödinger's tentative interpretation and see how much can we stretch out a reading of the equation as the equation for a classical matter wave. It will be enough to consider the simple case of a one-electron system. We will see that Schrödinger's difficulties with the two-fold aspect of his tentative interpretation can be traced back to an 'ambiguity' in the physical interpretation (in terms of a particle equation or a matter wave equation) of the one-electron Schrödinger equation (Becker, 1964, Vol 2., pp. 92-107;Tomonaga, 1962, Vol 2., pp. 14-115).

In 1927 Clinton J. Davisson and Lester H. Germen presented clear experimental evidence for matter waves propagating in space. The experiment consisted in the bombardment of a metal plate by an electron beam. Davisson expected that by analyzing the angular distribution of the electrons scattered by a metal plate it would be possible to obtain information regarding the shell structure of the electrons inside the atoms of the metal plate. In the early stages of the sequence of experiments (from 1921 to around 1925) there was no evidence of any wave properties of the electron beams. The first view on the results was that

> all the main features of the distribution curves so far observed for the scattering from nickel seem reasonably accounted for on the supposition that a small fraction of the bombarding electrons actually do penetrate one or more of the shells of electrons which are supposed to constitute the outer structure of the nickel atom and, after executing simple orbits in a discontinuous field, emerge without appreciable loss of energy. (Quoted in Jammer, 1966, pp. 249-250)

The experimental finding of the diffraction of the electron beams by a metal plate resulted from an accident in Davisson's laboratory in 1925. In their paper Davisson and Germen tell the story of the discovery of the diffraction of electrons:

> The investigation reported in this paper was begun as the result of an accident, which occurred in this laboratory in April 1925. At that time we were continuing an investigation, first reported in 1921, on the distribution-in-angle of electrons scattered by a target of ordinary (polycrystalline) nickel. During the course of this work a liquid-air bottle exploded at a time when the target was at a high temperature; the experimental tube was broken, and the target heavily oxidized by inrushing air. The oxide was eventually reduced and a layer of the target removed by vaporization, but only after prolonged heating at various high temperatures in hydrogen and in vacuum.
>
> When the experiments were continued it was found that the distribution-in-angle of the scattered electrons had been completely changed … This marked alteration in the scattering pattern was traced to a re-crystallization of the target that occurred during the prolonged heating. Before the accident and in previous experiments we had been bombarding many small crystals, but in the tests subsequent to the accident we were bombarding only a few large ones … It seemed probable from these results that the intensity of scattering from a single crystal would exhibit a marked dependence on crystal direction, and we set about at once preparing experiments for an investigation of this dependence. (Davisson & Germen, 1927, p. 706)

The 'marked alteration in the scattering pattern' made Davisson and Germen change their research towards an investigation of a possible dependency of the scattered beams on the crystal direction. It was clear that, in this case of a single nickel crystal, the

intensity variation of the angular distribution was not simply related with the internal structure of the atoms of the plates, since in the older experiments they also used plates of nickel, which in that case consisted in ordinary (polycrystalline) nickel. An explanation for these results must be found elsewhere. Here is how Davisson and Germen addressed the new experimental findings:

> We must admit that the results obtained in these experiments have proved to be quite at variance with our expectations. It seemed to us likely that strong beams would be found issuing from the crystal along what may be termed its transparent directions – the directions in which the atoms in the lattice are arranged along the smallest number of lines per unit area. Strong beams are indeed found issuing from the crystal, but only when the speed of bombardment lies near one or another of a series of critical values, and then in directions quite unrelated to crystal transparency.
>
> The most striking characteristic of these beams is a one to one correspondence, presently to be described, which the strongest of them bear to the Laue beams that would be found issuing from the same crystal if the incident beam were a beam of x-rays. Certain others appear to be analogues, not to Laue beams, but of optical diffraction beams from plane reflection gratings – the lines of these gratings being lines or rows of atoms in the surface of the crystal. Because of these similarities between the scattering of electrons by a crystal and the scattering of waves by three- and two- dimensional gratings a description of the occurrence and behavior of the electron diffraction beams in terms of the scattering of an equivalent wave radiation by the atoms of the crystal, and its subsequent interference, is not only possible, but most simple and natural. This involves the association of a wave-length with the incident electron beam, and this wave-length turns out to be in acceptable agreement with the value h/mυ of the undulatory mechanics, Planck's action constant divided by the momentum of the electron. (Davisson & Germen, 1927, pp. 706-707)

In this way Davisson and Germen found that they could make sense of the experimental results by resorting to the idea of de Broglie waves, finding that the de Broglie expression $\lambda = h/p$ relating the wavelength λ and the momentum p of the electron was verified.

We can choose to see Schrödinger's equation as the equation for this matter wave, as we in part have in Schrödinger's two-fold interpretation. In this way Schrödinger's equation can describe the wave properties of the electrons as revealed for example in Davisson and Germen experiments or in Schrödinger's account from a wave perspective of the Compton effect. But as we have seen this approach does not gives us a description of the electron's corpuscular aspects as revealed in several other experiments, since Schrödinger was unable to provide an account of the electron's particle-like characteristics as simplyj a wave-crest (more exactly a wave packet), and Schrödinger was forced to associate a charge (or mass) density to the wave function, which in the case of several electrons results in a highly abstract entity: a weight function.

Looking at the simple case of the hydrogen atom it is clear to what point we can take this use of Schrödinger's equation as an equation for a matter wave (Becker, 1964, Vol 2., pp. 92-107;Tomonaga, 1962, Vol 2., pp. 14-115). Returning to Schrödinger's initial treatment of the hydrogen atom, considering the Schrödinger wave equation for the proper oscillation of a de Broglie wave in a central potential, now writing it in terms of the de Broglie wave frequency:

$$\Delta\phi + 8\pi^2 m\left(\nu + \frac{e^2}{h}\frac{1}{r}\right)\phi = 0\,,$$

we obtain, in a totally classical treatment, for the proper frequencies of the de Broglie wave

$$\nu = -\frac{2\pi^2 me^4}{h^3}\frac{1}{(n_r+l+1)^2}, \text{ where } n_r, l = 0, 1, 2, \ldots.$$

By analogy to the case of light quanta we can consider that the proper frequencies of the de Broglie wave inside the atom have an energy given by $E = h\nu$. From this 'quantum rule' it follows that the energy levels of the hydrogen atom are given by

$$E = -\frac{2\pi^2 me^4}{h^2}\frac{1}{(n_r+l+1)^2},$$

a result that agrees with that derived previously in Bohr's theory. The difference with Schrödinger's original derivation is that Schrödinger took from the start the energy-frequency relation for granted, providing in reality a quantum wave mechanics equation that resembles (in the case of one-electron systems) a classical wave equation. Here we see that if we start from a classical wave perspective we need to take into account a quantization rule applied to the wave so that we can reach agreement with some experimental results for which a wave description is not enough. We will see briefly in the next chapter that an appropriate quantum formalism can be obtained by considering Schrödinger's equation as a classical wave equation, but only when submitted to a quantization procedure which is valid also in the case of many-electron systems. I will look at this in detail for the case of the Dirac equation.

CHAPTER 3

THE DIRAC EQUATION AND ITS INTERPRETATION

1 Introduction

Once upon a time, Richard P. Feynman wrote that "we know so very much and then subsume it into so very few equations that we can say we know very little (except these equations – Eg. Dirac, Maxwell, Schrod.). Then we think we have the physical picture with which to interpret the equations. But these are so very few equations that I have found that many physical pictures can give the same equations" (quoted in Schweber, 1994, p. 407). He wrote this having in mind, in particular, the Dirac equation: $i\partial\!\!\!/\psi = m\psi$ (Feynman, 1961, p. 57).

In this chapter, the Dirac equation will be used as a guideline to reveal the importance of the concept of quanta in the description of interactions in quantum electrodynamics. To this end the historical evolution and interpretation of the Dirac equation is considered. In sections 2, 3, 4, and 5, I present the evolution of the Dirac equation from its first formulation as a relativistic wave equation for an electron, to a classical field equation from which an electron-positron quantum field is obtained. In this transition, the Dirac equation went from being a relativistic 'update' of the Schrödinger equation in the calculation of energy levels in atoms (basically of hydrogen) to becoming one of the cornerstones of the most successful quantum field theory: quantum electrodynamics. In section 6, I will try to clarify the relation between the different interpretations of the Dirac equation. In this way the results provided by Dirac's equation as a relativistic one-electron equation are reinterpreted from the perspective of the quantized Dirac field. Doing this, the importance of the concept of quanta in the description of bound states becomes clear. By contrast, bound states are usually only described at the level of the one-electron interpretation of the Dirac equation, which gives a distorted idea of the physical description of bound states that should be described from the perspective of quantum fields. In particular, an analysis of a two-body description of the hydrogen atom reveals a distinctive feature of quantum electrodynamics: the interaction between fermions described as an exchange of photons.

2 Before the Dirac equation: some historical remarks

Schrödinger's first attempt at a wave equation was the development of a relativistic wave equation for the hydrogen atom. As in the case of the non-relativistic wave equation, Schrödinger considered the problem of determining the eigenvibrations of the hydrogen atom. As we have seen in the previous chapter, Schrödinger took the de Broglie relations generalizing them to the case of an electron in a central Coulomb

potential and by inserting them in a second-order differential equation obtained the relativistic wave equation

$$\Delta\psi = -\frac{4\pi^2 m^2 c^2}{h^2}\left[\left(\frac{h\nu}{mc^2}+\frac{e^2}{mc^2 r}\right)-1\right]\psi = 0$$

Using this wave equation Schrödinger determined the energy levels for the hydrogen atom, and arrived at a result that was not in agreement with Sommerfeld's result for the hydrogen spectrum obtained, within the so-called old quantum theory, through the quantization of the relativistic Bohr atom. Sommerfeld's result was

$$E_{n,k} = \frac{mc^2}{\sqrt{1+\frac{\alpha^2}{\left(n-k-\sqrt{k^2-\alpha^2}\right)^2}}} - mc^2,$$

where α is the fine structure constant, n the principal quantum number, and k the azimuthal quantum number. Schrödinger obtained an expression that did not depend on n – k and k but on n – k + 1/2 and k – 1/2 (Kragh, 1981, p. 33). This meant the failure of Schrödinger's relativistic wave mechanics. Schrödinger set aside his attempt at a relativistic wavefunction and developed a non-relativistic wave equation (Schrödinger 1926a). The relativistic wave equation, later known by the name of Klein-Gordon equation, was presented by several physicists during 1926, but since it did not give the fine structure of the hydrogen spectrum it was not accepted as the correct relativistic equation for an electron (Kragh, 1984).

Another factor that would complicate matters in what regards the wave mechanics description of the electrons was the discovery of spin. In Bohr's theory each spectral term of the hydrogen atom is labeled by three quantum numbers n, k, and m. Due to an external magnetic field a spectral term labeled by n and k splits into 2k + 1 levels, the new sub-levels being distinguished by the quantum number m. This is called the Zeeman effect (Tomonaga, 1997, pp. 1-2; Sánchez Ron, 2001, pp. 336-341). Before 1900 it was already known that the spectral lines, latter described by n and k, where not unique and in reality, when an external magnetic field was applied, consisted in closely spaced lines: they showed a multiplet structure. This was called the anomalous Zeeman effect (Jammer, 1966, p. 122). In 1920 Sommerfeld introduced a new quantum number j that enabled the classification of the different energy levels within one multiplet term (characterized by n and k). Under this new classification m is still related to the specification of sublevels but now of a level specified by n, k and j. Also m must satisfy the inequality $-j \leq m \leq j$. To explain the spectroscopic evidence available Alfred Landé (and also Sommerfeld) set forward a tentative model in which it was assumed that the core of the atom had an angular momentum. There would then be a magnetic moment μ_K related to the orbital angular momentum **K** of the electron in the outermost orbit (the valence electron), given by $\mu_K = -\mathbf{K}$ (in units of the Bohr magneton). Also there would be a magnetic moment μ_R associated to the core angular momentum **R** (corresponding to a quantum number related not to the electron but to the core). The relation between μ_R and **R** is given by $\mu_R = -g_0\mathbf{R}$, where g_0 has to be determined by

fitting the model to experimental results. F. Pachen and E. Back's study of the Zeeman effect in the case of a strong magnetic field, enabled to set the value of g_0 as 2. The interaction between the two magnetic moments μ_K and μ_R of the atom leads to a slight energy change in the atomic energy levels, which results in the multiplet structure of the spectral lines (Tomonaga, 1997, pp. 11-20).

In 1924 Wolfgang Pauli showed that the association of μ_R with the atom's core was inconsistent, and considered it to be associated with the valence electron. In this way the four quantum numbers are all related to the electrons. Upon reading Pauli's ideas G. E. Uhlenbeck and S. Goudsmit proposed in 1925 to reinterpret the core angular momentum **R** as an intrinsic angular momentum of the electron. Uhlenbeck and Goudsmit had the idea that to each quantum number should correspond a degree of freedom of the electron. This led them to the idea of an intrinsic rotation of the electron, the spin, as a fourth degree of freedom to which a quantum number would be associated. As in the case of Landé's model, Uhlenbeck and Goudsmit got a discrepancy, by a factor of 2, between the theoretical and the experimental results in the case of doublet levels of alkali atoms. In 1926 L. H. Thomas presented a relativistic calculation where the missing 1/2 factor, later called the Thomas factor, was obtained (Jammer, 1966, pp. 149-152). So by 1926 there was no relativistic wave equation for the electron and there was the further complication of having to account also for the electron's spin.

In 1927 Pauli attempted to incorporate spin into wave mechanics by considering a Schrödinger wave function depending also on a degree of freedom related to spin (Kragh, 1981, pp. 45-46). The intrinsic (spin) angular momentum in any direction takes only the two values $\pm \hbar/2$. This made Pauli consider a two-component wave function, with one component corresponding to an electron's spin up $\psi(\mathbf{x}, +1/2)$ and another to an electron's spin down $\psi(\mathbf{x}, -1/2)$. This two-component wave function must be solution of two coupled equations with the form

$$H\left(\frac{\hbar}{i}\frac{\partial}{\partial q}, s\right)\psi = E\psi$$

The question was how to define in the wave equation the spin operators **s**. Pauli defined the spin operators as $s_x = 1/2\ \sigma_x$, $s_y = 1/2\ \sigma_y$, $s_z = 1/2\ \sigma_z$, where σ_x, σ_y, σ_z are the so-called Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

In the Hamiltonian for his equation Pauli considered two new terms, besides the term corresponding to an electron (without spin) in a central potential, which was already present in Schrödinger's equation. One of these terms resulted from the interaction of an external magnetic field and the valence electron, which, as we have seen, possesses besides an orbital angular momentum an intrinsic spin momentum. The other resulted from the interaction between the spin magnetic moment and the central potential due to the orbital motion of the electron: the spin-orbit coupling. In this approach Pauli considered only first-order relativistic corrections, and the way the spin operators (and g_0 and the Thomas factor) where put in the Hamiltonian was arbitrary. Most importantly Pauli was unable to extend this approach into a fully relativistic form.

3 The Dirac equation as a one-electron equation

Things changed by the end of 1927, when Paul Dirac was able to formulate a relativistic wave equation. In his first attempts towards a relativistic theory, Dirac consider a Klein-Gordon type equation written in terms of a relativistic Hamiltonian (Dirac, 1926):

$$\{p_x^2 + p_y^2 + p_z^2 - E/c^2 + m^2c^2\}\psi = 0$$

$$\left\{\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{h^2}\right\}\psi = 0\,.$$

Upon reading Dirac's articles using this equation, Ehrenfest asked Dirac in a letter on the motive for using a particular form for the Hamiltonian:

Why do you write the Hamilton equation in the form:

$$E^2/c^2 - p_1^2 - p_2^2 - p_3^2 = m^2c^2$$

and not:

$$mc^2\sqrt{1-(p_1^2+p_2^2+p_3^2)/m^2c^2} = E$$

Does it make a difference? (quoted in Kragh, 1990, p. 53)

By that time also Pauli was proposing to adopt instead of a second order equation a first order equation involving a square-root (Mehra & Rechenberg, 2000, p. 293).

Dirac felt that neither form of the relativistic Hamiltonian was appropriate for the development of a relativistic wave equation. Dirac considered that this equation should maintain the formal structure of the Schrödinger equation (Kragh, 1990, p. 54). On one side Dirac knew he needed an equation that was linear in the time derivative so that he could maintain in the relativistic case the statistical interpretation of the wave function adopted in the non-relativistic case (Mehra & Rechenberg, 2000, p 294, Kragh, 1990, p. 64). On the other side, this meant, due to relativistic considerations, that the equation should be linear also in the spatial derivatives. According to Dirac "an appropriate formulation of quantum mechanics will only be possible when we succeed in treating space and time as equal to one another" (quoted in Kragh, 1990, p. 54). This means that space and time must appear in the equation as the coordinates of a Minkowski space-time.

It seems that what resulted fundamental to Dirac's development of his relativistic equation was Dirac's realization of the identity:

$$|\vec{p}| = \sqrt{p_1^2 + p_2^2 + p_3^2} = \sigma_1 p_1 + \sigma_2 p_2 + \sigma_3 p_3\,,$$

where σ_1, σ_2, σ_3 are the Pauli matrices. According to Dirac:

I was playing around with the three components σ_1, σ_2, σ_3, which I had used to describe the spin of an electron, and I noticed that if you formed the expression $\sigma_1 p_1 + \sigma_2 p_2 + \sigma_3 p_3$ and squared it, p_1, p_2 and p_3 being the three components of momentum, you got $p_1^2 + p_2^2 + p_3^2$, the square of the momentum. This was a pretty mathematical result. I was quite excited over it. It seemed that it must be of some importance. (Quoted in Mehra & Rechenberg , 2000, p. 295)

This mathematical identity was the insight that made Dirac search for a relativistic counterpart involving a term corresponding to the electron's rest mass. The problem facing Dirac was that with the Pauli matrices it was not possible to write down an expression with four squares:

$$|\vec{p}| = \sqrt{p_1^2 + p_2^2 + p_3^2 + m^2c^2} = \alpha_1 p_1 + \alpha_2 p_2 + \alpha_3 p_3 + \alpha_4 mc\,.$$

Dirac considered that from the wave equation developed using the previous expression $\{p_0 - (m^2c^2 + p_1^2 + p_2^2 + p_3^2)^{1/2}\}\psi = 0$ one should be able to recover the equation $\{p_0^2 - m^2c^2 - p_1^2 - p_2^2 - p_3^2\}\psi = 0$, "which is of a relativistically invariant form" (Dirac, 1958, p. 255). That is, Dirac expected his relativistic equation to contain the Klein-Gordon equation as its square, since this equation involves the relativistic Hamiltonian in its normal invariant form. This implied a set of relations for the unknown coefficients:

$$\alpha_\mu\alpha_\nu + \alpha_\nu\alpha_\mu = 0 \ (\mu \neq \nu);\ \mu, \nu = 1, 2, 3, 4,$$

$$\alpha_\mu^2 = 1.$$

There is no set of four 2×2 matrices that satisfies the previous conditions. According to his recollections, at some point Dirac "realized that there was no need to stick to quantities, which can be represented by matrices with just two rows and columns. Why not go to four rows and columns? Mathematically there was no objection to this at all. Replacing the σ-matrices by four-row and column matrices, one could easily take the square root of the sum of four squares, or even five squares if one wanted to" (quoted in Mehra & Rechenberg, 2000, p. 295). With this insight Dirac arrived at his relativistic wave equation. Dirac choose a representation where the coefficients are given by:

$$\sigma_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\rho_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \qquad \rho_2 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix} \qquad \rho_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

and $\alpha_1 = \rho_1\sigma_1$, $\alpha_2 = \rho_1\sigma_2$, $\alpha_3 = \rho_1\sigma_3$, $\alpha_4 = \sigma_3$.

In this way, Dirac had immediately the relativistic wave equation for a free electron:

$$[p_0 - \rho_1(\boldsymbol{\sigma}, \mathbf{p}) - \rho_3 mc]\psi = 0\,,$$

where $p_0 = i\hbar\,\partial/(c\partial t)$ and $\mathbf{p} = (p_1, p_2, p_3)$, where $p_r = -i\hbar\,\partial/(c\partial x_r)$ with r = 1, 2, 3; $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is a vector formed with the above 4×4 matrices.

Dirac generalized his equation to the case of an electron in an external electromagnetic field. Dirac followed the rule of replacing p_0 by $p_0 + e/c.A_0$ and $\mathbf{p}$ by $\mathbf{p} + e/c.\mathbf{A}$ (where A_0 and $\mathbf{A}$ are the scalar and vector potentials). This gives us the equation

$$[p_0 + \frac{e}{c}A_0 - \rho_1(\boldsymbol{\sigma}, \mathbf{p} + \frac{e}{c}\mathbf{A}) - \rho_3 mc]\psi = 0\,,$$

which is the "fundamental wave equation of the relativistic theory of the electron" (Dirac, 1958, p. 257).

Dirac had developed his equation by considering the relativistic Hamiltonian of a free point particle, that is, Dirac did not take into account in his Hamiltonian (as for example Pauli did in the derivation of his equation) any term related to the spin of the electron. It was a surprise to Dirac that "the simplest possible case did involve the spin" (quoted in Kragh, 1981, p. 55).

Dirac set out to explore the relation between his wave equation with external potentials and the Klein-Gordon equation (based on a classical relativistic Hamiltonian), which was according to Dirac "the wave equation to be expected from analogy with the classical theory" (Dirac, 1958, p. 264):

$$\left\{\left(p_0 + \frac{e}{c}A_0\right)^2 - \left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)^2 - m^2c^2\right\}\psi = 0\,.$$

By squaring his equation, Dirac obtained a differential equation that included the operator of the Klein-Gordon equation and two additional terms:

$$\left\{\left(p_0 + \frac{e}{c}A_0\right)^2 - \left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)^2 - m^2c^2 - \frac{\hbar e}{c}(\boldsymbol{\sigma}, \mathbf{H}) + i\rho_1\frac{\hbar e}{c}(\boldsymbol{\sigma}, \mathbf{E})\right\}\psi = 0\,.$$

Dirac concluded that

> the electron will therefore behave as though it has a magnetic moment $eh/4\pi mc \cdot \boldsymbol{\sigma}$ and an electric moment $ieh/4\pi mc \cdot \rho_1\boldsymbol{\sigma}$. This magnetic moment is just that assumed by the spinning electron model. The electric moment, being a pure imaginary, we should not expect to appear in the model. It is doubtful whether the electric moment has any physical meaning, since the Hamiltonian … that we started from is real, and the imaginary part only appeared when we multiplied it up in an artificial way to make it resemble the Hamiltonian of previous theories. (Dirac, 1928, p. 619)

Dirac showed how this internal magnetic moment resulted from the electron having a spin angular momentum. According to Dirac

> the spin angular momentum does not give rise to any potential energy and therefore does not appear in the result of the preceding calculation. The simplest way of showing the existence of the spin angular

momentum is to take the case of the motion of a free electron or an electron in a central field of force and determine the angular momentum integrals [of the motion]. (Dirac, 1958, p. 266)

By setting $\mathbf{A} = 0$ and A_0 a function of the radius r, the Hamiltonian in Dirac's equation takes the form $H = - eA_0(r) + c\rho_1(\boldsymbol{\sigma}, \mathbf{p}) + \rho_3 mc^2$. Considering, for example, the equation of motion of the x_1-component of the orbital angular momentum $m_1 = x_2p_3 - x_3p_2$, we have $i\hbar \dot{m}_1 = i\hbar c\rho_1\{\sigma_2p_3 - \sigma_3p_2\}$. We see that m_1 is not a constant of the motion. By considering also the equation $i\hbar \dot{\sigma}_1 = 2ic\rho_1\{\sigma_3p_2 - \sigma_2p_3\}$, Dirac found that $\dot{m}_1 + \hbar/2 \cdot \dot{\sigma}_1 = 0$. This means that the vector $\mathbf{m} + \hbar/2 \cdot \boldsymbol{\sigma}$ is a constant of the motion. According to Dirac "we can interpret this result by saying that the electron has a spin angular momentum of $\hbar/2 \cdot \boldsymbol{\sigma}$, which, added to the orbital angular momentum **m**, gives the total angular momentum **M**, which is a constant of the motion" (Dirac, 1928, p. 620). In this way Dirac found that his relativistic wave equation described an electron with a spin angular momentum (and corresponding magnetic moment).

Dirac did not provide an exact solution of his equation for an electron in a central potential. He only made a first order calculation. In this treatment of the hydrogen atom, Dirac was able to obtain Pauli's results on the energy levels, but without using any arbitrary assumptions: the spin angular momentum, gyromagnetic ratio (g_0) and Thomas factor all came out right. Just a few weeks after the publication of Dirac's paper on the relativistic wave equation, it was shown independently by C. G. Darwin and W. Gordon that an exact solution of Dirac's equation gave an expression for the discrete energy levels of the hydrogen spectrum which was identical to Sommerfeld's original formula derived in 1915, which was in good agreement with experimental results.

4 The problem with the negative energy solutions

Since Dirac was using 4×4 matrices in his equation, the wave function had four components (recall that Schrödinger's original equation had one component, and Pauli's equation had two components due to the spin degree of freedom). Initially Dirac thought that he could simply drop two of the components, since "half of the solutions must be rejected as referring to the charge +e on the electron" (Dirac, 1928, p. 618). This was possible in a first-order approximation. Looking at the exact solution we can see that the situation is far from that simple. Dirac's equation can be written as a set of two coupled differential equations for a pair of two-component wave functions ψ_A and ψ_B, where Dirac's wave function is given by

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}.$$

These two wave functions are essential in the solution of Dirac's equation and cannot be disregarded in the calculation of the energy levels. What happens is that the lower two-components (ψ_B) are smaller that the upper two-components (ψ_A), roughly by a ratio of $\upsilon/2c$, where υ is the 'velocity' of the orbiting electron in Bohr's theory. Now, when considering the solution of Dirac's equation for a free electron with momentum **p**, we see that there are two solutions corresponding to electron states with momentum **p** and energy E_p, and two solutions corresponding to states with momentum $-\mathbf{p}$ and energy $-E_p$, or as Dirac mentioned to an electron with charge +e (and positive energy E_p). In the case of the exact solution for an electron in an external electromagnetic field, as we

have seen, we have a four-component wave function, which we can say, by resort to the free electron case, to 'have' positive and negative energy components, or as Dirac mentions, solutions referring to a charge –e and +e.[11] In this way we must take, as Dirac did, the reference to positive and negative energy components as a "rough one, applying to the case when such a separation is approximately possible" (Dirac, 1958, p. 274). When taking the non-relativistic limit of Dirac's equation, the equation for the upper two-components, takes the form of the Schrödinger-Pauli two-component wave equation (corresponding to a negative energy state), and as mentioned, the lower components are smaller than the upper components and can be disregarded. This is the procedure taken by Darwin to 'derive' Schrödinger's equation from Dirac's equation (Mehra & Rechenberg, 2000, p. 302). That is we can only disregard two of the components of the four-component wave function in the non-relativistic limit. Now, Dirac's results are not non-relativistic. The whole point of Dirac's approach was to develop and apply a relativistic wave equation.

Dirac soon recognized that there was a fundamental difficulty with his equation. Already in his early work with the Klein-Gordon equation Dirac had noticed the possibility of solutions corresponding to a charge +e (this is a general characteristic of any relativistic equation due to the relativistic formula for the Hamiltonian involving E^2). The problem is that when considering any small external electromagnetic field, "in general a perturbation will cause transitions from states with E positive to states with E negative" (quoted in Mehra & Rechenberg, 2000, 306). Accordingly Dirac considered that

> such a transition would appear experimentally as the electron suddenly changing its charge from –e to +e, a phenomenon which has not been observed. The true relativity wave equation should thus be such that its solutions split up into two non-combining sets, referring respectively to the charge –e and the charge +e. (Dirac, 1928, p. 612)

As we have seen, also in the case of an electron in a central potential as described by Dirac's equation, that is not the case. Dirac knew that; he recognized in the beginning of his paper on the relativistic wave equation that he was unable to remove this difficulty and considered that his theory "is therefore still only an approximation" (Dirac, 1928, p. 612). However Dirac expected "the probability of these transitions [to be] extremely small" (quoted in Mehra & Rechenberg, 2000, p. 306). That was not the case. Soon afterwards Werner Heisenberg showed that the probability for transitions in which an electron in a state corresponding to a charge –e goes into a state corresponding to a charge +e (a negative energy state) was much larger than Dirac's estimation. Also, Heisenberg showed that the negative-energy states where necessary to obtain the correct dispersion formulae (Mehra & Rechenberg 2000, pp. 306-307). The problem with the negative-energy solutions was highlighted by O. Klein, when, in the end of 1928, he showed that the simple case of a positive-energy wave incident on a potential barrier could give rise to a transmitted negative-energy wave (Mehra & Rechenberg, 2000, pp. 309-311).

By the end of 1929 Dirac had found a way to solve the '± difficulty' of his electron theory. In late March 1929 Heisenberg wrote to Dirac mentioning that H. Weyl thought he had a solution to the ± difficulty and asked Dirac if he knew and could give him any

[11] According to Dirac, "it is not possible, of course, with an arbitrary electromagnetic field, to separate the solutions of [the relativistic wave equation] definitely into those referring to positive and those referring to negative values [of energy], as such a separation would imply that transitions from one kind to the other do not occur". (Dirac, 1958, p. 274)

details about it. Weyl's idea consisted in suggesting that the two extra components might be ascribed not to the electron but to the proton (Dirac's equation would be in this way describing simultaneously electrons and protons). Dirac worked on Weyl's ideas and set forward a new interpretation of his equation that might provide a solution to the problem of the negative energy solutions.

Dirac's first written accounts of his new views were made in an exchange of letters with Bohr. In a letter to Dirac from November 24, Bohr had put forward the idea that there might not be a strict conservation of momentum and energy in some nuclear processes and that this might lead to a solution of the negative energy problem, resulting from the fact that, according to Klein, the potential that confines the electron in the nucleus induces transitions to negative energy states (by that time it was believed that there were electrons in the nucleus of the atoms). Dirac answered, on November 26, that "I should prefer to keep rigorous conservation of energy at all costs", and that "there is a simple way of avoiding the difficulty of electrons having negative kinetic energy" (quoted in Kragh, 1990, p. 90). Dirac then elaborate on his views:

Let us suppose the wave equation $[w/c + e/c\cdot A_0(r) + \rho_1(\boldsymbol{\sigma}\cdot\boldsymbol{\gamma} + e/c\cdot\mathbf{A}) + \rho_0 me)]\,\psi = 0$ does accurately describe the motion of a single electron. This means that if the electron is started off with a +ve energy, there will be a finite probability of its suddenly changing into a state of negative energy and emitting the surplus energy in the form of high-frequency radiation. It cannot then very well change back into a state of +ve energy, since to do so it would have to absorb high-frequency radiation and there is not very much of this radiation actually existing in nature. It would still be possible, however, for the electron to increase its velocity (provided it can get the momentum from somewhere) as by so doing its energy would be still further reduced and it would emit more radiation. Thus the most stable states for the electron are those of negative energy with very high velocity.

Let us now suppose there are so many electrons in the world that all these most stable states are occupied. The Pauli principle will then compel some electrons to remain in less stable states. For example if all the states of –ve energy are occupied and also few of +ve energy, those electrons with +ve energy will be unable to make transitions to states of –ve energy and will therefore have to behave quite properly. The distribution of –ve electrons, will, of course, be of infinite density, but it will be quite uniform so that it will not produce any electromagnetic field and one would not expect to be able to observe it.

It seems reasonable to assume that not all the states of negative energy are occupied, but that there are a few vacancies or "holes." Such a hole which can be described by a wave function like an X-ray orbit would appear experimentally as a thing with +ve energy, since to make the hole disappear (i.e. to fill it up,) one would have to put –ve energy into it. Further, one can easily see that such a hole would move in an electromagnetic field as though it had a +ve charge. These holes I believe to be the protons. When an electron of +ve energy drops into a hole and fills it up, we have an electron and proton disappearing simultaneously and emitting their energy in the form of radiation.

I think one can understand in this way why all the things one actually observes in nature have positive energy. One might also hope to be able to account for the dissymmetry between electrons and protons; one could regard the protons as the real particles and the electrons as the holes in the distributions of protons of –ve energy. However, when the interaction between the electrons is taken into account this symmetry is spoilt. I have not yet worked out mathematically the consequences of the interaction. It is the "Austausch" effect that is important and I have not yet been able to get a relativistic formulation of this. One can hope, however, that a proper theory of this will enable one to calculate the ratio of the masses of proton and electron. (Quoted in Kragh, 1990, pp. 90-91)

Bohr answered a few days later (in December 5), after discussing Dirac's letter with Klein:

We do not understand, how it works out in detail. Before all we do not understand, how you avoid the effect of the infinite electric density in space. According to the principles of electrostatics it would seem that even a finite uniform electrification should give rise to a considerable, if not infinite, field of force. *In the difficulties of your old theory I still feel inclined to see a limit of the fundamental concepts on which atomic theory hitherto rests rather than a problem of interpreting the experimental evidence in a proper way by means of these concepts. Indeed according to my view the fatal transition from positive to*

negative energy should not be regarded as an indication of what may happen under certain conditions but rather as a limitation in the applicability of the energy concept.

In the case of electrons impinging on a potential barrier examined by Klein we have, on the one hand, a striking example of the difficulties involved in an unlimited use of the concept of potentials in relativistic quantum mechanics. On the other hand, we have just in this case an example of the actual limit of applying the idea of potentials in connection with possible experimental arrangements. In fact, due to the existence of an elementary unit of electrical charge we cannot build up a potential barrier of any height and steepness desired without facing a definite atomic problem. In Klein's example the critical height of the barrier is of order mc^2, and the rise of potential shall take place within a distance of the order h/mc which is the order of magnitude of the wavelength of the electrons concerned. But if the dimensions of the barrier perpendicular to the electric force shall be large compared with this wavelength λ_0, it claims the presence of a double layer of electricity of such a strength that a surface element of size λ_0^2 of the negative layer contains al least hc/e^2 electrons. It is therefore clear that the problem in question cannot legitimately be treated as that of one electron moving in a given potential field, but is essentially a many electron problem which falls outside the range of present quantum mechanics.

On the whole it appears that the circumstance that hc/e^2 is large compared with unity does not only indicate the actual limit of the applicability of the quantum theory in its present form, but at the same time ensures its consistency within these limits. In fact the radius r_0 of the electron estimated on classical theory is $e^2/mc^2 = (h/me)(e^2/hc)$, and we can therefore never determine the position of an electron within an accuracy comparable with r_0 without allowing an uncertainty in its momentum larger than mc, thus entailing an uncertainty of energy surpassing the critical value mc^2. The idea that the reach of quantum mechanics is bound up with the actual existence of the electron would also seem to be in harmony with the fact that the symbols e and m appear in the fundamental equations of the present theory … As regards the transitions from positive to negative energy accompanied by radiation I am not sure that they present as serious a difficulty for your wave equation as it might appear. The question is, how much those features of the theory which claim the transitions in question are involved in the problems, where your theory has been found in so wonderful agreement with experiments. In this connection I must correct the statement in my former letter regarding the probability of these transitions which is not nearly so large as I believed. In discussing the problem more closely with Klein we convinced ourselves that the estimation of this probability did not take sufficient regard to the smallness of the wavelength of the radiation concerned compared with atomic dimensions. We have not made an actual calculation of any such probability, and if you have considered the problem in detail I should be very thankful for any information regarding this point. My hope is that it should be possible to defend all the successful applications of your wave equation, but I suspect that the natural limitation of these applications prevents an extrapolation of the kind you describe in your letter. (Quoted in Moyer, 1981, pp. 1057-1058 [my emphases])

It is important to notice that Bohr started seeing the Klein paradox as resulting from an unlimited mathematical application of the concept of potential (or more generally of field) in relativistic quantum mechanics. Bohr called attention to the necessity of taking into account the elementary unit of electrical charge in the determination of the actual potential barrier. Calculations made not taking into account this fact and the limits in the determination of the electron's position (and its associated uncertainty in momentum, and according to Bohr also in energy) would be beyond the 'actual limit of applicability' of the theory and any 'possible experimental arrangement'. Accordingly, Bohr considered that the elimination of Klein's paradox passed through an essential limitation of the mathematical use of the concept of field (see also Darrigol, 1991, pp. 154-155). However Bohr considered that within the domain of applicability of the theory, the concepts (being used in a restricted context) and the results obtained were consistent (in chapter 5 I will return to Bohr's view on relativistic quantum theory). Due to this, the problem of the transitions to negative-energy states would not occur in 'all the successful applications of the theory'. In this way there would be no need for the hole theory.

Dirac did not agree with Bohr's views and in a letter sent to Bohr in December 9, stressed his differences with Bohr and gave a further elaboration of his views:

I do not completely agree with your views. Although I believe that quantum mechanics has its limitations and will ultimately be replaced by something better, (and this applies to all physical theories,) I cannot see any reason for thinking that quantum mechanics has already reached the limit of its development. I think it will undergo a number of small changes, mainly with regard to its method of application, and by these means most of the difficulties now confronting the theory will be removed. If any of the concepts now used (e.g. potentials at a point) are found to be incapable of having an exact meaning, one will have to replace them by something a little more general, rather than make some drastic alteration in the whole theory … There is one case where transitions of electrons from positive to negative energy levels does give rise to serious practical difficulties, as has been pointed out to me by Waller. This is the case of the scattering of radiation by an electron, free or bound. A scattering process is really a double transition, consisting of first an absorption of a photon with the electron jumping to any state and then an emission with the electron jumping to its final state (as in Raman effect) (or also of first the emission and then the absorption). The initial and final states of the whole system have the same energy, but not the intermediate state, which lasts only a very short time. One now finds, for radiation whose frequency is small compared with mc/h, that practically the whole of the scattering comes from double transitions in which the intermediate state is of negative energy for the electron. Detailed calculations of this have been made by Waller. If one says the states of negative energy have no physical meaning, then one cannot see how the scattering can occur.

On my new theory the state of negative energy has a physical meaning, but the electron cannot jump down into it because it is already occupied. There is, however, a new kind of double transition now taking place, in which first one of the negative-energy electrons jumps up to the proper final state with emission (or absorption) of a photon, and secondly the original positive-energy electron jumps down and fills the hole, with absorption (or emission) of a photon. This new kind of process just makes up for those excluded and restores the validity of the scattering formulas derived on the assumption of the possibility of intermediate states of negative energy.

I do not think the infinite distribution of negative-energy electrons need cause any difficulty. One can assume that in Maxwell's equation div $E = -4\pi\rho$, the ρ means the difference in the electric density from its value when the world is in its normal state (i.e when every state of negative energy and none of positive energy is occupied.) Thus ρ consists of a contribution $-e$ from each occupied state of positive energy and a contribution $+e$ from each unoccupied state of negative energy.

I have not made any actual calculation of the transition probabilities from +ve to –ve, but I think they are fairly small. (Quoted in Kragh, 1990, pp. 92-93)

A paper containing Dirac's hole interpretation of his equation was published in early 1930. In this work Dirac first made clear his departure from Weyl's original idea of associating the negative energy solutions directly to the protons. According to Dirac:

One cannot, however, simply assert that a negative-energy electron is a proton, as that would lead to the following paradoxes:

(i) A transition of an electron from a state of positive to one of negative energy would be interpreted as a transition of an electron into a proton, which would violate the law of conservation of electric charge.

(ii) Although a negative-energy electron moves in an external field as though it has a positive energy, yet, as one can easily see from a consideration of conservation of momentum, the field it produces must correspond to its having a negative charge, e.g. the negative-energy electron will repel an ordinary positive-energy electron although it is itself attracted by the positive-energy electron.

(iii) A negative-energy electron will have less energy the faster it moves and will have to absorb energy in order to be brought to rest. No particles of this nature have ever been observed. (Dirac, 1930, p. 362)

Dirac then presented in more details his hole theory as described in the letters to Bohr. Dirac gave in particular an account of the scattering of radiation by an electron according to his hole theory. Dirac mentions that in a scattering process two types of intermediate states can occur. In one case we have a

transition process, consisting of first an absorption of a photon with the electron simultaneously jumping to any state, and then an emission with the electron jumping into its final state, or else of first the emission and then the absorption. (Dirac, 1930, p. 364)

In the other case

first one of the distribution of negative-energy electrons jumps up into the required final state for the electron with absorption (or emission) of a photon, and then the original positive-energy electron drops into the hole formed by the first transition with emission (or absorption) of a photon. Such processes result in a final state of the whole system indistinguishable from the final state with the more direct processes, in which the same electron makes two successive jumps. (Dirac, 1930, p. 365)

In this second case we have an intermediate state with two electrons (or one electron and the hole). It is clear that the description of the light scattering by an electron involves more than just the original electron: we are faced with a many-body theory. Dirac with his hole theory changed the character of his equation from a single-electron equation into an equation describing a many-body (in reality infinite) electron system.

Even before the publication of his paper on the hole theory, several physicists, knowing the general lines of Dirac's ideas, had a sceptical reaction to it. In particular Heisenberg made a rough calculation of the electron-proton interaction in the new theory. Heisenberg concluded that the electron and the proton had to have the same mass (Kragh 1990, p. 94). Dirac had already recognized this problem in one of his letters to Bohr, but expected that a future detailed theory of the interaction between electrons and protons (holes) might solve this difficulty. A further objection was given a few months latter, in a note by J. R. Oppenheimer (1930a) in which the author calculated the transition probability for the annihilation of an electron and a proton that corresponds to the filling of a hole in the sea. The result was not very promising. Oppenheimer obtained a mean lifetime of a free electron in matter that was too low, and totally inconsistent with the observed stability of matter (Kragh, 1990, pp. 101-102). Oppenheimer's proposition was to "return to the assumption of two independent elementary particles of opposite charge" (quoted in Kragh, 1990, p. 102). That is, to consider the electron and the proton as dissociated particles, each one being related to its 'Dirac sea' of negative-energy particles. In this way there would not be a problem of a possible proton-electron annihilation. More importantly, in 1931 Weyl published a paper in which he proved by symmetry properties of Dirac's equation that the negative-energy electrons must have the same mass as the positive-energy electrons. In this same year Dirac rethought his hole theory in face of the objections being made and presented a new view on the problem:

It thus appears that we must abandon the identification of the holes with protons and must find some other interpretation for them. Following Oppenheimer, we can assume that in the world as we know it, all, and not merely nearly all, of the negative-energy states for electrons are occupied. A hole, if there were one, would be a new kind of particle, unknown to experimental physics, having the same mass and opposite charge to an electron. We may call such a particle an anti-electron. We should not expect to find any of them in nature, on account of their rapid rate of recombination with electrons, but if they could be produced experimentally in high vacuum they would be quite stable and amenable to observation. (Dirac 1931, p. 61)

In 1932 a brief article by C. D. Anderson was published presenting experimental evidence for a new kind of positively charged particle with a mass much smaller than that of the proton. These experimental findings were presented without taking into account Dirac's theory. By that time P. Blackett and G. Occhialini had independent evidence for the positrons and previous to publication they discussed their findings with

Dirac. They published their results after Anderson's publication, mentioning Dirac's theory and presenting some ideas regarding the origin of the positive particle. According to Blackett and Occhialini "one can imagine that negative and positive electrons may be born in pairs during the disintegration of light nuclei" (quoted in Schweber, 1994, p. 69). However they were cautious regarding their proposed mechanism:

> when the behavior of the positive electrons has been investigated in more detail, it will be possible to test these predictions of Dirac's theory. There appears to be no evidence as yet against its validity, and in its favour is the fact that it predicts a time of life for the positive electron that is long enough for it to be observed in the cloud chamber but short enough to explain why it had not been discovered by other methods. (quoted in Schweber, 1994, p. 69)

After a thorough revision of the experimental evidence for positrons Blackett and Occhialini published another article where their support to Dirac's theory was stronger:

> these conclusions as to the existence and the properties of positive electrons have been derived from the experimental data by the use of simple physical principles. That Dirac's theory of the electron predicts the existence of particles with just these properties, gives strong reason to believe in the essential correctness of his theory. (quoted in Schweber, 1994, p. 69)

Even with the experimental evidence for the positron there was resistance to Dirac's hole theory. In relation to this discovery, Bohr considered that "even if all this turns out to be true, of one thing I am certain: that it has nothing to do with Dirac's theory of holes!" (quoted in Kragh, 1990, p. 112). And Pauli wrote to Dirac saying: "I do not believe on your perception of 'holes', even if the existence of the 'antielectron' is proved" (quoted in Kragh, 1990, p. 112). It turns out they were right and a different – field theoretical – approach was possible without any need for an infinite sea of negative-energy particles with some holes in it.

5 The field theoretical interpretation of Dirac's equation

To understand how this field theoretical interpretation of Dirac's equation came to be, we need (at least) to go back to a work by Dirac published in 1927. In this work, Dirac presented a non-relativistic treatment of the interaction of electromagnetic radiation and atoms, which enabled him to give a dynamical derivation of Einstein's laws for the emission and absorption of radiation, which Einstein had obtained by statistical considerations (Darrigol, 1986, p. 226). Dirac followed initially an approach in which he considered an assembly of classical particles (that would interact with an atom), which were described by the Schrödinger equation. For the case of light quanta, Dirac knew that he could not use all the available wave functions, but had to select only symmetrical wave functions, corresponding to Bose-Einstein statistics: "The solution with symmetrical eigenfunctions must be the correct one when applied to light quanta, since it is known that the Einstein-Bose statistical mechanics leads to Planck's law of black-body radiation" (Dirac, 1926, p. 672).

In his 1927 work, Dirac did not follow the simpler procedure of imposing symmetrical wave functions (Dirac, 1958, p. 225), but a procedure more complex and physically unclear. This so-called 'second quantization' turns out to be simply a method that guaranteed that the (quantized) particles, that is particles described by a Schrödinger equation, satisfied Bose-Einstein statistics (Schweber, 1994, p. 28). Dirac did not arrive at the method by some physical insight. According to his words:

I remember the origin of that work was just playing about with equations. I was intending to get a theory of radiation at the time. I was just playing about with the Schrödinger equation. I got the idea of applying the quantization to it and worked out what it gave and found out it just gave the Bose statistics. (Quoted in Darrigol, 1984, p. 461)

In this work Dirac provided a different approach to the interaction of radiation and atoms, by considering the electromagnetic radiation as a classical wave (and not as constituted by particles), which after quantization satisfies Bose-Einstein statistics. Dirac made the bold move of quantizing not directly the electric and magnetic field but the vector potential (Dirac, 1927a, p. 262; Miller, 1994, p. 22; Kragh, 1990, p. 126), which is resolved into its Fourier components. Using a non-relativistic approximation consistent with the one adopted for the light quanta case, Dirac found it possible – by making a necessary reinterpretation of the state corresponding to zero light quanta as a state with an infinite number of unobservable light quanta with zero energy and momentum – to find a Hamiltonian for the system constituted by a (quantized) electromagnetic field interacting with an atom, that "takes the same form as in the light-quantum treatment" (Dirac, 1927, p. 265). This result led Dirac to consider that:

Instead of working with a picture of the photons [light quanta] as particles, one can use instead the components of the electromagnetic field. One thus gets a complete harmonizing of the wave and corpuscular theories of light. One can treat light as composed of electromagnetic waves, each wave to be treated like an oscillator; alternatively, one can treat light as composed of photons, the photons being bosons and each photon state corresponding to one of the oscillators of the electromagnetic field. One then has the reconciliation of the wave and corpuscular theories of light. They are just two mathematical descriptions of the same physical reality. (Quoted in Schweber, 1994, p. 31)

The fact that Dirac considers that there is "a complete harmony between the wave and light-quantum description" (Dirac, 1927a, p. 245), does not mean that he takes over this equivalence to the case of the electrons. In fact, as Dirac clearly states in this article, he makes a sharp distinction between the case of electromagnetic radiation and matter. For Dirac there simply is no real de Broglie wave that, after quantization, permits the description of the electrons (Dirac, 1927a, p. 247).

Jordan's reading of Dirac's work was quite different. Going back to the cumbersome method of second quantization that for Dirac was "nothing but a convenient way to take Bose statistics into account" (Darrigol, 1986, p. 229), Jordan interpreted the scheme of second quantization as the quantization of a classical wave described by a classical wave equation that could be the Maxwell-Lorentz equations for the case of the electromagnetic field or a Schrödinger equation for the case of electrons seen not as particles but as de Broglie waves (Darrigol, 1986, pp. 229-230). This view of Jordan had the advantage to make it possible to treat the quantized waves in a three-dimensional space (or four-dimensional Minkowski space-time) instead of using a 3n (multidimensional) space in the case of an n-particle system (Schweber, 1994, p. 36). In a paper sent to publication in July 1927, Jordan made a conceptual turnaround on Dirac's approach, and applied his method to the quantization of quanta obeying Pauli's exclusion principle, [12] that is to electrons. Contrary to the case of photons (light quanta), in which there is no limit to the number of particles that may occupy the same state, the electrons (according to Pauli's exclusion principle) cannot be in the same state, that is, the occupation number for each possible state can only be 0 or 1 (another way of making this statement is to say that the electrons are fermions, that is, they obey Fermi-

[12] Regarding Pauli's exclusion principle see e.g. Sánchez Ron (2001, pp. 348-350).

Dirac statistics). Jordan's approach was to take the method used by Dirac with the light quanta, and to apply it to the electron as a de Broglie wave – for which there was experimental evidence (Darrigol, 1986, p. 219) – that was a solution of a (classical) Schrödinger equation. In this way, Dirac's 'second quantization' was from Jordan's perspective a 'first quantization' of a classical wave. This was simply implemented by taking the coefficients of each normal mode to be matrices satisfying certain commutation relations. In this work, Jordan did not take correctly into account the phase factors in the matrices "necessary to guarantee that the creation operators for different energy states anticommute with one another" (Schweber, 1994, p. 37). This point was settled by the end of the year in a collaboration with E. Wigner, where the correct anticommutation relations were given. In any case, already in his first incomplete work Jordan was able, by his quantization of the wave, to obtain "an evolution identical to the one given by anti-symmetrical wave functions in configuration space" (Darrigol, 1986, p. 231). That is, Jordan showed the equivalence, for the electrons, of adopting as a classical starting point, not the electrons as particles but electrons as classical de Broglie waves. With this procedure there was no need for a multidimensional abstract configuration space, since it was possible with the wave approach to maintain the description solely in terms of a quantized wave described in a three-dimensional space. In this way, already in this first incomplete work, Jordan was able to conclude that "a quantum-mechanical wave theory of matter can be developed that represents electrons by quantum waves in the usual three-dimensional space" (quoted in Darrigol, 1986, p. 232). This conclusion made possible for Jordan to make the 'programmatic' assertion: "The natural formulation of the quantum theory of electrons will be attained by conceiving light and matter as interacting waves in three-dimensional space" (quoted in Darrigol, 1986, p. 232). In the abstract of the work done with Wigner similar considerations were made:

> The problem at hand is to describe an ideal or nonideal gas that satisfies the Pauli exclusion principle with the idea of not using any relation in the abstract (3N-dimentional) configuration space of the atoms of the gas, but using only three-dimensional space. This is made possible by representing the gas by a three-dimensional quantized wave, for which the particular non-commutative properties for multiplying wave amplitudes are simultaneously responsible for the existence of corpuscular atoms of the gas and for the validity of Pauli's exclusion principle. (Quoted in Schweber, 1994, p. 38)

Heisenberg and Pauli adopted Jordan's approach in the development of a quantum field approach to the description of the interaction of radiation and matter. In their case they took Dirac's equation as a classical wave equation. The 'de Broglie' solution of Dirac's equation is then quantized according to the procedure set forward by Jordan. The elementary excitations (quanta) of the field resulting from the quantization are the particles. In a sense this field theoretical approach as applied by Heisenberg and Pauli is incomplete. The point is that the energy of the field can be negative. This is so due to the presence of the negative energy quanta. This means it was still necessary to make use of Dirac's hole theory to make sense of the field quantization. The negative energy states where taken to be full and a positron was identified with an empty negative-energy state. That is, a positron in this field theoretical view was taken to be the lack of an elementary excitation in an infinite sea of negative-energy elementary excitations.

In November 1933, V. Fock published a paper where he made a symmetrical treatment of free electrons and positrons without using negative-energy particles, following a procedure by Heisenberg from 1931 in which he explored "a far-reaching analogy between the terms of an atomic system with n electrons and those of a system in which n electrons in a closed-shell are lacking" (quoted in Pais, 1986, p. 379). In a

letter to Pauli from July 1933 Heisenberg had presented that same approach, and used it in a paper published in 1934, considering the case where an external field was present (Darrigol, 1984, p. 479; Miller, 1994, p. 63). In this paper he required that "the symmetry of nature in the positive and negative charges should from the very beginning be expressed in the basic equations of [the] theory" (Heisenberg 1934, p. 169). Taking the Dirac equation and its adjoint equation as classical field equations derived from a classical Lagrangian, an arbitrary field can be expanded in terms of the complete set of free-particle solutions (Schweber, 1961, pp. 222-223):

$$\psi(\mathbf{x}) = \int \frac{d^3p}{(2\pi)^{3/2}} \left(\frac{m}{E_{\mathbf{p}}} \right)^{1/2} \left\{ \sum_{r=1}^{2} b_r(\mathbf{p}) w^r(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} + \sum_{r=3}^{4} b_r(-\mathbf{p}) w^r(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{x}} \right\}.$$

The quantization scheme consists in replacing the expansion coefficients by operators satisfying the anticommutation relations $[b_n, b_m]_+ = [b_n^*, b_m^*]_+ = 0$ and $[b_n, b_m^*]_+ = \delta_{nm}$. With this procedure $\psi(\mathbf{x})$ and the adjoint spinor field $\psi^*(\mathbf{x})$ become operators that act on state vectors of a Fock space;[13] and $b_r(\mathbf{p})$ and $b_r^*(\mathbf{p})$ are interpreted as the annihilation and creation operators of an electron in the state $(\mathbf{p}, r)$. Redefining the operators for the negative-energy states as $b_{r+2}(-\mathbf{p}) = d_r^*(\mathbf{p})$ and $b_{r+2}^*(-\mathbf{p}) = d_r(\mathbf{p})$ with r = 1, 2, these operators can be interpreted as the creation and annihilation operators for a positive-energy positron (Schweber, 1961, p. 223; Miller, 1994, p. 56), and the expansion of the $\psi(\mathbf{x})$ operator is now given by

$$\psi(\mathbf{x}) = \int \frac{d^3p}{(2\pi)^{3/2}} \left(\frac{m}{E_{\mathbf{p}}} \right)^{1/2} \sum_{r=1}^{2} \left\{ b_r(\mathbf{p}) w^r(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} + d_r^*(\mathbf{p}) v^r(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{x}} \right\}.$$

With this formulation there are no negative-energy states (identified as the positive-energy positrons), and so no need for the infinite sea of negative-energy electrons. Also in the field operators $\psi(\mathbf{x})$ and $\psi^*(\mathbf{x})$ we have simultaneously components related to electrons and positrons. Let us consider the total charge operator

$$Q = \sum_r \int d^3p [-a_r^*(\mathbf{p}) a_r(\mathbf{p}) + b_r^*(\mathbf{p}) b_r(\mathbf{p})] = \int d^3p [n^+(\mathbf{p}) - n^-(\mathbf{p})],$$

where $n^-(p)$ is the number of the quanta identified as electrons and $n^+(p)$ is the number of quanta identified as positrons (Jauch & Rohrlich, 1976, p. 64). As we can see from this expression, as Jordan proposed, the quantization of charge and subsequent emergence of a particle-like concept of an electron can be seen as a result of the quantization of the classical field.

[13] Considering the vacuum state, which is the state with no quanta, an n-quanta Hilbert space can be defined by n applications of creation operators. The Fock space is the (infinite) product of the n-quanta Hilbert spaces: $H^{(0)} \oplus H^{(1)} \oplus H^{(2)} \ldots$ (Schweber, 1961, pp. 134-137; Gross, Runge & Heinonen, 1991, p. 21).

6 Combining results from the different views on Dirac's equation

With this field theoretical reinterpretation of Dirac's equation we are still facing a problem. We know that the original one-electron interpretation is not consistent: how then can we relate the solutions of Dirac's equation as a relativistic wave equation for an electron to the view imposed by the quantum field perspective?[14]

I will look again into the case of the hydrogen atom. As Dirac mentioned "in the general case of an arbitrary varying electromagnetic field we can make no hard-and-fast separation of the solutions of the wave equation into those referring to positive and those to negative kinetic energy" (Dirac, 1930, p. 361). L. L. Foldy and S. A. Wouthuysen gave a more detailed account of the situation:

> If we regard the electric field as a perturbation, then one can say that the electric field induces transitions of the particle between the positive- and negative-energy states of a free particle. This is one way of viewing the physical situation.
>
> On the other hand, one knows that for sufficiently weak fields the Hamiltonian above possesses a complete set of eigenfunctions with energy eigenvalues which may be classified according to whether they are positive or negative. There exists for these weak fields a clear-cut distinction between these two sets of stationary states since they are separated by a relatively large energy gap of order 2m. Furthermore, the wave functions corresponding to positive energies show a behavior of the particle appropriate to a particle of positive mass, in that the particle tends to be localized in regions of low potential energy; while the negative-energy solutions show a behavior of the particle appropriate to a particle of negative mass, in that the particle tends to be localized in regions of high potential energy.
>
> Either of the two descriptions of the behavior of the particle in a weak field given above is of course correct, although the distinction between what are called the positive- and negative-energy states is different in the two descriptions. However, the question of terminology for positive- and negative-energy states being left to our own choice, we are free to choose our definitions in such a way as to give the more graphic (and perhaps more intuitively satisfying) description of the actual physical events which are being described. In this spirit we feel that the second description is to be preferred since it has a perfectly reasonable classical limit. It would be difficult indeed to picture classically the motion of a particle in a weak field in terms of transitions between free-particle motions with positive and negative mass.
>
> Consider now what happens when the particle interacts with strong rather than weak fields. Under such circumstances, the division of states into those of positive and negative mass is no longer clear-cut, since the energy separation of the two sets of states is reduced to a relatively small amount. Furthermore, the wave functions describing these states no longer appropriately describe the motion of a particle of fixed sign of mass according to our customary notions. In fact, if we try to interpret the wave function in these terms, we encounter certain well-known paradoxes – the Klein paradox, for example. While the energy of any stationary state will still have a definite sign, the statement that the particle is in a state of positive energy will no longer carry with it the validity of any intuitive conceptions as to the behavior of a classical particle with positive energy, and there will be little qualitative difference between certain states of positive energy and certain states of negative energy. Hence, in the presence of strong fields, the usefulness of a description in terms of positive and negative-energy states will be lost. (Foldy & Wouthuysen, 1949, pp. 33-34)

[14] A simple answer in what regards the equation itself is that we can see the Dirac one-electron equation as a 'semi-classical' equation resulting from using the so-called external field approximation (Jauch & Rohrlich, 1976, p. 303), where there appears to be a classical potential within the quantum formalism, but that really is due to a quantum field theoretical description of the interaction with a very heavy charged particle (described by a quantum field) when its recoil is neglected (Schweber, 1961, p. 535). It is within the external field approximation that a Dirac field operator equation with an 'external' field appears, and from which the relativistic one-electron equation with a 'classical' potential can be seen to emerge from the full quantum electrodynamics (Jauch & Rohrlich, 1976, pp. 307 & 313).

When considering the exact solution of the one-electron Dirac equation in a central potential (the hydrogen atom) we have a four-component wave function. In simple terms we can say that in the four-component wave function we have components that, from a quantized field perspective, are related to both electrons and positrons. As we have seen, the quantized field perspective relates the (free) positive-energy solutions to the electrons and the (free) negative-energy solutions to the positrons. If we want, taking into account this perspective, a simple model for the hydrogen atom with only one electron, while using the Dirac equation as a relativistic one-electron equation, we must develop a model that uses only two-component positive-energy wave functions to describe the electron. This approach is also important if we want to make a clear connection between the relativistic and non-relativistic equations, that is, between the Dirac and the Schrödinger equations.

Considering the four-component solutions of the Dirac equation in the presence of electromagnetic coupling $\psi = (\psi_A \ \psi_B)$, in the non-relativistic limit the lower two components ψ_B are smaller than the upper two ψ_A. When calculating matrix elements like $(\psi, \gamma_4\psi) = \psi_A^*\psi_A - \psi_B^*\psi_B$, neglecting terms of order $(v/c)^2$, we obtain an expression only in terms of the large components $\psi_A^*\psi_A$, reducing the matrix element to its non-relativistic form in terms of two-component wave functions (Mandl, 1957, pp. 214-215). In the non-relativistic limit the large components can be seen as the solution of the Schrödinger-Pauli two-component wave equation. Concerning this approach to the problem of the non-relativistic limit of the Dirac equation, Foldy and Wouthuysen argued that "the above method of demonstrating the equivalence of the Dirac and Pauli theories encounters difficulties […] when one wishes to go beyond the lowest order approximation" (Foldy & Wouthuysen, 1949, p. 29). Foldy and Wouthuysen proposed a new method (using a different representation than Dirac's original one) which would not only provide better results for higher-order approximations but also the definition of new operators for position and spin "which pass over into the position and spin operators in the Pauli theory in the non-relativistic limit" (Foldy & Wouthuysen, 1949, p. 29).

In the case of the Dirac equation for a free electron it is possible to perform a canonical transformation on the Hamiltonian that enables the decoupling of the positive- and negative-energy solutions of Dirac's equation, each one becoming associated to a two-component wave equation. This means we get two independent equations for two-component wave functions, and that we can identify the equation with positive-energy solution as the Schrödinger-Pauli equation. The case of an electron interacting with an external electromagnetic field is more involved. The trick is to consider the electromagnetic field as a perturbation and to make a sequence of transformations to obtain the separation of negative- and positive-energy solutions. In the non-relativistic limit, like in the previous method, the Schrödinger-Pauli equation is obtained.

It is then possible to rework the relativistic Dirac one-electron equation in a way in which only positive-energy solutions are considered. Foldy and Wouthuysen applied their method to the case where a Dirac electron interacts with an external electromagnetic field. By making three canonical transformations and using only terms of order $(1/m)^2$ they obtained a Hamiltonian (incorporating relativistic correction to this order) that enabled a clear separation of positive- and negative-energy solutions. With this method the non-relativistic limit of Dirac's equation results in two uncoupled equations one with positive-energy solutions and the other with negative-energy solutions. With their three canonical transformations Foldy and Wouthuysen were able to obtain the same wave equation as in the Pauli theory. However it is important to

notice that in the previous method we are not taking into account directly the quantized Dirac field, and we are basically maintaining the inconsistent one-electron interpretation of Dirac's equation. Also, Foldy and Wouthuysen's definition of the positive-energy solutions was made by taking into account the classical limit, and as they mentioned it is not unique. As we have seen the quantization of the (free) Dirac field leads to an association of the quanta to individual terms of a plane-wave expansion of the field corresponding to either positive or negative energy eigenvalues, which implies choosing another definition of positive-energy solutions.

This leads us to the necessity of taking a quantum field approach to the case of the hydrogen atom. One possibility is to use the so-called Furry or bound interaction representation within the external field approximation. This gives a method for calculating corrections (due to a quantized electromagnetic field) to the energy levels of a bound electron (due to a static external potential) determined by the Dirac equation as a relativistic one-electron equation (Berestetskii, Lifshitz & Pitaevskii, 1982, p. 487). But the starting point is the field operator defined by

$$\psi(x) = \sum_{r} u_r(\mathbf{x}) a_r e^{-iE_r t} + v_r(\mathbf{x}) b_r^* e^{iE_r t},$$

where $u_r(\mathbf{x})$ and $v_r(\mathbf{x})$ are obtained by solving the Dirac equation for a positive-energy particle representing the electron, and a negative-energy particle representing de positron: $Hu_a(\mathbf{x}) = E_a u_a(\mathbf{x})$ and $Hv_b(\mathbf{x}) = -E_b v_b(\mathbf{x})$, where $H = i\gamma^0\boldsymbol{\gamma}.\nabla - e\gamma^0\gamma_\mu\varphi^\mu + i\gamma^0 m$, with φ^μ a static external field (Jauch & Rohrlich, 1976, p. 313). The first equation is exactly the one solved in the case of the one-electron interpretation of the Dirac equation. This means that E_a gives the positive energy levels obtained by this method, and that in spite of identifying $u_a(\mathbf{x})$ as the electron's positive-energy wave function, it contains what in the limit of a free-particle solution are positive- and negative-energy components (Schweber, 1961, p. 566). Now, what is needed is a method in which the free particle positive-energy characteristic of the electron is maintained during the interaction with no mixing of positive- and negative-energy components.

As we will see in the following chapters, the main working tool in quantum electrodynamics, the S-matrix, was designed for scattering problems where we have free particles in the beginning and free particles in the end of an interaction (scattering). This means that the S-matrix is not very appropriate to deal with the case of a bound particle, at least not in a direct way. Moreover, one of the most important characteristics of quantum field methods is that the interaction between fermions is represented by the exchange of photons: quanta of the electromagnetic field (e. g. Carson, 1996, pp. 127-129). If we make a model of the atom in which a classical Coulomb field gives the effect of the nucleus, this quanta view is lost (as in the external field method previously discussed). A way to overcome these difficulties is to address directly the two-body problem using the Bethe-Salpeter equation. In this method, the two-body problem is addressed by considering directly the two-particle propagator for an electron and a proton (which in the calculations is taken to be a 'big' positron with the same mass as the proton).[15] Considering a power series expansion of the two-particle propagator, the binding energy between a proton and an electron is basically calculated using what is known as the ladder approximation (Schweber, 1961, p. 713). Concerning this

[15] There is an indirect method to calculate the energy levels of bound states from the S-matrix, which consists in determining the poles of the exact scattering amplitude. But in practice this approach leads to a summation of an infinite series of diagrams that corresponds to solving the Bethe-Salpeter equation (Berestetskii, Lifshitz & Pitaevskii, 1982, p. 553-556).

approximation, H. A. Bethe and E. E. Salpeter remarked that "although the probability for the exchange of a quantum during a small time interval is fairly small, during the infinite time of existence of the bound state an indefinite number of quanta may be exchanged *successively*. It is just such processes that the ladder-type graphs deal with" (Salpeter & Bethe, 1951, p. 1234). Thus, in the quantum field theory approach, the binding of the electron in the atom is achieved by an exchange of photons with the proton. We see that from a quantum field theory perspective, the description of the hydrogen atom (as a two-body problem) leads to a physical picture of the process going on in the atom quite different from the one obtained when using inconsistently the Dirac equation as a one-electron equation. That is, we see, when going from a central potential approach to a quantum field two-body treatment of the hydrogen atom, the importance of the quanta concept in the description of interactions in quantum electrodynamics. The exchange of quanta is a basic characteristic of the description of physical processes in quantum electrodynamics. We will look at this in detail in later chapters.

CHAPTER 4

THE QUANTIZATION OF THE ELECTROMAGNETIC FIELD AND THE VACUUM STATE

1 Introduction

There is a widespread idea that we can associate with the concept of quantum vacuum important measurable consequences, and even, like in the case of the commonly accepted interpretation of the Casimir effect, clear dynamical effects. To better address the problem of what vacuum concept we really have in quantum electrodynamics, I start in section 2 with an historical account of the coming to be of the quantized electromagnetic field and in section 3 with a brief 'technical' presentation of the quantized electromagnetic field. We will see in particular how Einstein's light quanta (photons) can be seen as resulting from the quantization of the electromagnetic field. The quantized electromagnetic field's vacuum or ground state is the state with the lowest energy, corresponding to no (transverse) photons present.

Due to the quantization, in all the quantum electromagnetic field states corresponding to a defined number of quanta, the variance of the electric and magnetic fields is not zero. This situation also occurs in the ground state (or vacuum state), and it has measurable consequences. This is in clear contrast to the classical counterpart where the vacuum state corresponds to a null electromagnetic field in some region of space.

In section 4, I will focus on the properties of the ground state of the quantized electromagnetic field. Following Peter Milonni I will make a case for an interpretation of the Casimir effect that does not rely on zero-point energy fluctuations. This does not mean that the vacuum of the quantized electromagnetic field can be disposed of. Contrary to the classical case where it is possible to consider charged matter in an empty region of space – where there is no external electromagnetic field but only the field of the charged matter itself –, in the case of quantized fields this is no longer possible. According to Milonni, for the formal consistency of the theory, when considering a charged particle in an empty region of space, we must take into account that the charged particle is always interacting with an *external* quantized electromagnetic field even if just in its ground state. In this way, together with charged matter, we must always consider at least an 'empty-space' or 'space-vacuum' field in its vacuum or ground state with its associated non-zero variance; and this is not just a formal aspect of the theory, it can be related to experimental results. To clarify things, first, in section 5, I will explain the physical meaning of variance, making the case for an interpretation in terms of a statistical spread (distribution) in the results of independent measurements made on identically prepared systems. This interpretation is made within the broader framework of the 'ensemble' interpretation of quantum mechanics. Then, in section 6, we will see that using the balanced homodyne detection method it is possible to obtain experimental results corresponding to the non-vanishing

variance of the vacuum state. This implies that we can retain a notion of vacuum with experimental meaning that is consistent with an interpretation of the variance in terms of a statistical spread (distribution) in the results of independent measurements made on identically prepared systems.

It seems then that we cannot recover the 'nothingness' of the classical notion, but, nevertheless, the physical properties we can really associate with the vacuum concept are much more subtle than usually thought, and do not present any experimental particularities that are not found in all quantum states corresponding to a defined number of quanta: the non-vanishing variance is a common characteristic of all these states, not only the ground state. In this way, I will be making a case for an empirically demonstrable notion of the vacuum in quantum electrodynamics independent of dynamical fluctuations.

2 The historical emergence of the quantized electromagnetic field

Though the story of quantum theories began around 1900 with Planck's theoretical work on the so-called blackbody radiation, a working quantum theory of the electromagnetic field (and its interaction with matter) was not available until the late 1940s. The quantum theory of radiation can be seen to have its first development not in Planck's early and subsequent work, but in an article published in 1905 that its author referred to as "very revolutionary" (quoted in Kragh, 1999, p. 66). As we have seen, in this article Einstein presented what he called a heuristic viewpoint on the nature of radiation, considering in particular the emission, absorption, and propagation of light in space. Einstein proposed that in the limit where Wien's law is valid light shows atomistic features behaving in "a thermodynamic sense, as if it consisted of mutually independent energy quanta" (Einstein, 1905, p. 102).

An important step forward was made by the end of 1908, when Einstein came up with a new argument in favor of the light quanta hypothesis. Einstein studied the energy fluctuations of radiation enclosed in a cavity (Einstein, 1909a). Let us consider radiation inside an isothermal enclosure at a constant temperature, and take the radiation system to be composed of two parts one of them with a small volume v (and the other with a volume V). The idea is to determine the (mean square) energy fluctuation in v of the instantaneous energy η from the equilibrium value η_0. Denoting the entropies of the two parts as Σ and σ (for the volume v), and taking Σ_0 and σ_0 to be the equilibrium values, the total entropy can be written as

$$S = \Sigma + \sigma = \Sigma_0 + \sigma_0 + \left\{\frac{d(\Sigma+\sigma)}{d\varepsilon}\right\}_0 \varepsilon + \frac{1}{2}\left\{\frac{d^2(\Sigma+\sigma)}{d\varepsilon^2}\right\}_0 \varepsilon^2 \cdots,$$

where $\eta = \eta_0 + \varepsilon$. By taking V to be much larger than v, the deviation of the entropy from its equilibrium value is given by

$$\Delta S = \frac{1}{2}\left\{\frac{d^2(\Sigma+\sigma)}{d\varepsilon^2}\right\}_0 \varepsilon^2,$$

to second order in ε. By combining this result with Einstein's reinterpretation of the Boltzmann principle it is possible to obtain the probability of an energy fluctuation between ε and $\varepsilon + d\varepsilon$ (Klein, 1964, pp. 10-11):

$$dW = const. \cdot e^{-\frac{1}{2}\frac{N}{R}\left\{\frac{d^2\sigma}{d\varepsilon^2}\right\}_0 \varepsilon^2} \cdot d\varepsilon \ .$$

From this it is immediate to determine

the mean value $\overline{\varepsilon^2}$ of the square of the energy fluctuation of the radiation occurring in v

$$\varepsilon^2 = \frac{1}{\frac{N}{R}\left\{\frac{d^2\sigma}{d\varepsilon^2}\right\}_0} \text{. (Einstein, 1909a, p. 365)}$$

The essential point now is to consider the Planck's law as empirically given and use it to calculate σ. After a simple calculation, Einstein obtained the result

$$\varepsilon^2 = \frac{R}{N\kappa}\left\{\nu h\eta_0 + \frac{c^3}{8\pi\nu^2 d\nu} \cdot \frac{\eta_0^2}{v}\right\},$$

for the mean value of the fluctuations of the radiation energy present in v.

According to Einstein, from the classical Maxwell-Lorentz electrodynamics we would expect only to obtain the second term. The appearance of the first term was a new piece of evidence for the light quanta hypothesis. According to Einstein "the first term, if present alone, would yield a fluctuation of the radiation energy equal to that produced if the radiation consisted of point quanta of energy hν moving independently of each other" (Einstein, 1909a, p. 366). Einstein made a first remark on his results, mentioning that it was as though there was two independent causes for the energy fluctuations: "the formula says that in accordance with Planck's formula the effects of the two causes of fluctuation mentioned act like fluctuations (errors) arising from mutually independent causes (additivity of the terms of which the square of the fluctuation is composed)" (Einstein, 1909a, p. 369).

In a conference held at Salzburg in September 1909, Einstein made further remarks related to his results. At this conference Einstein set forward the idea of a dual character of light:

> light possesses certain fundamental properties that can be understood far more readily from the standpoint of Newton's emission theory of light than from the standpoint of the wave theory. It is my opinion that the next stage in the development of theoretical physics will bring us a theory of light that can be understood as a kind of fusion of the wave and emission theories of light. (Einstein, 1909b, p. 379)

Einstein proposed a tentative model in which each light quantum could be regarded as a singularity in space surrounded by a field. This was meant simply as a suggestion to make plausible the idea that "the two structural properties (the undulatory structure and the quantum structure) simultaneously displayed by radiation according to the Planck formula should not be considered as mutually incompatible" (Einstein, 1909b, p. 394).
A theory taking into account the dual nature of light would have to wait for the development of quantum mechanics.

In two articles published in 1925, Heisenberg's formalism – based on a particular law of multiplication of quantum-theoretical quantities derived by correspondence

arguments – was developed with more formal mathematics by using matrices (van der Waerden, 1967, pp. 36-57; Sánchez Ron, 2001, pp. 419-443). In these articles the question of the quantization of the electromagnetic field was considered. In the first article an unsuccessful attempt was made to treat a quantized electromagnetic field in interaction with a Hertzian dipole oscillator (Mehra & Rechenberg, 2000, p. 200; Darrigol, 1986, p. 220). The advance brought by this method was made clearer in the second article, where in the last section Jordan treated solely the situation of a free electromagnetic wave in a cavity. In a mathematically unrigorous way, Jordan was able to obtain Einstein's formula of 1909 for the average squared energy fluctuations in radiation (Darrigol, 1984, p. 450; Darrigol, 1986, p. 221-222). To arrive at this result Jordan took advantage of the possibility to treat a wave as an infinite set of linear harmonic oscillators corresponding each to a normal mode of the wave. By using the recently formulated formalism of matrix mechanics it was a simple task to quantize a system of independent linear harmonic oscillators (Kramers, 1964, p. 422), which corresponds to imposing the quantum commutation conditions to each normal mode (Schweber, 1994, p. 11).

To avoid calculational complications Jordan considered the simplified case of a one-dimensional string fixed at both ends of the cavity. The lateral displacement u (x, t) of a string with length l is given, when expressed as a Fourier series, by

$$u(x,t) = \sum_{\kappa=1}^{\infty} q_k(t) \sin \kappa \frac{\pi}{l} x \,.$$

The energy in a part (0, a) of the string is given by

$$E = \frac{1}{2} \int_0^a \sum_{j,\kappa=1}^{\infty} \left\{ \dot{q}_j \dot{q}_k \sin j\frac{\pi}{l} x \ \sin \kappa \frac{\pi}{l} x + q_j q_k \, jk \left(\frac{\pi}{l}\right)^2 \cos j\frac{\pi}{l} x \ \cos \kappa \frac{\pi}{l} x \right\} dx \quad .$$

Using the previous expression, the fluctuation in the energy is given by

$$\overline{\Delta^2} = \frac{\overline{E^2}}{2a} \,.$$

This is exactly the term in Einstein's derivation resulting form the interference of classical electromagnetic waves.

Up till now this is a totally classical derivation applied to any classically described wave phenomena. Going over to quantum mechanics the previous expressions for u(x, t) and E become matrix equations. The coefficients of the Fourier expansion q_k become matrix elements q_k (n, m) which vanish except when

$n_j - m_j = 0$ for $j \neq k$,

$n_k - m_k = \pm 1$.

Following a straightforward quantum mechanical calculation Jordan now obtained the result Einstein had obtained for the fluctuation in the energy by purely statistical methods:

$$\overline{\Delta^2} = h\nu\bar{E} + \frac{\overline{E^2}}{z_\nu V} \quad ,$$

where z_ν is the number of characteristic frequencies in the interval $d\nu$ and V is the volume that contains the string.

The most important aspect of this, otherwise straightforward, procedure was the conceptual implications brought with it. As said before, in the procedure followed by Jordan " each individual eigenvibration [normal mode] is to be treated as a simple linear oscillator" (Born, Heisenberg & Jordan, 1925, p. 375). The fundamental conceptual change was that "Jordan saw that he could relate light quanta to wave excitations, and elucidate Bose's counting as the natural counting for quantized waves … Furthermore, energy discontinuities in the field appeared as properties of radiation itself, and not of the material emitters" (Darrigol, 1986, p. 221). That is, Jordan found a relation between the light quanta concept of Einstein satisfying Bose-Einstein statistics – light quanta that cannot be seen as classical independent particles, but that show statistical dependence – with the quantized normal modes of the electromagnetic field. According to Jordan, "so strong an association between the eigenvibrations of a cavity and the light quanta postulated formerly can nonetheless be drawn that every statistics of cavity eigenvibrations corresponds to a definite statistics of light quanta and conversely" (Born, Heisenberg & Jordan, 1925, p. 376). Also we have that

> the states of the system of oscillators [corresponding to the normal modes of the electromagnetic field] can be characterized by 'quantum numbers' n_1, n_2, n_3,… of the individual oscillators, so that apart from a additive constant the energies of the individual states are given by $E_n = h\sum_k \nu_k n_k$. (Born, Heisenberg & Jordan, 1925, p. 377)

Following Jordan we must also see n_1, n_2, n_3,... as the number of light-quanta (photons) inside the cavity with a frequency ν_1, ν_2, ν_3,….

Further developments were made by Dirac. In his 'The quantum theory of the emission and absorption of radiation', published in February 1927, Dirac developed a quantum treatment of the electromagnetic field from two different approaches, which at the quantum level gave the same mathematical result. In the final part of his paper he extended Jordan's initial work on the quantization of the electromagnetic field (Schweber, 1994, pp. 9-11). However, the main aspect of Dirac's work was not the quantization of a wave; on the contrary his paper is mainly a treatment of an assembly of identical quantized particles. As we have already seen, for Dirac this method, later called 'second quantization', turns out to be simply a different procedure to impose the Bose-Einstein statistics on the particles. He could instead have simply selected symmetrical wave functions as the physically admissible wave functions for this type of particle (Dirac, 1926, p. 672).

Dirac started with an assembly of N similar independent particles (subject to an interaction with an atomic system), whose wave function, solution of the Schrödinger equation, is $\psi = \Sigma_r a_r \psi_r$ (where ψ_r is the eigenfunction of a particle in the state r). Dirac took the expansion coefficients a_r to be canonical conjugates. Working with the canonical variables $b_r = a_r e^{-iw_r t/\hbar}$ and $b_r^* = a_r^* e^{iw_r t/\hbar}$ (where w_r is the energy of a particle in the state r), Dirac assumed that these variables were "q-numbers satisfying the usual quantum conditions instead of c-numbers" (Dirac, 1927a, p. 251). This gives the false impression that an additional quantization scheme is being used, but what is being done is changing from a configuration space representation to an occupation number representation (Cao, 1997, pp. 166-167). The commutation relation $[b_r, b_s^*] = \delta_{rs}$ holding

between b_r and b_r* serves to impose the symmetrization of the wave functions. This implies that the particles obey Bose-Einstein statistics (Dirac, 1927a, pp. 252-255; Schweber, 1994, p. 28).

As mentioned previously, in the final part of his work Dirac considered the quantization of a classical electromagnetic wave. Starting with the classical Hamiltonian describing an atom in interaction with radiation, the field was described by canonical variables, which in the quantization procedure were taken to be q-numbers satisfying the usual quantum commutation relations. Dirac took the field to be described by "the canonical variables N_r, θ_r, of which N_r is the number of quanta of energy of the component r, θ_r, is its canonically conjugate phase, equal to $2\pi h\nu_r$ times ϕ_r [as determined by $\dot{\phi}_r = \partial H / \partial E_r = 1$, where H is the field's Hamiltonian, and E_r is the energy of a component labelled r]" (Dirac, 1927a, p. 244). We see here Dirac following Jordan's interpretation of the normal modes of the field in terms of the number of light-quanta associated to each eigenvibration.

With this procedure Dirac obtained a Hamiltonian for the quantized system, which was, according to his view, consistent with the Hamiltonian obtained using the particle view (Dirac, 1927a, p. 263). Dirac considered that this work demonstrated the equivalence between a quantized electromagnetic wave and a system of bosons (light-quanta). Implicit in this conclusion is the identification of the quanta of energy with the particles (light-quanta). In order to get this result, a particle cannot cease to exist when it is apparently absorbed, or be created when it is emitted. It is therefore necessary to have an infinite sea of light-quanta (photons), in a state in which their momentum and energy are zero, from which the particle can jump from or into (Cao, 1997, pp. 163-164; Dirac, 1927a, p. 261).

In his approach to the quantization of a classical electromagnetic wave, Dirac "resolved the radiation into its Fourier components, and supposed that their number is very large but finite. Let each component be labelled by a suffix r … each component r can be described by a vector potential k_r chosen so as to make the scalar potential zero" (Dirac, 1927a, p. 262). That is, in modern term, Dirac quantized the vector potential in the Coulomb gauge. This meant to consider the vector potential (usually taken in classical electrodynamics to be a subsidiary concept when compared with the electric and magnetic fields) as an operator, and in this way more fundamental quantum-mechanically than the electric and magnetic fields strengths. This had never been tried before (Kragh, 1990, p. 126).

Another important contribution in the development of a quantum theory of the electromagnetic field (and its interaction with matter) was made in 1928. In parallel with a line of work based on the quantization of de Broglie waves (mentioned in the previous chapter), Jordan worked out with Pauli a relativistic quantization of the free electromagnetic field. Dirac's quantization method was not relativistically invariant (as was also the case with Jordan's quantization of de Broglie waves).

The fields, taken to be in a cavity of volume V, were expanded in Fourier series, each term corresponding (mathematically) to a harmonic oscillator

$$\mathbf{E}_k = i(\hbar\omega_\kappa/2V)^{1/2}\, \boldsymbol{\varepsilon}_\alpha\{a_{k,\alpha} \exp(-i\omega_k t + i\mathbf{k}.\mathbf{r}) - a^*_{\kappa,\alpha} \exp(i\omega_k t - i\mathbf{k}.\mathbf{r})\},$$

$$\mathbf{B}_k = i(\hbar/2V\omega_\kappa)^{1/2}\, \mathbf{k} \times \boldsymbol{\varepsilon}_\alpha\{a_{k,\alpha} \exp(-i\omega_k t + i\mathbf{k}.\mathbf{r}) - a^*_{k,\alpha} \exp(i\omega_k t - i\mathbf{k}.\mathbf{r})\}$$

($\boldsymbol{\varepsilon}_\kappa$ is a unit linear polarization vector), where the operators for the total electric and magnetic fields are given by

$$E = \sum_k E_k \,,$$

$$B = \sum_k B_k \,.$$

The amplitude (normal mode) coefficients were taken to be operators satisfying the commutation relations:

$$[a_{k,\alpha}, a^*_{k',\alpha}] = \delta_{kk'}\delta_{\alpha\alpha},$$

$$[a_{k,\alpha}, a_{k',\alpha'}] = [a^*_{k,\alpha}, a^*_{k',\alpha'}] = 0.$$

From this it follows immediately (as in the simplified case taken by Jordan in 1925) that the energy of the quantized electromagnetic wave is given by

$$E = \sum_k N_{k,\alpha}\hbar\omega_k \,,$$

where $N_{k,\alpha}$ is the number of light quanta in a state with momentum k and polarization α.

From these commutation relations, Jordan and Pauli determined the commutation relations for the electric and magnetic fields strengths themselves:

$$\left[E_j(r,t), E_k(r',t')\right] = 4\pi i\hbar c\left[\frac{\delta_{jk}}{c^2}\frac{\partial}{\partial t}\frac{\partial}{\partial t'} - \frac{\partial}{\partial r_j}\frac{\partial}{\partial r_k}\right]\cdot D(r-r', t-t') \,,$$

$$\left[E_j(r,t), E_k(r',t')\right] = \left[B_j(r,t), B_k(r',t')\right],$$

$$\left[E_x(r,t), B_y(r',t')\right] = -\left[B_x(r,t), E_y(r',t')\right] = -4\pi i\hbar c\frac{\partial}{\partial z}\frac{\partial}{\partial t'}D(r-r', t-t') \,,$$

with cyclic permutations of x, y and z in this last expression.

Essential to achieve the goal of an expression that was manifestly relativistically invariant, was the introduction by Pauli of a relativistic generalization D (r, t) = $1/4\pi r$ $\{\delta(r + ct) - \delta(r - ct)\}$ of the Dirac delta-function $\delta(r)$ appearing in the non-relativistic commutation relations (Mehra & Rechenberg, 2000, p. 220).

By that time, Pauli and Heisenberg were considering the possibility of trying to develop a relativistic quantum electrodynamical theory picking up Jordan's idea on the quantization of matter and radiation fields. By taking into account correspondence ideas (Miller, 1994, p. 31; Mehra & Rechenberg, 2000, p. 318; Darrigol, 1984, p. 484), in 1928 Pauli and Heisenberg took as their theoretical starting point the classical Lagrangian field theory of continuous systems (that can be applied for example to classical sound waves). In general the Lagrangian density for a classical field can be written as

$$L = L(\psi_\alpha, \text{grad}\,\psi_\alpha, \dot{\psi}_\alpha).$$

By calculating the conjugate momentum of each field (described, as Dirac did, by the scalar and vector potentials), the quantization of the field followed from imposing commutation relations between field components and their canonically conjugate momentum. The canonical momentum π_α conjugated to each field component is

$$\pi_\alpha = \frac{\partial L}{\partial \dot{\psi}_\alpha}.$$

The Hamiltonian density can be written as

$$H(\pi_\alpha, \psi_\alpha) = \sum_\alpha \pi_\alpha \dot{\psi}_\alpha - L.$$

The canonical cuantization results from treating π_α and ψ_α as operators and imposing the commutation relations:

$$[\pi_\alpha, \psi_\alpha] = \hbar/i.$$

This approach revealed itself inapplicable (as it stood) to the electromagnetic field, because the conjugate momentum of the scalar potential was identically zero. The Lagrangian density for the electromagnetic field is in terms of potentials defined as

$$L = \frac{1}{8\pi}\left[(\text{curl } A)^2 - \left(\frac{1}{c}\frac{\partial A}{\partial t} - \nabla\varphi \right)^2 \right].$$

We do not have $dA_4/dt = id\varphi/dt$ in the expression for L (where φ is the scalar potential). This implies that its conjugate momentum $\pi_4 = 0$. From this we have the commutation relation $[\pi_4, \psi_4] = 0$, instead of $\hbar/i$. This made impossible the quantization of the electromagnetic field by this method.

In January 1929, Heisenberg came up with a formal trick that made it possible to circumvent this difficulty and quantize the electromagnetic field; it consisted in adding a new term to the electromagnetic field Lagrangian depending on a parameter ε that was taken to zero ($\varepsilon \to 0$) in the end of the calculations (Darrigol, 1984, p. 484; Schweber, 1994, p. 41):

$$L' = \frac{\varepsilon}{2}\left(\frac{\partial \varphi_\alpha}{\partial x_\alpha} \right)^2.$$

In their work Pauli and Heisenberg demonstrated the equivalence of their quantization method, when applied to the free electromagnetic field, with the previous procedure adopted in the work of Pauli and Jordan (Mehra & Rechenberg, 2000, pp. 322-323). When Pauli and Heisenberg sent their work to publication in 19 march 1929, it was still very incomplete, in particular it was lacking clear applications (Mehra & Rechenberg, 2000, p. 326), and it did not deal with the problem of the infinite self-energy of the charged particles, which was simply discarded (Miller, 1994, p. 34).

Independently of the Pauli and Heisenberg approach, in 1929, Enrico Fermi developed a more straightforward approach in which, contrary to Dirac's 1927 work, not only the radiation field was quantized, but the full electromagnetic field described by the vector and scalar potentials, which can be seen as the components of a covariant four-vector electromagnetic potential (in modern terms Dirac worked in the Coulomb gauge, where only the two components of the transverse radiation field are quantized). To achieve this goal Fermi considered "an electromagnetic field of the most general type" (Fermi 1932, 125; see also Fermi, 1929), using the d'Alembert equation for the vector and scalar potentials: $\Box A_\mu = j_\mu$. To make this equation equivalent to Maxwell's equations, Fermi had to take into account the so-called Lorentz condition $\partial_\mu A^\mu = 0$, which he regarded as a condition to be satisfied by the field operators. Making a Fourier expansion of the vector and scalar potentials, Fermi easily obtained a Hamiltonian depending on the charged particle variables and the coefficients of the Fourier series expansions of the electromagnetic potentials. From this a quantization procedure was immediately possible: "it is sufficient to consider the Hamiltonian expression as an operator in which, according to the usual rules, the momenta are equivalent to the operator of differentiation with respect to the corresponding coordinate and to multiplication by – h/2πi" (quoted in Schweber, 1994, p. 74).

In the months following their first paper on quantum electrodynamics, Pauli and Heisenberg improved their approach, in particular avoiding formal tricks like the use of the ε parameter and others (Carson, 1996, pp. 111 & 113). The key was gauge invariance. According to Pauli:

> In the new paper of Heisenberg and myself it will be shown that exactly with the help of gauge invariance these ε-terms can be avoided. As gauge invariance I consider a substitution [of the matter fields ψ and $\overline{\psi}$ and the electromagnetic potentials Φ_μ]
>
> $$\psi' = e^{i\lambda}\psi,\ \psi' = e^{-i\lambda}\overline{\psi},\ \Phi'_\mu = \Phi_\mu - \frac{\partial\lambda}{\partial x_\mu},$$
>
> where λ may even be a q-number but one connecting with ψ and $\overline{\psi}$ on every space-like section t = const. (Quoted in Mehra & Rechenberg, 2000, p. 328)

By taking into account gauge invariance, Pauli and Heisenberg were able to adopt a gauge that made the calculations simpler, the Coulomb gauge, already used (implicitly) by Dirac in 1927, in this way avoiding the use of artificial parameters in the quantization procedure. Since they dominated the aspect of proving the relativistic invariance of the formalism, they were able to show that the Coulomb gauge, which is not manifestly covariant, did not affect the relativistic invariance of the theory: "all statements about gauge invariant quantities satisfy the condition of relativistic invariance" (quoted in Mehra & Rechenberg, 2000, p. 329). They also showed that their formalism reduced to Dirac's theory in the non-relativistic limit (Mehra & Rechenberg, 2000, p. 330).

In this second work, Pauli and Heisenberg noticed Fermi's note on quantum electrodynamics, and re-worked it using their Lagrangian formalism instead of the Hamilton formalism adopted by Fermi. They showed that by changing the electromagnetic Lagrangian by the term $-1/2\ (\partial A_\mu/\partial x_\mu)^2$ the d'Alembert equation used by Fermi as his starting point could be derived. Also they noticed that the subsidiary condition $\partial_\mu A^\mu = 0$ (which implied working in the Lorentz gauge) necessary to make the d'Alembert equation equivalent to Maxwell's equations, could not, as Fermi initially

thought, be imposed as an operator identity but solely as a supplementary condition on admissible state vectors: $(\partial_\mu A^\mu)\Psi = 0$ (Schweber, 1994, p. 75).

Fermi in part elucidated the physical meaning of the subsidiary condition in a subsequent note. Contrary to Dirac's work of 1927, in Pauli and Heisenberg's first paper they did not consider solely the radiation field (described by a transverse vector potential with two degrees of freedom, corresponding to two polarizations perpendicular to the direction of propagation of the wave), but like Fermi they considered the four degrees of freedom associated with the full vector and scalar potentials (Carson, 1996, p. 110). But they did not discuss the relation between the scalar and vector potentials adopted and the transverse vector potential of the radiation field (Carson, 1996, p. 112). Neither did Fermi address this point in his first note, he solely mentioned that he wanted to develop a more general theory than Dirac's by taking into account the full electromagnetic interaction. Some elucidation on the role of the non-transverse components of the four-vector electromagnetic potential was given by L. Rosenfeld also in 1929 by showing (choosing a particular reference frame) that the four polarizations of each normal mode can be put in a simple relation to the wave vector: two components corresponding to transversely polarized light, one to a longitudinal polarization and another to a time-like polarization (Carson, 1996, p. 113; Källén, 1972, p. 19).[16]

Adopting Pauli and Heisenberg's view on the condition to be imposed on the available states, Fermi knew that this subsidiary condition "determine[s] the form of the dependence" (Fermi, 1932, p. 130; see also Fermi, 1930) of the system's wave function on the scalar potential and the longitudinal component of the vector potential. Knowing this, Fermi also developed an approach where "the coordinates Qs and χs representing the scalar potential and one component of the vector potential are completely eliminated" (Fermi, 1932, p. 131; see also Fermi, 1930). By this procedure Fermi obtained a Hamiltonian whose electromagnetic part had a term corresponding to a transverse (radiation) field and a term corresponding to the Coulomb interaction between the charged particles (this procedure corresponds to going from the Lorentz gauge to the Coulomb gauge).[17] With this approach, Fermi showed that we can regard the scalar and longitudinal components of the field – that are not independent degrees of freedom of the field as implied in the subsidiary condition – as a representation of the Coulomb interaction between charged particles.

At this point the problem of the quantization of the electromagnetic field in interaction with charges was basically settled. In more general terms the theory of quantum electrodynamics was still very imperfect; the problem of the infinite self-energy of the charged particles was not solved. In fact, the theory faced even more problems with divergences in the calculations (Schweber, 1994, chapter 2). In practice, only a few second-order calculations using perturbation theory were available (Pais, 1986, pp. 374-376). The 'serious' divergences in the theory (Jauch & Rohrlich, 1976, pp. 174-175) were only circumvented in the late forties with the renormalization program, which made possible to obtain finite results in higher-order calculations. This was done by attaching the higher-order contributions – that from a physical point of

[16] This situation already occurs (as should be expected) in classical electrodynamics. For each normal mode we can always choose a particular reference frame in which the electromagnetic potential is represented by two transverse, one longitudinal and one time-like components, and due to the Lorentz condition, the contribution of the longitudinal and time-like components compensate each other (Bogoliubov & Shirkov, 1959, pp. 55-57).

[17] This result is not particular to the quantum theory of the electromagnetic field; it is also derived in the classical theory when considering the Fourier expansion of the field produced by charges, and not only the free radiation field (Landau & Lifshitz, 1971, pp. 124-125).

view should be smaller and smaller, but that in the mathematical calculations appear in integrals that are divergent – to the mass and charge of the electrons (and positrons), whose values are not determined by the theory but from experiments (Pais, 1986, pp. 374 & 462).

The quantization of the electromagnetic field in the (manifestly covariant) Lorentz gauge as realized by Fermi, Pauli and Heisenberg, with the adopted Lorentz subsidiary condition, showed not to lead to any incongruence in practical applications, as can be seen in the work done in the forties by R. P. Feynman (Carson, 1996, pp. 128). In his approach Feynman always considered that a "photon can be polarized in any one of the four directions" (Feynman, 1961, p. 122). This was no fortuitous event. Feynman wanted a scheme that was relativistically invariant: "Everything I was computing was covariant. The way others had formulated everything, they had separated the Coulomb potential and the transverse waves … I knew which terms went together … and how to generalize to four dimensions from the two transverse dimensions" (quoted in Mehra, 1994, p. 229). Nevertheless when looking closely at the consequences of the subsidiary condition adopted in the quantum electrodynamics developed by Fermi, Pauli and Heisenberg, this approach is strictly speaking not consistent (Pais, 1986, p. 355). A solution to the inconsistency was given around 1950 by the development of a formalism based on the use of an indefinite metric for the Hilbert space (Schweber, 1961, pp. 245-251). But in the usual way in which covariant calculations are done, where the four polarizations of the field are simultaneously taken into account – a typical case being the description of the electron-electron interaction –, the indefinite metric operator does not appear explicitly (Heitler, 1954, pp. 129-130). This gives an *a posteriori* justification for the procedure of Feynman and others.

3 The quantization of the electromagnetic field

In simple terms, the quantization of the electromagnetic field can be presented as follows. In the case of an electromagnetic field in a region free of charges, the Maxwell Lorentz equations are:

$$\nabla \cdot \mathbf{E} = 0$$

$$\nabla \times \mathbf{B} = \frac{\partial \mathbf{E}}{c \partial t}$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{c \partial t}.$$

From the second pair of equations we see that the electric and magnetic fields (strenght) can be defined in terms of a scalar and vector potentials $\phi(\mathbf{x},t)$ and $\mathbf{A}(\mathbf{x}, t)$:

$$\mathbf{B} = \nabla \times \mathbf{A}$$

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{c \partial t}.$$

This enables us to write down Maxwell-Lorentz equations for free space in terms of the scalar and vector potentials. In a four-vector notation we have that the Maxwell-Lorentz equations become

$$\left(\frac{\partial^2}{c\partial t^2} - \nabla^2\right)A_\mu - \frac{\partial}{\partial x_\mu}\left(\frac{\partial A_\nu}{\partial x_\nu}\right) = 0 \cdot$$

The potentials are not uniquely determined, since it is possible to leave the fields unaltered when doing the following transformation

$$A_\mu \rightarrow A'_\mu = A_\mu + \frac{\partial \Lambda(x)}{\partial x_\mu},$$

(where $\Lambda(x)$ is an arbitrary function). This means the theory is invariant regarding what is called a gauge transformation (of the second kind). The Maxwell-Lorentz equations in free space can be simplified in a manifestly covariant way by taking the potential to satisfy the so-called Lorentz condition $\partial_\mu A^\mu(x) = 0$. In this case the Maxwell-Lorentz equations reduce to the wave equation $\Box A_\mu = 0$ (the d'Alembert equation in the free charge case).

In the quantization of the electromagnetic field we take initially the components of the four-vector-potential to be independent, that is, we disregard the Lorentz condition. We then make a Fourier expansion (in terms of a complete set of solutions of the wave equation) of the free electromagnetic field (as given by the four-vector potential) $A_\mu(x)$:

$$A_\mu(x) = A_\mu^{+}(x) + A_\mu^{-}(x)$$

$$A_\mu^{+}(x) = \sum_{\mathbf{k}}\sum_{r=0}^{3}\left(\frac{\hbar c^2}{2V\omega_{\mathbf{k}}}\right)^{1/2} \varepsilon_r^\mu(\mathbf{k}) a_r(\mathbf{k}) e^{-ikx}$$

$$A_\mu^{-}(x) = \sum_{\mathbf{k}}\sum_{r=0}^{3}\left(\frac{\hbar c^2}{2V\omega_{\mathbf{k}}}\right)^{1/2} \varepsilon_r^\mu(\mathbf{k}) a_r^*(\mathbf{k}) e^{ikx}.$$

For each k there are four independent mutually orthogonal unit vectors or 'polarizations'. It is useful to choose the vectors as given by $\varepsilon^\mu{}_0(\mathbf{k}) = (1, 0, 0, 0)$, and $\varepsilon^\mu{}_r(\mathbf{k}) = (0, \varepsilon_r(\mathbf{k}))$, with r = 1, 2, 3, where $\varepsilon_1(\mathbf{k})$ and $\varepsilon_2(\mathbf{k})$ are mutually orthogonal unit vectors also orthogonal to $\mathbf{k}$, and $\varepsilon_3(\mathbf{k})$ is a unit vector longitudinal to $\mathbf{k}$. With this choice, the vector-potential dependent on $\varepsilon^\mu{}_1(\mathbf{k})$ and $\varepsilon^\mu{}_2(\mathbf{k})$ refers to transversely polarized light; the vector-potential dependent on $\varepsilon^\mu{}_3(\mathbf{k})$ refers to a longitudinal polarization; and the vector-potential dependent on $\varepsilon^\mu{}_0(\mathbf{k})$ refers to a so-called scalar or 'time-like' polarization.

Up till now we are still in the classical realm. By imposing equal time canonical commutations on the vector potentials, the Fourier expansion coefficients become operators satisfying the commutation relations

$$[a_r(\mathbf{k}), a^*{}_s(\mathbf{k}')] = \zeta_r \delta_{rs} \delta_{\mathbf{k}\mathbf{k}'}$$

$$[a_r(\mathbf{k}), a_s(\mathbf{k}')] = [a^*{}_r(\mathbf{k}), a^*{}_s(\mathbf{k}')] = 0,$$

where $\zeta_r = 1$ for r =1, 2, 3 and $\zeta_0 = -1$ for r = 0. Following the Gupta-Bleuler approach, $a^*_r(\mathbf{k})$ are taken to be creation operators and $a_r(\mathbf{k})$ as absorption operators, even if in the case r = 0 their role seems to be interchanged due to the minus sign. This would mean that $A_0(x)$ is an anti-Hermitian operator. In the Gupta-Bleuler method, this problem does not arise due to the use of an indefinite metric. The number operators are defined as $N_r(\mathbf{k}) = \zeta_r a^*_r(\mathbf{k})a_r(\mathbf{k})$, implying that the total energy operator is given by

$$H = \sum_{\mathbf{k}} \sum_{r=0}^{3} \hbar\omega_{\mathbf{k}} \xi_r a^*_r(\mathbf{k}) a_r(\mathbf{k}) \cdot$$

With this choice of absorption and creation operators, and corresponding definition of number and energy operators there is a consistent interpretation of these operators, because we do not have any negative number of photons or energy appearing (due to the scalar photons). However there would be a problem of having states of the quantized field with negative norm. Still we must recall that we are taking the creation and absorption operators to be independent, and that cannot be the case, since we must take into account Lorentz condition. In the Gupta-Bleuler method, use is made of a Lorentz condition ($\partial_\mu A^{\mu+}(x)\psi = 0$) less stringent than its classical counterpart. This is necessary to have no contradiction with the commutation relations. The subsidiary condition selects the physically realizable states, all with a positive-defined norm, in which we have $[a_3(k) - a_0(k)]\psi = 0$. This implies that the physical states have an admixture of longitudinal and scalar photons. As a result of this constraint regarding longitudinal and scalar photons, all observable quantities of the field in free space will depend only on the transverse photons. For example the expectation value of the energy is given by

$$\langle \psi | H | \psi \rangle = \langle \psi | \sum_{\mathbf{k}} \sum_{r=1}^{2} \hbar\omega_{\mathbf{k}} \xi_r a^*_r(\mathbf{k}) a_r(\mathbf{k}) | \psi \rangle \cdot$$

This does not mean that the longitudinal and scalar photons are irrelevant. In reality they cannot be seen as independent dynamical degrees of freedom of the field as the transverse part is. When considering for example the electron-electron scattering the longitudinal and scalar photons represent (in a covariant way) the Coulomb interaction between the electrons.

With this approach it is guaranteed that the Hamiltonian (energy) operator cannot have negative values. This means that we have a lower bound to the energy of the quantized electromagnetic field. As is easily seen from the previous expression the state corresponding to the lowest value of energy is a state with no transverse photons. This does not impose any restriction on the number of time-like and longitudinal photons in this ground state (besides the one provided by the subsidiary condition that implies there is an equal number of them in the allowed states). However states with different admixtures of time-like and longitudinal photons correspond to a particular choice within the Lorentz gauge, since the Lorentz condition does not specify the potential uniquely (Mandl & Shaw, 1984, p. 89). This means that there really is no physical difference between 'different' ground states with different admixtures of non-transverse photons (Schweber, 1961, p. 251; Källén, 1972, p. 42). In this way, we may simply characterize the ground state (without choosing a particular Lorentz gauge) by requiring the occupation number for the transverse photons to be zero (Jauch & Rohrlich, 1976, p. 47). The classical counterpart of this ground-state is simply the space vacuum: a region of space without any electromagnetic field.

4 The Casimir effect and formal aspects related to the vacuum state

Contrary to the classical case, the ground state of the (free) quantized electromagnetic field is presented as having quite a few very 'visible' physical effects, in particular the so-called Casimir effect. In the usual interpretation of the Casimir effect the ground state of the electromagnetic field could have a dynamical effect on macroscopic conducing plates located face to face, in the form of an attractive force between the plates. Another so-called (electromagnetic) vacuum effect would be the spontaneous emission of radiation by atoms in an excited state without radiation present (Aitchison, 1985, pp. 342-345; Milonni, 1994, pp. 79-111). A different physical interpretation can be given to these (and others) so-called vacuum effects without explicit resort to the ground state of the field (e.g. Milonni, 1994, pp. 115-138; Zinkernagel, 1998, 48-60). I will look only into the case of the Casimir effect.[18]

When considering the quantization of the electromagnetic field (or even a simple harmonic oscillator) the canonical quantization procedure does not enforce a specific choice of the ordering of the creation and absorption operators appearing in the field operators, energy operators, momentum operators, etc. Following Dirac (1958, pp. 84-88) we may recall that in classical mechanics a dynamical system can be described in terms of generalized coordinates q_j and momenta p_j. Let u and v be two dynamical variable functions of q_j and p_j. The Poisson bracket of these two functions is

$$[u, v] = \sum_r \left\{ \frac{\partial u}{\partial q_r} \frac{\partial v}{\partial p_r} - \frac{\partial u}{\partial p_r} \frac{\partial v}{\partial q_r} \right\}.$$

Some of the main properties of the Poisson bracket are

$$[u, v] = - [v, u],$$

$$[u, c] = 0,$$

where c is a number. In the canonical quantization procedure, a quantum equivalent of the Poisson bracket is introduced:

$$uv - vu = i\hbar[u, v],$$

where u and v are now taken to be operators. This method is the one used in the case of the quantization of the electromagnetic field (in the case of the de Broglie field anticommutation rules are used). Looking into the case of the quantization of one field mode (mathematically equivalent to the quantization of the harmonic oscillator), in terms of creation and absorption operators, we have

[18] The main difference between Zinkernagel's views and mine is that I consider that we do not need to go beyond standard quantum electrodynamics to show that the Casimir effect is not a vacuum effect. In this way I will not consider for example Schwinger's source theory (see e.g. Rugh, Zinkernagel and Cao, 1999). I will frame my discussion within standard quantum electrodynamics by considering Milonni's approach like Zinkernagel did. This does not mean that there are no other standard quantum electrodynamics calculations which enable to calculate the Casimir effect without reference to the vacuum state (see e.g. Jaffe 2003, Jaffe 2005, Graham et al. 2004). Simply, choosing Milloni's work makes it easier to see the difference between my views and Zinkernagel's.

$$H = \frac{\hbar\omega}{2}\left(aa^* + a^*a\right).$$

Since $[a, a^*] = 1$, we can write the previous expression as

$$H = \hbar\omega\left(a^*a + \frac{1}{2}\right).$$

Here we see a term $\hbar\omega/2$ corresponding to the so-called zero-point energy of the field mode. This would imply that the electromagnetic field, when in its vacuum state, would have an energy different from zero (formally infinite). This would correspond physically to the infinite sea of photons in the vacuum state prescribed by Dirac in 1927. Like in the case of electrons the sea can be dealt with by recalling (with Dirac) that energy measurements are made in relation to the ground-state energy, which enables us to set it to zero:

$$H - \langle 0|H|0\rangle = \frac{1}{2}\hbar\omega\left(aa^* + a^*a\right) - \frac{1}{2}\hbar\omega = \frac{1}{2}\hbar\omega\left(2a^*a + 1\right) - \frac{1}{2}\hbar\omega = \hbar\omega a^*a \ .$$

A different way of addressing this question is to take away any physical meaning and to see the term $\hbar\omega/2$ as resulting simply from an imprecision in the quantization procedure. In fact at a classical level there is no difference between $\hbar\omega/2(aa^* + a^*a)$ and $\hbar\omega a^*a$. This means that there is an ambiguity in the ordering of the operators, since depending on our starting classical expression we obtain a different quantum Hamiltonian. In this way we can consider the zero-point energy as an artifact of an improper application of the quantization rule, and use the so-called normal ordering in which we have the operator $H = \hbar\omega a^*a$, where there is no zero-point energy (this is what I have been doing all the time). Contrary to this view, H. B. G. Casimir presented in 1948 a calculation sustaining that there are dynamical consequences of this zero-point energy.

In the quantization of the electromagnetic field space is (for practical purposes) considered to be divided in 'boxes' with a volume $V = L^3$, and one imposes on the field the periodic boundary conditions $\mathbf{A}(x + L, y + L, z + L, t) = \mathbf{A}(x, y, z, t)$. This implies (since $\mathbf{A} \sim \exp i\mathbf{k}\cdot\mathbf{r}$) that $(k_x, k_y, k_z) = 2\pi/L\ (l, m, n)$, where l, m, n are integers. It is standardly held that "this artificial periodic boundary condition will be of no physical consequences if L is very large compared with any physical dimensions of interest" (Milonni, 1994 , p. 44). If we suppose that there are two (infinite) parallel conducting plates located, say, at z = 0 and Z = d, Casimir made the heuristic move of considering that this would change the set of modes describing the quantized electromagnetic field which would not anymore be simply given by free-space plane-wave modes. This would mean that matter would affect radiation by simply changing its quantization boundary conditions.

According to Casimir since we are considering perfect conductors the tangential component of the electric field must vanish on the walls of the conductors. This implies that

$$k_x = \frac{l\pi}{L}, k_y = \frac{m\pi}{L}, k_z = \frac{n\pi}{d}.$$

In this way the allowed frequencies will be

$$\omega_{lmn} = k_{lmn}\, c = \pi c \left[\frac{l^2}{L^2} + \frac{m^2}{L^2} + \frac{n^2}{d^2} \right]^{1/2} .$$

The zero-point energy is given by

$$\sum_{l,m,n} \frac{1}{2} \hbar \omega_{lmn} = \sum_{l,m,n} \pi \hbar c \left[\frac{l^2}{L^2} + \frac{m^2}{L^2} + \frac{n^2}{d^2} \right]^{1/2} ,$$

(in the summation a factor of 2 must be considered due to the polarization, when l, m, n $\neq 0$).
The difference of the zero-point energy of the field with and without plates U(d) = E(d) – E(∞) is taken to be the potential energy of the system plates + vacuum field. That is, U(d) is now taken to be the energy required to bring the plates from a large distance to d. From the previous expression one derives the expression for the force per unit area F(d) = – U'(d) between the plates:

$$F(d) = -\frac{\pi^2 \hbar c}{240 d^4} .$$

This is, we might say, the conventional derivation of the Casimir effect as a vacuum effect. However, as P. W. Milloni and M.-L. Shih(1992) have shown, it is possible to arrive at the Casimir force between the plates without having to consider any vacuum field in the calculation. This is done simply by adopting the normal ordering of the operators and by taking explicitly into account that the conducting plates are not mathematical boundary conditions but must be considered as constituted by matter (we consider two semi-infinite dielectric slabs with dielectric constants ε_1 and ε_2 at a distance d separated by a layer with dielectric constant ε_3; the Casimir result is derived in the limiting case of a perfect conductor). There will be an induced dipole moment in each atom of the slabs induced by source fields. In the Milonni and Shih calculation the approximation that "each dipole interacts, in effect, only with its own field; this field is modified from its free-space form by the presence of all the other dipoles" (Milonni & Shih, 1992, p. 4245) was made. The energy of this system (of two dielectric slabs separated by a medium) is given by

$$\langle E \rangle = -\frac{1}{2} \int d^3 r \langle \mathbf{P}(\mathbf{r}, t) \cdot \mathbf{E}(\mathbf{r}, t) \rangle ,$$

where $\mathbf{P}(\mathbf{r}, t)$ is the polarization due to the dipoles and $\mathbf{E}(\mathbf{r}, t)$ is the electric field present. The electric field can be written as $\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0(\mathbf{r}, t) + \mathbf{E}_s(\mathbf{r}, t)$, where $\mathbf{E}_0(\mathbf{r}, t)$ is

the source-free (or vacuum) part of the electric field and $\mathbf{E}_s(\mathbf{r}, t)$ is the part due to the dipoles present. By using a normal ordering of the field operators we have

$$\langle E \rangle = -\frac{1}{2}\int d^3 r \langle \mathbf{P}(\mathbf{r}, t) \cdot \mathbf{E}_s(\mathbf{r}, t) \rangle ,$$

in which we have only source fields. Milonni and Shih then calculated the change in the energy due to an infinitesimal change δd in d, and from this the force between the dielectric slabs. The general expression is

$$F(d) = -\frac{\hbar}{2\pi^2 c^3}\int_1^\infty dp\, p^2 \int_0^\infty d\xi\, \xi^3 \varepsilon_3^{3/2} \left[\left[\frac{\varepsilon_3 s_1 + \varepsilon_3 p}{\varepsilon_3 s_1 - \varepsilon_1 p} \frac{\varepsilon_3 s_2 + \varepsilon_2 p}{\varepsilon_3 s_2 - \varepsilon_2 p} e^{2\xi p \sqrt{\varepsilon_3} d/c} - 1 \right]^{-1} + \left[\frac{s_1 + p}{s_1 - p} \frac{s_2 + p}{s_2 - p} e^{2\xi p \sqrt{\varepsilon_3} d/c} - 1 \right]^{-1} \right].$$

I will not go into the details of this expression, but simply cnote what force this approach predicts in the same case as the one considered by Casimir. We have empty space between the slabs, which means that $\varepsilon_3 = 1$; also we must consider the case of two perfectly conducting plates, which implies taking $\varepsilon_{1,2} \to \infty$. Under these conditions the previous expression reduces to

$$F(d) = -\frac{\pi^2 \hbar c}{240 d^4} ,$$

which is the Casimir force. In this way, Milonni and Shih have shown that "the Casimir effect can be understood in terms of source fields in conventional quantum electrodynamics, with no explicit reference to the zero-point energy" (Milonni & Shih, 1992, p. 4241).

A different view was taken by Simon Saunders, who wrote: "I do not think we can do without appeal to the zero-point energy in explaining the Casimir effect" (Saunders, 2002, p. 23). Saunders develops his argumentation without taking into account Milonni's work (or any other work where the Casimir effect is derived without any reference to the vacuum state). He mentions for example Lifshitz's macroscopic theory, concluding that "Lifshitz's methods are perfectly consistent with the interpretation of the effect in terms of vacuum fluctuations" (Saunders, 2002, p. 19). This is highly doubtful since as we have seen, according to Milonni & Shih, the Casimir force can "be calculated in terms of source fields, with no explicit reference to zero-point-field energy" (Milonni & Shih, 1992, p. 4241). Also they show that "the general Lifshitz expression, and therefore the Casimir force in particular, may be derived in terms of sources alone in conventional QED" (Milonni & Shih, 1992, p. 4243).

Even when agreeing with Milonni's interpretation, this does not mean that the ground state of the quantized electromagnetic field becomes a sort of 'nothingness' without any physical relevance, as when we consider the classical electromagnetic vacuum. That is not the case. As Milonni has remarked, "the vacuum field is absolutely necessary in the quantum theory of radiation, if only to preserve commutation relations and the formal consistency of the theory" (Milonni, 1994, p. 138). In the classical case

we can conceive a single dipole in empty space. In this case "the only field acting on the dipole is its own radiation reaction field" (Milonni, 1994, p. 52). The difference from the classical case is that when considering the quantized electromagnetic field "there is an 'external' field, namely, the source-free or vacuum field" (Milonni, 1994, p. 52). Milonni shows that, in contrast to the classical case, the ground state of the free electromagnetic field cannot be disregarded as soon as a charged body (which can be seen as a source of electromagnetic field) is considered, as it is necessary to take into account the source-free field variables for the preservation of the commutation relations (Milonni, 1994, p. 53).

Let us look at this in more detail. The Hamiltonian for the dipole oscillator in interaction with the quantized electromagnetic field can be written as

$$H = \frac{1}{2}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + \frac{1}{2}m\omega_0^2\mathbf{x}^2 + H_F,$$

where H_F is the field Hamiltonian, $\mathbf{x}$ is the operator corresponding to the classical coordinate of the oscillator, $\mathbf{p}$ is the operator for the dipole momentum, and ω_0 is the frequency of oscillation of the dipole. In the Heisenberg representation we have (in the electric dipole approximation):

$$\ddot{\mathbf{x}} + \omega_0^2\mathbf{x} = \frac{e}{m}\mathbf{E} = i\frac{e}{m}\sum_{\mathbf{k}\lambda}\left(\frac{2\pi\hbar\omega_k}{V}\right)^{1/2}\left[a_{\mathbf{k}\lambda}(t) - a^*_{\mathbf{k}\lambda}(t)\right]e_{\mathbf{k}\lambda},$$

$$\dot{a}_{\mathbf{k}\lambda} = a_{\mathbf{k}\lambda}(0)e^{-i\omega_k t} + ie\left(\frac{2\pi}{\hbar\omega_k V}\right)^{1/2}\int_0^t dt' e_{\mathbf{k}\lambda}\cdot\dot{\mathbf{x}}(t')e^{i\omega_k(t'-t)}$$

(where $a_{\mathbf{k}\lambda}$ and $a^*_{\mathbf{k}\lambda}$ are respectively the photon annihilation and creation operators for the field mode ($\mathbf{k}$, λ), $e_{\mathbf{k}\lambda}$ are the polarization vectors, and $\mathbf{E}$ is the electric field operator). In this way the Heisenberg equation for the operator x can be written as:

$$\ddot{\mathbf{x}} + \omega_0^2\mathbf{x} = \frac{e}{m}\mathbf{E}_0(t) + \frac{e}{m}\mathbf{E}_{RR}(t),$$

where we have

$$\mathbf{E}_0(t) = i\sum_{\mathbf{k}\lambda}\left(\frac{2\pi\hbar\omega_k}{V}\right)^{1/2}\left[a_{\mathbf{k}\lambda}(0)e^{-i\omega_k t} - a^*_{\mathbf{k}\lambda}(0)e^{i\omega_k t}\right]e_{\mathbf{k}\lambda},$$

$$\mathbf{E}_{RR}(t) = -\frac{4\pi e}{V}\sum_{\mathbf{k}\lambda}\int_0^t dt'\left[e_{\mathbf{k}\lambda}\cdot\dot{\mathbf{x}}(t')\right]e_{\mathbf{k}\lambda}\cos\omega_k(t'-t) = \frac{2e}{3c^3}\dddot{\mathbf{x}}.$$

According to Milonni,

$\mathbf{E}_0(t)$ is the free or zero-point field acting on the dipole. It is the homogeneous solution of the Maxwell equation for the field acting on the dipole, i.e. the solution, at the position of the dipole, of the wave

equation $[\nabla^2 - c^{-2}\,\partial^2/\partial t^2]\mathbf{E} = 0$ satisfied by the field in the (source-free) vacuum. For this reason $\mathbf{E}_0(t)$ is often referred to as the *vacuum field* … $\mathbf{E}_{RR}(t)$ is the source field, the field generated by the dipole and acting *on* the dipole. (Milonni, 1994, p. 52)

Considering the previous operator equation for **x** that can be written as

$$\ddot{\mathbf{x}} + \omega_0^2\mathbf{x} - \tau\dddot{\mathbf{x}} = \frac{e}{m}\mathbf{E}_0(t)$$

(where, as mentioned, $\mathbf{E}_0(t)$ is the vacuum electric field operator, and $\tau = 2e^2/3mc^3$), and the corresponding equation for the momentum operator **p**, we have the following commutation relation between the two operators

$$\left[z(t), p_z(t)\right] \cong \frac{2ei\hbar e^2}{3\pi mc^3}\omega_0^3\int_{-\infty}^{\infty}\frac{dx}{x^2 + \tau^2\omega_0^6} = \frac{2ei\hbar e^2\omega_0^3}{3\pi mc^3}\frac{\pi}{\tau\omega_0^3} = i\hbar\,,$$

as is expected according to general quantum mechanics rules. Now if we had not considered the vacuum field $E_0(t)$, then in the operator equation for x, "the operator x(t) would be exponentially damped, and commutators like $[z(t), p_z(t)]$ would approach zero for $t >> (\tau\omega_0^2)^{-1}$," (Milonni, 1994, p. 53). Because of this Milonni concluded that "the free field is in fact *necessary* for the formal consistency of the theory" (Milonni, 1994, p. 53).

This result and Milonni's derivation of the Casimir effect in the context of standard quantum electrodynamics have been questioned. In Rugh, Zinkernagel & Cao (1999, p. 129) two critical remarks are made on Milonni's (and collaborators) approach. One point is that Milonni's approach regarding the derivation of the Casimir effect as due only to source fields is not conclusive, because in higher orders of perturbative calculations we will have contributions to the vacuum energy from the so-called vacuum blob diagrams. But this is the case only when considering the 'interacting' vacuum (e.g. Rugh & Zinkernagel, 2002, p. 675), it has nothing to do with the quantized (source-free) electromagnetic field and its possible quantum states. The other point, also made in Rugh & Zinkernagel (2002, p. 683, footnote 50), is that Milonni uses the so-called fluctuation-dissipation theorem for linearly dissipative systems to arrive at his result that the source-free field is necessary for consistency reasons (i.e. the preservation of commutation relations), and this is not a sound approach. However, that is not the case, even if Milonni presents his results as an example of the theorem (see e.g. Milonni, 1988, p. 106). As we have seen the need for the source-free field for the preservation of the commutation relations is derived by Milonni without any need for the fluctuation-dissipation theorem (see e.g. Milonni, 1984, p. 342; Milonni, 1988, p. 106; Milonni 1994, pp. 50-54).[19] That is, according to Milonni, we must have simultaneously with a system consisting of charged matter a different system corresponding to the quantized free electromagnetic field, *even if only in its ground state (when considering charged matter in empty space)*. However for a different reason than the one presented by Rugh & Zinkernagel I regard Milonni's view regarding the

[19] This, as mentioned, is the main difference between Zinkernagel's views on the Casimir effect and my own. Zinkernagel considers that Milloni's work is not sound and we must go beyond standard quantum electrodynamics to show that the Casimir effect is not a vacuum effect. My view is that Milloni's work is sound and shows that we do not have to see the Casimir effect as a vacuum effect (see also Jaffe 2003, Jaffe 2005, Graham et al. 2004).

need of the free field for the formal consistency of the theory as not conclusive. The point is that Milonni arrives at his result by considering a quantum model of a dipole oscillator; it is not an *ab initio* derivation from the formalism of the theory. In this way we cannot conclude that Milonni's consistency claim follows directly from the formalism of the theory. Nevertheless, as we will see in the next sections, this (proposed) formal aspect related to the vacuum adjusts well with experimental results.

5 The physical meaning of variance

As is well known, in the ground state of the quantized electromagnetic field the expectation value of the electric and magnetic fields vanishes, that is $\langle 0|\mathbf{E}|0\rangle = \langle 0|\mathbf{B}|0\rangle = 0$, but not its variance, because $\langle 0|\mathbf{E}^2|0\rangle$ and $\langle 0|\mathbf{B}^2|0\rangle$ are non-zero in the ground state. What to make of this result? There is a tendency in the literature to refer to the non-vanishing variance as 'fluctuations' of the vacuum state (Sakurai, 1967, pp. 32-33; Aitchison, 1985, pp. 246-247). For example, according to I. J. R. Aitchison "the vacuum can now be thought of as a state in which the fields are all in their ground states, but executing random fluctuations (even at T = 0) about their zero average values" (Aitchison, 1985, p. 347). We must take some care in adopting this type of terminology. As has been noticed, we cannot associate the non-vanishing variance of the ground state of the quantized electromagnetic field to some sort of fluctuation in time: "there is no time evolution of this vacuum state" (Rugh & Zinkernagel, 2002, p. 673). I will defend here that the mathematical result of a non-vanishing variance of the quantized electromagnetic field can be given an interpretation that has a clear experimental meaning.

According to the interpretation of quantum mechanics adopted here, the non-zero variance (or its square root, the standard deviation) is determined by considering a large (ideally infinite) number of measurements performed in similarly prepared systems (Isham, 1995, pp. 80-81; Peres, 1995, pp. 24-26; Ballentine, 1998, pp. 225-227, Falkenburg, 2007, pp. 205-207). According to what C. J. Isham called the minimal interpretation of quantum theory (which as other authors I refer to as the ensemble interpretation):

> Quantum theory is viewed as a scheme for predicting the probabilistic distribution of the outcomes of *measurements* made on suitably prepared copies of a system.
>
> The probabilities are interpreted in a statistical way as referring to the *relative frequencies* with which various results are obtained if the measurements are repeated a sufficiently large number of times. (Isham, 1995, p. 80)

The view of A. Peres is that

> A *quantum system* is a useful abstraction … defined by an *equivalent class of preparations*. For example there are many equivalent macroscopic procedures for producing what we call a photon, or a free hydrogen atom, etc. The *equivalence* of different preparation procedures should be verifiable by suitable tests…. While quantum systems are somewhat elusive, quantum *states* can be given a clear *operational* definition, based on the notion of test. Consider a given preparation and a set of tests … if these tests are performed many times, after identical preparations, we find that the statistical distribution of outcomes of each test tends to a limit. Each outcome has a definite probability. We can then define a state as follows: *A state is characterized by the probabilities of the various outcomes of every conceivable test*…. Before we examine concrete examples, the notion of *probability* should be clarified. It means the following. We *imagine* that the test is performed an infinite number of times, on an infinite number of replicas of our quantum system, all identically prepared. This infinite set of experiments is called a *statistical ensemble*.

… In this statistical ensemble, the occurrence of event A has relative frequency P{A}; it is this relative frequency which is called *probability*. (Peres, 1995, pp. 24-25)

Under this view we cannot associate for example the Schrödinger wave function to a single system. We must consider a large number of identical 'quantum systems' prepared in the same way and then subjected to the same measurement procedure. From the wave function we can calculate the relative frequencies (probabilities) of particular outcomes regarding physical observables of the system.[20]

Now we can address the meaning of having $\langle 0|\mathbf{E}^2|0\rangle \neq 0$. We must consider a particular experimental setup that will enable us to make measurements on a quantum electromagnetic field. We can consider successive measurements made on a field, which can be taken to be in the same initial state at each successive measurement, or we may think in terms of different identical experimental setups being used at the same time to make measurements of identically prepared fields (in this case all in the vacuum state). Then on each of a large number of similarly prepared systems a measurement is made of the electric field. According to the adopted interpretation of the theory, there will be a frequency distribution for the results of the independent measurements according to a standard deviation of $\sqrt{\langle 0|\mathbf{E}^2|0\rangle}$ from a measurement corresponding to no transverse photos. That is, sometimes an electric field will be measured different from zero even if the electromagnetic field is in its ground-state. Is this again a formal aspect of the theory, even if a formal aspect of its interpretation? Or is there any real experiments where a measurement is made on the vacuum field and results are obtained corresponding to a frequency distribution of results deviating from 'nothingness'?

6 Experimental results on the vacuum state using the balanced homodyne detection method

In experiments using the method known as balanced homodyne detection it is possible to determine what can be interpreted as quadrature fluctuations of the vacuum or simply vacuum noise which corresponds to the non-zero standard deviation predicted by the theory (Leonhardt, 1997, pp. 23, 47 & 84-88).

In the balanced homodyne method, the signal under study is sent into one of the ports of a beam splitter. In the present case since we are making a measurement of the vacuum electromagnetic field, the port is left unused, that is, there is no external field present. The other port receives a strong coherent laser field (called the local oscillator), which will provide the phase reference for measuring the quadrature statistics of the signal field, which in this case is the vacuum.

We can write the quantum field operator for a single-mode field as

$$E_x = \left(\frac{\hbar\omega}{\varepsilon_0 V}\right)^{1/2} \left(a e^{-i\omega t} + a^* e^{i\omega t}\right) \sin(kz),$$

[20] In the appendix, I will give a presentation of part of Bohr's interpretation of quantum mechanics, providing a Bohrian reinterpretation, or better, an integrated view on Bohr's ideas, enlightening the internal consistency of Bohr's ideas, and showing its compatibility with the so-called minimal or ensemble or statistical interpretation addressed in the main text.

where ω is the frequency of the mode and k is the wave number related to the frequency according to k = ω /c. Defining the quadrature operators

$$q = \frac{1}{\sqrt{2}}(a^* + a),$$

$$p = \frac{i}{\sqrt{2}}(a^* - a),$$

the field operator can be written as

$$E_x = \sqrt{2}\left(\frac{\hbar\omega}{\varepsilon_0 V}\right)^{1/2} \sin(kz)(q\cos(\omega t) + p\sin(\omega t)).$$

The balanced homodyne detection makes it possible to make a measurement of these quadrature components of a quantum field.

The beam splitter will combine the incoming fields. Taking, for simplicity, each incoming field to be described by the mode operators a and b, the output modes are

$$c = \frac{1}{\sqrt{2}}(a + ib),$$
$$d = \frac{1}{\sqrt{2}}(b + ia).$$

After the optical mixing of the signal and the local oscillator, each beam is directed towards a photodetector, which enables a measurement of the field intensities. The photodetectors respond to the intensity of the incident light, generating the photocurrents $I_c = \langle c^* c \rangle$ and $I_d = \langle d^* d \rangle$. By assuming that the photocurrents are proportional to the photon numbers of the beams striking each detector we have that the difference $I_{21} = I_1 - I_2$ is proportional to the difference in the photon numbers of each beam

$$n_{21} = n_2 - n_1 = 2^{1/2}|\alpha| q_\theta,$$

where $|\alpha|^2$ is the intensity of the coherent field (local oscillator), and q_θ is a quadrature component of the vacuum field (signal). By changing the phase of the coherent field it is possible to measure an arbitrary quadrature of the signal field. In particular if the phase was initially chosen so as to measure X_1 by changing the phase by $\pi/2$ it is possible to measure X_2 and in this way a balanced homodyne detector enables one to measure the quadrature components defining the quantum state of the field (Gerry & Knight, 2005, pp. 167-168).

Let us see in more detail what the experiment tell us about the vacuum state. First we must recall the interpretation of the quantum formalism. If we use the balanced homodyne detector to make one measurement of a quadrature component that by itself does not give us any valuable result:

It must be distinguished between an individual (single) and an ensemble measurement (i.e. in principle, an infinitely large number of repeated measurements on identically prepared objects). Performing a single measurement on the object, a totally unpredictable value is observed in general. (Vogel & Welsch & Wallentowitz, 2001, p. 225)

In this way we need an experimental procedure that may give us the relative rate at which a particular value for a quadrature component q_θ is observed, i.e. the probability distribution pr(q, θ), where θ is the relative phase between signal and local oscillator. Thus, making a large number of measurements of the observable q_θ yields pr(q, θ), i.e. the probability distribution of its eigenvalues. In general the experimental procedure goes as follows:

The phase θ can be easily varied using a piezo-electric translator. To measure quadrature distributions, we may fix the phase angle θ and perform a series of homodyne measurements at this particular phase to build up a quadrature histogram pr(q, θ). Then the [local oscillator] phase should be changed in order to repeat the procedure at a new phase, and so on [, in such a way that we obtain results for a set of different phase angles between 0 and π]. (Leonhardt, 1997, p. 99)

The probability distribution pr(q, θ) is equal to $\langle q|U(\theta)\rho U^{*}(\theta)|q\rangle$, where ρ is the density operator (which provides the most general description of a quantum state), and $U(\theta) = \exp(-i\theta n)$ is the phase-shifting operator (where n is the photon number operator). From the experimentally obtained probability distribution pr(q, θ), it is possible to reconstruct the so-called Wigner function W(q, p), which is closely related to the density operator. In reality both can be seen as "one-to-one representations of the quantum state" (Leonhardt, 1997, p. 40). The interesting part comes now. In the case of the vacuum field (like in all others), we have a good agreement between the experimentally reconstructed Wigner function and the theoretical Wigner function (Leonhardt, 1997, pp. 46-47). In particular, if we consider the quadrature wave function of the vacuum state

$$\psi_0(q) = \pi^{-1/4}\exp\left(-\frac{q^2}{2}\right),$$

the measured quadrature probability distribution $|\psi_0(q)|^2$ "is approximately Gaussian and already follows the theoretical expectation" (Leonhardt, 1997, p. 23).

In general there is a good agreement between the theoretical predictions for several quantum states of light (e.g. single-photon Fock states and squeezed states) and the experimental results (e.g. Breitenbach & Schiller & Mlynek, 1997; Bertet et al, 2002). This gives some assurance that the results obtained in the case of the vacuum state can be taken to be a property of the vacuum state and not as resulting from some other physical origin, for example, from the matter of the photodetectors. I mention this because in these experiments we are considering a high intensity field that is treated, by correspondence arguments, as a classical field that interferes with the vacuum field, producing two different beams. As I said, each beam is directed to a photodetector. Ideally each of the two photodetectors will produce a photocurrent that is proportional to the number of photons of the beams striking each one. It would seem that we are detecting individuated photons due to the vacuum field, which would imply that the photodetectors are receiving momentum and energy from the vacuum. However we

must recall that what is being detected are the beams resulting from the interference of (what can be considered) a classical field and the vacuum field. The possible 'photons' from the vacuum are not 'differentiated' from the 'photons' from the classical field. We must take into account the usual identification of a classical field with a quantum coherent field with a large expectation value of the photon number operator. The coherent state does not have a definite number of photons. In fact it can be defined by an infinite expansion in terms of photon number states, that is, by taking into account photon states corresponding to an infinite number of photons. Due care is needed in the physical interpretation of this situation, in particular in what concerns the possibility of detection of photons in the ground state, which I consider not to be possible (and theoretically nonsense), and this makes problematic the usual quantum theory of the photodetectors based on the idea of photon absorption (Vogel & Welsch & Wallentowitz, 2001, pp. 169-190). More than questioning the experimental results regarding the vacuum electromagnetic field, this points to a need of revision of the theoretical treatment of the interaction of photodetectors with the quantized electromagnetic free field. However, I believe that there is no final and conclusive approach to address this problem. In quantum electrodynamics we face an 'intrinsic' limitation in the description of the interaction of radiation and matter (since we are only able to make approximate calculations) that leads me to consider that we cannot go beyond a 'model' level of description of the interaction between the quantized electromagnetic field and the photodetectors. However, this problem is well beyond the scope of the present work. As I said, what gives me some confidence in the interpretation of the experimental results for the quantum electromagnetic vacuum is the coherence between the interpretation of $\langle 0|\mathbf{E}^2|0\rangle$ and the experimental results obtained for different quantum states of light, including the vacuum state. We see then that we can ascribe to the vacuum state of the quantized electromagnetic field a clear operational meaning in terms of the measurement of a non-zero variance, which is consistent with the adopted interpretation of the quantum formalism.

7 Conclusions

In this chapter I am more interested in a tentative clarification (or at least in a contribution towards it) of the concept of vacuum in quantum electrodynamics than in possible philosophical ramifications of the view presented. The lengthy, but necessary, technical discussions presented show that there are intricate aspects that make it very difficult to have any strong metaphysical commitment regarding the concept of vacuum; more than exploring possible metaphysical consequences of the conceptual analysis being presented, the intention here is to provide a 'frame' within which to make clear what we should not attribute to the concept of vacuum and what we might attribute to it even if with some reservations.

We have seen that there are subtle theoretical and experimental aspects related to the ground state of the quantized electromagnetic field, which represent a clear departure from the 'nothingness' of the classical concept of vacuum. However, we must be careful not to ascribe too much to the ground state of the quantized field. One difference with the classical theory is that (if accepting Milonni's consistency claim to be generally valid) when considering a charged particle we must consider it to be at least in 'interaction' with the ground state of an *external* quantized electromagnetic field. In a certain sense the quantized radiation and matter need a more integrated description, while maintaining a clear distinction between radiation and matter. As Milonni stressed,

"without [the source-free field] the whole quantum theory of a charged particle in vacuum becomes inconsistent" (Milonni, 1994, p. 125).

As we have seen the other aspect in which the quantum concept of vacuum presents a clear departure from the classical 'nothingness' is at the experimental level. We see experimental results that for their interpretation make it necessary to take into account the concept of quantum vacuum. The view defended here is that we can deflate the so-called experimental vacuum effects to a simple aspect common to any n-photon state of the quantum field: a non-vanishing variance of the electric and magnetic fields.[21] That is, there are no dynamical effects of the vacuum state. In this way the formal considerations (pointing to the need of an external 'independent' quantized electromagnetic field even if in its ground state) and the experimental results (giving observational meaning to the mathematical expression of the variance even in the case of the vacuum state) are consistent with each other and point to a concept of vacuum that has theoretical and experimental relevance. However the only experimental results that we can attribute with relative security to the vacuum state relate to a non-vanishing variance and not to some spectacular dynamical effects. This implies that we cannot attribute any feature to the vacuum state that makes it 'special' when compared with other states of the quantized electromagnetic field. In this way, whatever metaphysical ramifications might be related to the concept of vacuum they do not go beyond the ones we might endorse in relation to any other state of the quantized electromagnetic field, which is not an unexpected result since the quantized electromagnetic field is a more fundamental concept than the particular state it might be in. Looking from this perspective, if it was the case that the vacuum state had no experimental relevance (not being possible to give an observational meaning to its variance) this would lead to an awkward situation regarding the concept of quantum field. We would be in a situation in which the physical-mathematical structure of the theory would be inconsistent with the available experimental results. On one side, for example a one photon state of the quantized electromagnetic field would have experimental meaning (and we could relate the variance to observed outcomes of measurements made on the electromagnetic field in this state) while on the other side, another state of the field, the ground state, would be a sort of a formal artifact (and in this case the variance would be a physically meaningless mathematical expression). That is not the case. Thus we see that even when not accepting dynamical fluctuations as a property of the vacuum state we can retain an experimentally meaningful notion of vacuum state that is consistent with the adopted interpretation of the variance within the ensemble interpretation of quantum theories.

[21] We must recall that this variance is related with measurements made on identically prepared systems not one individual system. As mentioned, there is a tendency in the literature to refer to the non-vanishing variance as 'fluctuations' of the vacuum state (Sakurai, 1967, pp. 32-33; Aitchison, 1985, pp. 346-247). This view is misleading since the non-zero variance of the ground state of the quantized electromagnetic field cannot be related to a fluctuation in time: "there is no time evolution of this vacuum state" (Rugh & Zinkernagel, 2002, p. 673). Considering measurements made on equally prepared systems, they will show fluctuations in the results of the successive observations – according to the interpretation of the theory followed here (Isham, 1995, pp. 80-81; Peres, 1995, pp. 24-26; Ballentine, 1998, pp. 225-227, Falkenburg, 2007, pp. 205-207). The non-vanishing variance is not a temporal property of one single system. We observe a statistical fluctuation on the results of measurements made on equally prepared systems, not a temporal fluctuation of the same system.

CHAPTER 5

THE INTERACTION OF RADIATION AND MATTER

1 introducion

The more basic and fundamental elements of quantum electrodynamics are already present in Dirac's 1927 work. In it, the electromagnetic field and matter are described by classical Hamiltonians; a further term gives the interaction between the field and matter (Jordan's reinterpretation of matter as waves or Pauli and Heisenberg's Lagrangian formalism does not change the mathematical core of the theory and procedures used in its applications). All this can be developed within a correspondence approach with classical mechanics and field theory, that is, this type of Hamiltonian can be put to use in the Maxwell-Lorentz classical electrodynamics or a classical theory of fields in interaction (Barut, 1964, p. 138; Bogoliubov & Shirkov, 1959, p. 84). Then a second 'layer' is put on top of the classical description (in the fully developed theory, matter is described by the Dirac equation) through which the quantization of the individual fields is achieved (the so-called 'second quantization'). That is, the generalized coordinates (and conjugate momenta) of each field are submitted to commutation or anticommutation relations, and the terms in the Hamiltonian for each field become operators, as is also the case for the term describing the interaction between the fields. But it is important to notice that the fields are quantized as free non-interacting fields, each by itself. Then we are into the game. For practical purposes Dirac makes use of perturbation theory to treat the interaction of radiation and matter.[22] So it was then, and it still is now.

In section 2 we will look into the details of setting quantum electrodynamics (as the theory that describes the interaction of matter and radiation) into 'motion'. It turns out that quantum electrodynamics *is* a perturbative approach. Also quantum electrodynamics relies on the doubtful method of adiabatically switching on/off the interaction between radiation and matter. However, not looking too closely into the mathematical structure of the theory and considering only a few order terms perturbative calculations, quantum electrodynamics presents an astonishing agreement with experimental results.

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[22] The use of perturbative methods has a long history in celestial mechanics. One example is the development of an analytical perturbation theory for the three-body problem: the Sun-Earth-Moon system (Hoskin & Taton, 1995, pp. 89-107). From the planets, perturbative methods went to the planetary models of atoms, being a calculational tool present in the so-called old quantum theory (Darrigol, 1992, pp. 129 & 171). Also it became fundamental in the creation of matrix mechanics, as it was from the perturbative study of the anharmonic oscillator that Heisenberg developed his quantum-theoretical approach (Darrigol, 1992, pp. 266-267; Paul, 2007, pp. 4-5). Soon after, Heisenberg and Max Born put together a perturbation theory within the formalism of quantum mechanics recently developed (van der Waerden, 1967, pp. 43-50; see also Lacki, 1998).

Unfortunately there appear to be severe problems with the previous view. These will be addressed in section 3. According to John Earman and Doreen Fraser, the Haag theorem seems to imply the mathematical inconsistency of the usual treatment of interactions in quantum electrodynamics using perturbative methods (Earman & Fraser, 2006), in which the concept of quanta is central. Fraser presents the idea that "once infinite renormalization counterterms are introduced … it is no longer possible to prove Haag's theorem" (Fraser, 2006, p. 2). I shall argue that simply calling attention to the fact that renormalization "renders the theory mathematically not well-defined" (Fraser, 2006, p. 171), does not provide any answer to the question: "why perturbation theory works as well as it does" (Earman & Fraser, 2006, p. 307). This is not an unimportant question, since we are facing the puzzling situation that the predictions of quantum electrodynamics are so accurate, while the theory from which they are derived appears to be mathematically inconsistent. In this section I will try to provide an answer to this question. In the process I will try to show that Earman and Fraser's conclusion that "Fock representations are generally inappropriate for interacting fields" (Earman & Fraser, 2006, p. 330) or Fraser's related conclusion that "an interacting system cannot be described in terms of quanta" (Fraser, 2008, p. 842), are not valid in quantum electrodynamics: we do not have an interacting system but two weakly interacting fields (systems), and their interaction is described in terms of quanta.

In a nutshell my argument will be as follows: it turns out that quantum electrodynamics, because the series expansion of the S-matrix is divergent, is unable to treat radiation and matter as one closed system. Rather the theory can only give an approximate description (using a perturbative approach) of the interaction between radiation and matter as distinct systems. If we try to close the gap and treat radiation and matter as one closed system, corresponding to an exact solution of the coupled non-linear Maxwell-Lorentz and Dirac equations, our perturbative approach fails. My view is that there is a one-to-one correspondence between having meaningful mathematical results and being clear about the physical assumptions used to set up the theory (in quantum electrodynamics I take part of the input physical concepts to be radiation and matter taken to be independent systems that are independently quantized due to the weak interaction between then). This is so, because the physical concepts are defined in connection with a specific mathematical 'support', not beyond or independently of maths. In a situation where we have an infinity popping up we cannot have a well-defined use of the physical concepts involved. In the case of quantum electrodynamics this situation occurs when trying to give a full description of the (weak) interaction between matter and radiation, which would correspond to treating them as one closed system. I see the divergence of the S-matrix series expansion as a fingerprint of a tentative application of the mathematics of the theory beyond its physical content.

By focusing on the basic physical concepts used to set up the theory, and not solely on its (ill-defined) mathematical structure, we can make sense of the success of quantum electrodynamics (independently of the Haag theorem). This provides a different perspective than the one adopted by Earman & Fraser that not only contradicts several of their conclusions, but also, in my view, makes quantum electrodynamics more intelligible.

2. Quantum electrodynamics as a perturbative approach

In his 1927 paper Dirac dealt with a system consisting of an atom interacting with electromagnetic radiation. Dirac used a non-relativistic Hamiltonian and made his

calculations in what would be called the Coulomb gauge. As already mentioned, in this article Dirac was able to obtain a dynamical derivation of Einstein's coefficients for the spontaneous and stimulated emission of radiation by an atomic system. In a subsequent paper from April 1927 Dirac applied his techniques to the development of a quantum theory of the dispersion of radiation by an atom. The starting point was the classical Hamiltonian for an atom (an electron in a central potential ϕ) interacting with an electromagnetic field (a transverse radiation field with two polarization components) described by a vector potential **A**:

$$H = c\sqrt{m_0^2c^2 + (\vec{p} + \frac{e}{c}\vec{A})^2} - e\phi .$$

In the non-relativistic approximation we have

$$H = H_0 + \frac{e}{c}\vec{v}\cdot\vec{A} + \frac{e^2}{2m_0c}\vec{A}^2 .$$

Each Fourier component of the vector potential is written as

$$k_r = 2\left(\frac{h\nu_r}{c\sigma_r}\right)^{1/2} N_r^{1/2}\cos\theta_r / h ,$$

where in particular ν_r is the frequency of the radiation in the mode k_r. Then Dirac takes the field to be a quantum operator, by taking the canonically conjugated variables N_r and θ_r to be quantum operators (q-numbers in Dirac's approach). N_r is now the number of light-quanta of the component r, and θ_r is its corresponding phase (operator). They satisfy the commutation relation

$$[\theta_r, N_r] = ih.$$

As in his previous 1927 work Dirac is describing the radiation field by using the vector potential **A**, and making a Fourier expansion of **A**. It is the vector potential that is treated as a quantum operator by applying the quantum rules to each of its components.

To treat the dispersion of radiation Dirac found it necessary to use perturbation theory. According to Dirac:

In applying the theory to the practical working out of radiation problems one must use a perturbation method, as one cannot solve the Schrödinger equation directly. One can assume that the term (V say) in the Hamiltonian due to the interaction of the radiation and the atom is small compared with that representing their proper energy, and then use V as the perturbing energy … In the present paper we shall apply the theory to determine the radiation scattered by an atom … If V_{mn} are the matrix elements of the perturbing energy V, where each suffix m and n refers to a stationary state of the whole system of atom plus field (the stationary state of the atom being specified by its action variables, J say, and that of the field by a given distribution of energy among its harmonic components, or by a given distribution of light-quanta), then each V_{mn} gives rise to transitions from state n to state m; more accurately, it causes the eigenfunction representing state m to grow if that representing state n is already excited, the general formula for the rate of change of the amplitude a_m of an eigenfunction being

$$ih/2\pi\,\dot{a}_m = \sum_n V_{mn}a_n = \sum_n \upsilon_{mn}a_n e^{2\pi i(W_m - W_n)t/h} \quad (1)$$

where υ_{mn} is the constant amplitude of the matrix element V_{mn}, and W_m is the total proper energy of the state m. To solve these equations one obtains a first approximation by substituting for the a's on the right-hand side their initial values, a second approximation by substituting for the a's their values given by the first approximation, and so on. (Dirac, 1927b; pp. 711-712)

Up to second order Dirac found that the Hamiltonian operator gave rise to two processes of scattering of radiation by the electron in the atom. In one case, which Dirac called direct or true scattering processes, we have a transition "in which a light-quantum jumps directly from a state s to a state r" (Dirac, 1927b, p. 717). The other case, which shows up only when making an approximate second order calculation, Dirac named 'double scattering processes'. When considering two states m and m' without an appreciably difference in energy, there can be a scattering of radiation which "appears as the result of the two processes m' → n and n → m, one of which must be an absorption and the other an emission" (Dirac, 1927b, p. 712), where n is a third state different from m and m'. According to Dirac in neither of the two processes "is the total proper energy even approximately conserved" (Dirac, 1927b, p. 712).[23]

As we have already seen, Dirac's approach was improved by Pauli, Heisenberg, and Fermi, in the development of a relativistic theory of the interaction of quantized radiation and matter. Looking now at quantum electrodynamics from the established Lagrangian approach, we have two classical fields described by the Maxwell-Lorentz equations and the Dirac equation. As we have already seen, the Dirac equation can be taken to be a classical equation of a spinor field (and its adjoint field). Using the usual procedure of Fourier expansion of a wave function this field can be resolved into its Fourier components, whose amplitude coefficients become operators after the quantization and satisfy anticommutation relations according to Fermi-Dirac statistics. An equivalent procedure is taken for the quantization of the electromagnetic field (following Bose-Einstein statistics). Up to this point we are dealing with two independently quantized fields. Quantum electrodynamics is about the description of the interaction between radiation and matter as described by these quantum fields. In classical electrodynamics, the relativistic equation of motion of a charged particle in a given external field is

$$K = e\left(\vec{E} + \frac{1}{c}\left[\vec{v}\times\vec{H}\right]\right).$$

This equation can be derived from the Hamiltonian representing the total energy of the particle expressed as a function of the canonical coordinates and momenta

$$H = e\phi + \sqrt{m_0^2c^4 + (\vec{p} - e\vec{A})^2}\,,$$

where the total energy, which can be given by $T + e\phi$, is the fourth component of a four-vector p_μ given by

$$p_\mu = u_\mu + eA_\mu$$

[23] In chapter 7 I will look at what might be the physical meaning of these transitory states (the virtual states) that appear in the perturbative treatment of the interaction of radiation a matter.

(u_μ is the kinetic momentum given by the relativistic expression for the momentum-energy four-vector for a free particle).

From the Hamiltonian it is a simple task to derive the equation of motion for the charged particle in an external field:

$$\frac{1}{c}\frac{d}{dt}(p_x - eA_x) = e\left(E_x + \frac{1}{c}[vH]_\xi\right).$$

In this way the Hamiltonian for the particle contains also the term describing the interaction of the particle with the field.

In the application of Dirac's equation as a one-electron equation to the case of electrons in an external field (e.g. the hydrogen atom) we use the prescription of going from the 'kinetic momentum' to the 'total momentum' by making the replacement

$$p_\mu \rightarrow p_\mu - \frac{e}{c}A_\mu .$$

In this way, Dirac's equation in the presence of an external (classical) field is given by

$$\gamma^\mu\left(i\hbar\partial_\mu - \frac{e}{c}A_\mu(x)\right)\psi(x) = mc\,\psi(x),$$[24]

instead of simply

$$i\hbar\gamma^\mu\partial_\mu\psi(x) = mc\,\psi(x),$$

which is the case for a free field. As we have seen it is this last equation that is used when making the quantization of the Dirac field. The case of the electromagnetic field is similar. We quantize the free field, but the (operator) equation for the (quantized) electromagnetic field in the presence of (quantized) charges is

$$\left(\frac{\partial^2}{c\partial t^2} - \nabla^2\right)A_\mu = -\frac{\partial L}{\partial A^\mu} = -e\overline{\psi}\gamma_\mu\psi .$$

This set of coupled equations, for the Dirac and electromagnetic field, can be derived from a Lagrangian representing the Dirac field interacting with the electromagnetic field

$$L = -\frac{1}{2}\frac{\partial A_\mu}{\partial x_\nu}\cdot\frac{\partial A^\mu}{\partial x^\nu} - \frac{1}{2i}\left[\overline{\psi}\gamma^\mu\cdot\left(\frac{\partial}{\partial x^\mu} - ieA_\mu\right)\psi + im\overline{\psi}\cdot\psi\right]$$

$$+\frac{1}{2i}\left[\left(\frac{\partial\overline{\psi}}{\partial x^\mu} + ieA_\mu\overline{\psi}\right)\gamma^\mu\cdot\psi - im\overline{\psi}\cdot\psi\right].$$

[24] After quantization this equation becomes an operator equation for a quantized Dirac field in interaction with a quantized electromagnetic field.

This Lagrangian can be written in terms of the Lagrangians for the free Dirac field, the free electromagnetic field and a term representing the interaction between the two fields

$$L = L_m + L_{em} + e\overline{\psi}\gamma^{\mu} \cdot \psi A_{\mu} .$$

Since the interaction term in the Lagrangian does not contain any time derivatives of the field operators "the canonical momenta are therefore the same functions of the dynamical variables as [in the free field case], and we can immediately write down the equal time canonical commutation relations" (Källén, 1972, p.76). That is we could apparently start from the Lagrangian for the Dirac and electromagnetic fields in interaction to develop the quantization procedure. But contrary to the case of free field quantization it is not possible now to obtain commutation relations valid for all times since this implies solving first the coupled equations for the fields (Schweber, 1961, p. 276; Källén, 1972, p.76). The problem is that, as Freeman Dyson mentioned,

these equations are non-linear. And so there is no possibility of finding the general commutation rules of the field operators in closed form. We cannot find any solution of the field equations, except for the solutions which are obtained as formal power series expansions in the coefficient e which multiplies the non-linear interaction terms. It is thus a basic limitation of the theory, that it is in its nature a perturbation theory starting from the non-interacting fields as an unperturbed system. Even to write down the general commutation laws of the fields, it is necessary to use perturbation theory of this kind. (Dyson, 1952a, p. 79)

This implies that to treat the interaction of radiation with matter we must start from the quantized free fields and then by using perturbation theory treat the interaction between the two fields. According to Dyson

Since the perturbation theory treatment is forced on us from the beginning, it is convenient not to set up the theory in the Heisenberg representation but to use the interaction representation. The IR is just designed for a perturbation theory in which the radiation interaction is treated as small. In the IR the commutation rules can be obtained simply in closed form, and so the theory can be set up with a minimum of trouble. (Dyson , 1952a, p. 79)

I will consider for the time being that we can (apparently) describe the interaction of matter and radiation in terms of a wave function describing the fields as one closed system. We take, as Dirac did in 1927, this joint system to be described by a Hamiltonian $H = H_0 + V$, where H_0 describes the free non-interacting fields and V describes the interaction between them. In the Schrödinger picture (representation) the equation of motion of the system is the time-dependent Schrödinger equation

$$i\hbar\partial_t \left|\phi_S(t)\right\rangle = H_S \left|\phi_S(t)\right\rangle = (H_{0S} + V)\left|\phi_S(t)\right\rangle .$$

In the interaction representation (or Dirac picture) the state vector describing the system is defined in terms of the state vector in the Schrödinger representation as

$$\left|\phi_D(t)\right\rangle = e^{iH_{0S}t\hbar} \left|\phi_S(t)\right\rangle .$$

This state vector satisfies the equation

$$i\hbar\partial_t\left|\phi_D(t)\right\rangle = e^{iH_{0S}t\hbar}Ve^{-iH_{0S}t\hbar}\left|\phi_D(t)\right\rangle = V_D(t)\left|\phi_D(t)\right\rangle;$$

also, an operator in the interaction representation is related to the corresponding Schrödinger representation operator by

$$Q_D(t) = e^{iH_{0S}t\hbar}Q_S e^{-iH_{0S}t\hbar},$$

whose time dependency is determined in terms of the unperturbed Hamiltonian

$$i\hbar\partial_t Q_D(t) = \left[Q_D(t), H_0\right].$$

In this way we see that in the interaction representation the time evolution of the state vector (describing the two fields in interaction) is dependent only on the interaction term, while the time evolution of the operators depends on the free-field Hamiltonian.

In quantum electrodynamics, the majority of its applications are made using the S-matrix formalism. This formalism is particularly tailor-made for the description of scattering processes but is also applicable to bound-state problems (Veltman, 1994, pp. 62-67). I follow Dyson's presentation of a typical scattering process as described within quantum electrodynamics:

> The free particles which are specified by a state A in the remote past, converge and interact, and other free particles emerge or are created in the interaction and finally constitute the state B in the remote future. (Dyson, 1952a, p. 81)

Dyson calls attention to the fact that:

> The unperturbed states A and B are supposed to be states of free particles without interaction and are therefore represented by constant state-vector ϕ_A and ϕ_B in the interaction representation. The actual initial and final states in a scattering problem will consist of particles each having a self-field with which it continues to interact even in the remote future and past, hence ϕ_A and ϕ_B do not accurately represent the initial and final states.(Dyson, 1952a, p. 81)

Dyson presents what can be considered an operational justification for using the states of free particles (usually referred to as bare states) in the calculations, by taking into account how scattering experiments are really done (see Falkenburg, 2007, pp. 129-131):

> Let $\Psi_B(t)$ be the actual time-dependent state-vector of the state B in the IR. We are not interested in the dependence of $\phi_B(t)$ on t. In an actual scattering experiment the particles in state B are observed in counters of photographic plates or cloud-chambers and the time of their arrival is not measured precisely. Therefore it is convenient to use for B not the state-function $\Psi_B(t)$ but a state function ϕ_B which is *by definition* the state-function describing a set of bare particles without radiation interaction [that is without self-interaction with its own field], the bare particles having the same momenta, and spins as the real particles in state B. (Dyson, 1952a, p. 94)

The transition amplitude of the scattering process is given by $S_{AB} = (\phi^*_B S\phi_A)$, where S is the so-called S-matrix. This scattering amplitude S_{AB} can be written as (ψ_B^-, ψ_A^+), where we have: $\lim_{t_0\to-\infty} U(0,t_0)\phi_A = \psi_A^+$ and $\lim_{t\to+\infty} U(0,t)\phi_B = \psi_B^-$, where $U(t, t_0)$ is the time displacement unitary operator defined by

$$U(t,t_0)\left|\psi(t_0)\right\rangle = \left|\psi(t)\right\rangle$$

(where we are using the state vectors and operators in the Dirac picture), which satisfies the equation

$$i\hbar\partial_t U(t,t_0) = V(t)U(t,t_0)\,.$$

In this way the S matrix is simply related to the operator $U(t, t_0)$ by the formal expression $S = U(\infty,-\infty)$. By using the boundary condition $U(t_0, t_0) = 1$ the previous equation for $U(t, t_0)$ is equivalent to the integral equation

$$U(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} V(t')U(t',t_0)dt'\,.$$

This equation is solved by an iteration procedure. We have

$$\begin{aligned} U(t,t_0) = 1 &+ \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t} dt_1 V(t_1) \\ &+ \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 V(t_1)V(t_2) \\ &+ \left(-\frac{i}{\hbar}\right)^3 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3 V(t_1)V(t_2)V(t_3) \\ &+ \ldots . \end{aligned}$$

By defining a chronological operator

$$P(V(t_1)\ldots V(t_n)) = \sum_P \theta(t_{\alpha_1} - t_{\alpha_2})\ldots\theta(t_{\alpha_{n-1}} - t_{\alpha_n})V(t_{\alpha_1})\ldots V(t_{\alpha_n})$$

(where we must sum over all permutations of $t_1, \ldots t_n$), so that we have

$$P(V(t_1)\ldots V(t_n)) = V(t_i)\ldots V(t_j)\ldots V(t_k)\,, \text{ with } t_i > \ldots t_j \ldots > t_k,$$

the expansion for $U(t, t_0)$ can be written as

$$U(t,t_0) = \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \ldots \int_{t_0}^{t} dt_n P(V(t_1)V(t_2)\ldots V(t_n))\,.$$

In applications to scattering problems we need to calculate the S-matrix, that is, $U(\infty,-\infty)$. This is the case because in the case of scattering processes we only have experimental access to the cross-section. In quantum electrodynamics the scattering cross-section is calculated from the transition probability per unit space-time volume, which is related to the S-matrix in a simple way (Jauch & Rohrlich, 1976, pp. 163-167). According to B. Falkenburg "the effective cross-section is the physical magnitude with which the current field theories come down to earth. As a *theoretical quantity*, the cross-section is calculated from the S-matrix of quantum mechanics … as an *empirical*

quantity, it is the measured relative frequency of scattering events of a given type" (Falkenburg, 2007, p. 107)

When calculating the S-matrix we must extend the initial time t_0 to $-\infty$ and the final time t to $+\infty$. As we have seen in Dyson's presentation the initial (and final) state of the system is taken to be an eigenstate of H_0 the Hamiltonian for the non-interacting fields. This idea can be given a more formal presentation by considering that the interaction between particles in a scattering process is adiabatically switched on in the remote past and adiabatically switched off in the remote future (Lippmann & Schwinger, 1950, p. 473; Bogoliubov & Shirkov, 1959, p. 197). What this means is that at infinity the interaction term is taken to zero, that is, there is no interaction between matter and radiation. This has important implications. One is that since there is no interaction we are really considering two uncoupled systems, the Dirac field, and the electromagnetic field. Another point is that in this case the state vectors are taken to be a product of Fock states of each field: bare states. Looking at this in terms of scattering of particles (quanta of each field), the initial and final states of the scattered particles are states of the (free-particle) Fock space.

As we have seen the S-matrix is given as a series expansion in powers of the interaction term V(t). We can look at the description of an interaction process as described by the S-matrix as a perturbative approach in which only Fock states are considered. The use of the interaction representation in the S-matrix approach can be seen then as part of a perturbative approach in which the interaction term is leading to a perturbation of the free states of the fields.

To see the importance of the adiabatic 'switching on' and 'switching off' of the interaction to this overall perturbative approach let us look into Dyson's take on this subject. As we have seen Dyson gave an operational justification to the use of a Fock state function ϕ_B to describe the initial and final state of the Dirac field, instead of $\Psi_B(t)$ the state-vector representing for example a self-interacting electron. Dyson asks the question: "what is the connection between $\Psi_B(t)$ and ϕ_B?"(Dyson, 1952a, p. 94). Let us look into his presentation of the adiabatic trick.

Suppose t_B to be a time so long in the future after the scattering process is over, that from t_B to $+\infty$ the state B consists of separated outward-travelling particles. Then the relation between $\psi_B(t)$ and ϕ_B is simple. We imagine a fictitious world in which the charge e occurring in the radiation interaction decreases infinitely slowly (adiabatically) from its actual value at time t_B to zero at time $(+\infty)$. In the fictitious world, the state $\psi_B(t_B)$ at time t_B will grow into the bare-particle state ϕ_B at time $+\infty$. Thus

$$\phi_B = \Omega_2(t_B)\, \psi_B(t_B) \tag{489}$$

where

$$\Omega_2(t_B) = \sum_{n=0}^{\infty}\left(\frac{e}{\hbar c}\right)^n \frac{1}{n!}\int_{t_B}^{\infty}\dots\int_{t_B}^{\infty} dx_1 \dots dx_n P\{\overline{\psi}\mathbb{A}\psi(x_1),\dots,\overline{\psi}\mathbb{A}\psi(x_n)\} g_B(t_1)\dots g_B(t_n) \tag{490}$$

and $g_B(t)$ is a function decreasing adiabatically from the value 1 at $t = t_B$ to zero at $t = \infty$. Similarly, when t_A is a time so far in the past that the state A consists of separated converging particles from $t = -\infty$ to $t = t_A$ we have

$$\Omega_1(t_A) = \sum_{n=0}^{\infty}\left(\frac{e}{\hbar c}\right)^n \frac{1}{n!}\int_{-\infty}^{t_A}\dots\int_{-\infty}^{t_A} dx_1 \dots dx_n P\{\overline{\psi}\mathbb{A}\psi(x_1),\dots,\overline{\psi}\mathbb{A}\psi(x_n)\} g_A(t_1)\dots g_A(t_n) \tag{492}$$

where $g_A(t)$ is a function increasing adiabatically from $t = -\infty$ to $t = t_A$.

The scattering matrix element between states A and B is given exactly by

$$M = (\psi_B^*(t_B) S_{t_A}^{t_B} \psi_A(t_A)) \tag{493}$$

$$S_{t_A}^{t_B} = \sum_{n=0}^{\infty} \left(\frac{e}{\hbar c}\right)^n \frac{1}{n!} \int_{t_B}^{t_A} \dots \int_{t_B}^{t_A} dx_1 \dots dx_n P\{\bar{\psi} A \psi(x_1), \dots, \bar{\psi} A \psi(x_n)\} g(t_1) \dots g(t_n) \tag{494}$$

Of course (493) is independent of the times t_A and t_B. When t_A and t_B are chosen so far in the past that (489) and (491) are satisfied, then (493) may be written in the form (487), where now

$$\begin{aligned} S &= \Omega_2(t_B) S_{t_A}^{t_B} \Omega_2(t_A) \\ &= \sum_{n=0}^{\infty} \left(\frac{e}{\hbar c}\right)^n \frac{1}{n!} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dx_1 \dots dx_n P\{\bar{\psi} A \psi(x_1), \dots, \bar{\psi} A \psi(x_n)\} g(t_1) \dots g(t_n) \end{aligned} \tag{495}$$

and g(t) is a function increasing adiabatically from 0 to 1 for $-\infty < t < t_A$, equal to 1 for $t_A \le t \le t_B$, and decreasing adiabatically from 1 to 0 for $t_A < t < \infty$. Thus we come to the important conclusion that [the] formula [$M = (\phi_B^* S \phi_A)$ (487)] for the matrix element is correct, using the bare particle state-functions ϕ_A and ϕ_B, provided that [the] formula

$$S = \sum_{n=0}^{\infty} \left(\frac{e}{\hbar c}\right)^n \frac{1}{n!} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dx_1 \dots dx_n P\{\bar{\psi} A \psi(x_1), \dots, \bar{\psi} A \psi(x_n)\} \tag{488}$$

for S is interpreted by putting in the slowly varying cut-off function $g(t_i)$ to make the integrals converge at $t_i = \pm\infty$. The cut-off functions are to be put in as they appear in (495), and then S is defined as the limit to which (495) tends as the rate of variation of g(t) is made infinitely slow.

The main practical effect of this limiting process in the definition of S is to justify us in throwing away all terms in the integrals which oscillate finitely at $t_i = \pm\infty$. There are however certain cases in which the integral (488) is in a more serious way ambiguous due to bad convergence at $t_i = \pm\infty$. In these cases the cut-off functions have to be kept explicitly until a late stage of the calculations before going to the limit g(t) = 1. In all cases, if the limiting process is done in this way, the matrix element M is obtained correctly and unambiguously.

The use of bare-particle wave-functions ϕ_A and ϕ_B in (487) is thus justified. (Dyson, 1952a, pp. 94-95)

In this way, in the S-matrix approach we will be calculating transition amplitudes between free-particle states ($M = (\phi_B^* S \phi_A)$). Since the interaction term is given by $e\bar{\psi}\gamma^\mu \cdot \psi A_\mu$, we can also see the series expansion of the S-matrix as given in powers of *e*, where *e* is the electric charge (or in powers of the so-called fine structure constant $\alpha = e^2/4\pi$): $S = 1 + eS^{(1)} + e^2S^{(2)} + \dots$ (Källén, 1972, p. 88).

Let us consider, for example, the quantum electrodynamical treatment of the two-photon annihilation of an electron and a positron (Sakurai, 1967, pp. 204-208): $e^+ + e^- \rightarrow 2\gamma$. The initial state corresponds to a Dirac field with two quanta, one corresponding to the electron, and the other to the positron (the electromagnetic field is taken to be in the vacuum state). In the final state after the 'scattering', the Dirac field is in the ground-state, that is, with no quanta, and the electromagnetic field is in a state with two photons. The second-order transition or scattering amplitude is given by

$$S_{fi} = (-e)^2 \int d^4x_1 \int d^4x_2 \left\langle 2\gamma \middle| A_\mu(x_1) A_\nu(x_2) \middle| 0 \right\rangle (\gamma_\mu)_{\alpha\beta} (\gamma_\nu)_{\gamma\delta}$$

$$\times\Big[\big\langle 0\big|\Psi_{\beta}^{(+)}(x_1)\overline{\Psi}_{\gamma}^{(-)}(x_2)\overline{\Psi}_{\alpha}^{(+)}(x_1)\overline{\Psi}_{\delta}^{(+)}(x_2)\big|e^{-}e^{+}\big\rangle\theta(t_1-t_2)$$
$$-\big\langle 0\big|\Psi_{\gamma}^{(+)}(x_2)\overline{\Psi}_{\beta}^{(-)}(x_1)\overline{\Psi}_{\alpha}^{(+)}(x_1)\overline{\Psi}_{\delta}^{(+)}(x_2)\big|e^{-}e^{+}\big\rangle\theta(t_2-t_1)\Big].$$

I will not go into the details of this expression but only address some relevant features. The expression is an example of the perturbative quantum electrodynamical treatment of the interaction between the Maxwell and Dirac fields. In it we have the description of the propagation of quanta between two space-time points x_1 and x_2 (corresponding to Dirac's 'third state'), and components related to the non-interacting states of each field (Fock states): $\left|e^{-}e^{+}\right\rangle$, $\left|2\gamma\right\rangle$, and the vacuum states of each field $\left|0\right\rangle$. That is, we use only the Fock space for each field to calculate the interactions in quantum electrodynamics. Also, each quantum field operates in different Fock spaces.

3 *Possible problems for quantum electrodynamics: the Haag theorem and the divergence of the S-matrix series expansion*

It seems then that we have a simple procedure to calculate whatever situation of interaction between radiation and matter we might have by simply addressing each case as if it is a scattering problem and dealing with it using the S-matrix approach with the adiabatic switching trick, where we can use as initial and final states Fock states of each field. However the situation is not that simple. One crucial aspect of all this adiabatic switching trickery is that the following supposition (called the adiabatic theorem) is being made: "If a state is an eigenstate of the Hamiltonian and if a parameter in the Hamiltonian is adiabatically changed …, then the same state is also an eigenstate, after the Hamiltonian is changed, but with a different eigenvalue" (Källén, 1972, pp. 52-53). As we have seen in Dyson's presentation this is being taken for granted: 'the state $\psi_B(t_B)$ at time t_B will grow into the bare-particle state ϕ_B at time $+\infty$. Thus $\phi_B = \Omega_2(t_B)\,\psi_B(t_B)$'. Is this really the case?

No! From Haag's theorem (Haag, 1955) we know that we cannot have a unitary transformation that relates the field operators corresponding to the free Hamiltonian H and the interacting field Hamiltonian H_I. Considering that at t_0 the Heisenberg picture and the Dirac picture (interaction representation) coincide (Earman & Fraser, 2006, p. 320), it would seem that the state vector in the interaction representation, in the limit $t \to \pm\infty$, corresponds to free particles due to the fact that the interaction part of the Hamiltonian is negligible. But from Haag's theorem it seems that "at times $t = \pm\infty$, all the assumptions of the theorem hold for the Heisenberg representation, which represents an interaction, and for the interaction representation, which is a Fock representation for a free system" (Earman & Fraser, 2006, p. 322). In informal terms Haag's theorem implies that the state vectors in the interaction representation, that for $t \to \pm\infty$ are *supposed* to represent the free field, and the state vector in the Heisenberg representation for the interacting fields, are not in a common domain of both H and H_I (Schweber, 1961, p. 416).

From Haag's theorem we can conclude that if we have a free field at $t = -\infty$, the interaction representation describes also a free field at any time t_0. This means that we need to have a state of the full interacting Hamiltonian from the start so that we can consistently give the interaction representation its usual interpretation as giving a different time dependency to the state vector and the operators (Schweber, 1961, p. 317).

Both the Heisenberg and Dirac pictures can hypothetically be used in either free or interacting systems, if we can separate the Hamiltonian in two parts. The change of representation does not change the physical situation whether it concerns free or interacting fields. There really is no "interaction picture's assumption that there is a time at which the representation for the interaction is unitarily equivalent to the Fock representation for a free system" (Fraser, 2006, p. 54).[25] This 'assumption' has nothing to do with the representation being used. The 'assumption' is that with an adiabatic switching on of the interaction, the state vector for the interacting systems can be constructed from the state vector of free fields (Schweber, 1961, p. 320):

$$\lim_{t\to-\infty} U(t_0,t)\left|\varphi_a\right\rangle = \left|\psi_a\right\rangle .$$

This is what is supposed to be achieved in the adiabatic switching on of the potential that 'connects' a free field Hamiltonian with the interacting field Hamiltonian (Jauch & Rohrlich, 1976, p. 134; Schweber, 1961, p. 322): $\lim_{t\to-\infty} H_\varepsilon(t) = \lim_{t\to-\infty}(H_0 + e^{-\varepsilon|t|}V(t)) = H_0$, where ε is a parameter that is taken to zero in the end of the computations. The point is, as we have seen, that at infinite times before and after the adiabatic switching on/off of the interaction potential, the state vector in either the Heisenberg or the Dirac picture is *assumed* to be describing free fields.

The question here is not thus the representation being used but whether it is possible to connect the interacting state to a free field state. It seems clear from the consequences of Haag's theorem that the usual adiabatic switching on/off of the interaction will not do the trick. In this way we are in the situation of explaining how it is that with a mathematically incorrect procedure it is possible to develop applications from the theory that give so good results when compared with experiments.

It is well known that in the applications of quantum electrodynamics there are problems with divergent integrals. These problems are circumvented in practice with renormalization techniques in which (basically) all the divergent integrals appearing in the series expansion of the S-matrix are related to corrections to the mass and charge of the fermions. Since the value of the mass and the charge are not defined by the theory but result from measurements, the terms in the series expansion that are divergent (but formally should be smaller and smaller) are taken to be part of the observed mass and charge.

It might seem that by using renormalization techniques the consequences of Haag's theorem might be evaded because "once infinite renormalization counter terms are introduced, the interaction picture is not mathematically well-defined" (Fraser, 2006, p. 2). From this it might seem that "renormalization addresses this problem not by refining the assumptions, but by rendering the canonical framework mathematically ill-defined" (Fraser, 2006, p. 90). But it would be rather strange, to say the least, that by considering

[25] Earman and Fraser's take it that in the infinite past and the infinite future "particles are assumed to be infinitely far apart and therefore not interacting" (Earman & Fraser, 2006, p. 321). In this case they consider that at t=±∞ "the representation is taken to be a Fock representation" (p. 321). And this is taken to be a Dirac picture (interaction representation) assumption: "In the interaction picture ... at $t = \pm\infty$ the representation is the Fock representation for the free field" (p. 321). At this point I thus disagree with Earman and Fraser's presentation of the consequences of the Haag theorem. I simply do not think that the assumption that at infinite past we can take the state of a particular field to be a free state as described by a Fock space has to be seen as part of the assumptions of the Dirac picture. But this is a question of detail. The main aspect of their presentation is irrefutable: according to the Haag theorem the perturbative approach used in quantum electrodynamics to describe interactions is mathematically inconsistent.

an impoverished mathematical structure, suddenly, something physically equivalent to a unitary transformation connecting free and interacting field operators might emerge. In reality this argument does not provide any explanation for why the theory is effective, and this is a central question which has correctly been considered to be relevant: "There is, however, unfinished business in explaining why perturbation theory works as well as it does" (Earman & Fraser, 2006, p. 307).

If we followed Fraser's account we would be back where we started since, without taking into account the ill-defined mathematics of renormalization (and this is possible by considering only the lowest-order calculations), one could say that the adiabatic switching on/off of the interaction is also of doubtful mathematical rigor precisely due to the Haag theorem. This means that when imposing the adiabatic switching on/off we are developing an ill-defined approach. The primary question of the effectivity of the theory would remain, independently of the probable impossibility of taking into account the Haag theorem in this ill-defined mathematical context (now due to the adiabatic switching on/off of the interaction).

Another aspect of not having a rigorous basis for a procedure to adiabatically construct the interacting states from the free states is the following. In the Fock space we have a direct connection of quanta to the normal modes of classical field configurations. It is from the Fourier splitting of a classical wave into positive and negative frequency normal modes, providing the basis for the configuration space, that the concept of quanta emerges (via a quantization procedure which results in associating quanta to each normal mode). In the case of interacting fields it is not possible to make this Fourier expansion (Fraser 2006, p. 136). This implies that it is not possible to use the Fock representation for a free field to represent the interacting Dirac and Maxwell fields (Earman & Fraser, 2006, p. 322). Following this line of reasoning, this means that the quanta concept is unavailable when we consider full interacting fields (Earman & Fraser, 2006, p. 330; Fraser, 2008, pp. 2-3). It could seem that the perturbative S-matrix approach could overcome this problem by providing a rigorous procedure to describe the interacting Dirac and Maxwell fields in the scattering problem by using only the Fock states representing free quanta from each field. According to the Haag theorem this is not possible. It seems then, according to Earman and Fraser, that we cannot use the concept of quanta when dealing with interacting fields.

It does not seem that the effectiveness of the perturbative approach, in spite of Haag's theorem, is a consequence of the need for a mathematical ill-defined mass and charge renormalization. At least there is no argument that shows how the efficiency of this scheme might result from developing it from a mathematical structure that is ill-defined due to renormalization. Moreover the renormalization technique is not the only element that makes the theory mathematically ill-defined. It seems that we cannot arrive at any solid conclusions by analysing from a mathematical perspective, what appears to be an ill-defined mathematical structure.

My view is that the explanation for the good results of the perturbation theory approach to scattering (and bound state) problems in spite of the Haag theorem, will not be found in the mathematical structure of quantum electrodynamics. As will be seen below, the point about Haag's theorem is that the question of its applicability, is not even addressed in the way the physical theory is really used: *we have to consider the physical input assumptions of the theory together with its mathematical formulation and application, not the mathematical structure all by itself.*

As mentioned above, the theory is developed from a canonical quantization of two independent classical fields. The description of the interaction between the fields is given, like in the classical counterpart, by an interaction term. Formally we can adopt

whatever representation is mathematically possible. But since we are (apparently) dealing with an ill-defined mathematical structure one should not consider formal aspects of the theory, like the full formal S-matrix for a scattering process (which in the applications turns out to be an asymptotic series). We must consider the applications of the theory that provide results that we can check with experiments. In these circumstances the use of the interaction representation only attains a physical meaning at the level of applications in which we can consider different systems with an interaction that can be considered as a perturbation of their independent states. In this way the fields maintain their identity as separated physical systems even during the interactions. In this sense the use of the interaction representation is part of the applications. We simply use part of the Hamiltonian, which is possible since the theory was developed considering distinct parts in the Lagrangian, one corresponding to the free Dirac field, another to the free Maxwell field, and another to the interaction. This is the one pulled apart from the others in the interaction representation.

The description of scattering is developed from the theory considering an initial state corresponding to a limited number of free particles (quanta), and with an adiabatic switching on of the interaction between the fields, a full interacting state ψ_b^- is *apparently* obtained. The interacting state ψ_a^+ that corresponds to a well-defined number of quanta in the final state is defined in an equivalent way. The scattering amplitude S_{ab} is given by (ψ_b^-, ψ_a^+) (Schweber, 1961, p. 323). The point is that we really do not work with these doubtful interacting states. What is going on is quite different. We are only considering a few terms of a perturbation expansion of the scattering matrix. When considering the applications we are taking advantage of the way the theory was developed. We always have clearly distinct fields. For the description of their interaction it is not necessary to have a description of both fields as a closed interacting system. On the contrary, as we will see next, if we try to make a full description of the interaction considering all the terms of the power series expansion of the S-matrix, it can "at best only be an asymptotic expansion" (Schweber, 1961, p. 644).

One of the major achievements of Dyson in the development of quantum electrodynamics was showing that the perturbative expansion of the S-matrix is renormalized to all orders. As mentioned previously, quantum electrodynamics (QED) had tremendous problems of divergent integrals that made impossible but a few lower order calculations. This problem was circumvented by the procedure of mass and charge renormalization. Dyson showed, in a paper published in 1949, that the renormalization procedure could be applied to all orders of the perturbative expansion of the S-matrix (Schweber, 1994, pp. 527-544).

Soon afterwards, in the summer of 1951, Dyson came out with a physical argument that strongly suggested that, after all, "all the power-series expansions currently in use in quantum electrodynamics are divergent after the renormalization of mass and charge" (Dyson, 1952b, p. 631). [26] According to Dyson, the series expansion of the S-matrix is divergent, and this has nothing to do with renormalization (Dyson 1952b). That is, even if there were no divergent integrals appearing in the terms of the S-matrix, the series would still be divergent. According to Dyson, if we try to make a full description of the interaction considering all the (infinite) terms of the power series expansion of the S-matrix, it can "only be an asymptotic series" (Schweber, 1994, p. 565). That is, according to Dyson's physical argument, we can expect at some point that the term of

[26] It is important to notice that Dyson's is a heuristic physical argument not a rigorous mathematical derivation. In my view, this is not a deficiency of Dyson's argumentation since we are considering a theory with an ill-defined mathematical structure.

order n+1 will not be smaller than the term of order n and the series starts to diverge: "the terms … will decrease to a minimum and then increase again without limit, the index of the minimum term being roughly of the order of magnitude 137" (Dyson, 1952b, p. 632). In Dyson's view the "divergence will not prevent practical calculations being made with the series" (Dyson, 1952b, p. 632). But Dyson's view was that in a certain way the theory only provided a basis for developing the S-matrix series expansion (Cushing, 1986, p. 122). In Dyson's own words: "I had this rather positivistic view that all QED was the perturbative series. So if that failed you didn't really have a theory" (quoted in Schweber, 1994, p. 565). Even if strict mathematical proof of the divergence of the S-matrix does not exist, further strong evidence in favor of Dyson's claim has been given in the last decades (Aramaki 1989, 91-92; West, 2000, 180-181; Jentschura, 2004, pp. 86-112; Caliceti et al, 2007, pp. 5-6). I will now look in more details into Dyson's argument and mention some of the contemporary results that reinforce his claims.

During the summer of 1951 while visiting the ETH In Zurich Dyson found a heuristic argument that convinced him that the perturbation theory, used trough the S-matrix series expansion, diverges. According to Dyson

> All existing methods of handling problems in quantum electrodynamics give results in the form of power-series in e^2. The individual coefficients in these series are finite after mass and charge renormalization ... The purpose of this note is to present a simple argument which indicates that the power-series expansions obtained by integrating the equations of motion in quantum electrodynamics will be divergent after renormalization … The argument for divergence is as follows. According to Feynman, quantum electrodynamics is equivalent to a theory of the motion of charges acting on each other by a direct action at a distance, the interaction between two like charges being given by the formula
>
> $$e^2\delta_+(s_{12}^2), \tag{1}$$
>
> where e is the electron charge. The action-at-a-distance formulation is precisely equivalent to the usual formulation of the theory, in circumstances where all emitted radiation is ultimately absorbed. We shall suppose that conditions are such as to justify the use of the Feynman formulation of the theory. Then let
>
> $$F(e^2) = a_0 + a_2e^2 + a_4e^4 + ... \tag{2}$$
>
> be a physical quantity which is calculated as a formal power series in e^2 by integrating the equations of motion of the theory over a finite or an infinite time. Suppose, if possible, that the series (2) converges for some positive value of e^2; this implies that $F(e^2)$ is an analytic function of e at e = 0. Then for sufficiently small values of e, $F(-e^2)$ will also be a well-behaved analytic function with a convergent power-series expansion.
>
> But for $F(-e^2)$ we can also make a physical interpretation. Namely, $F(-e^2)$ is the value that would be obtained for F in a fictitious world where the interaction between like charges is $[-e^2\delta_+(s_{12}^2)]$ instead of (1). In the fictitious world, like charges attract each other. The potential between static charges, in the classical limit of large distances and large numbers of elementary charges, will be just the classical Coulomb potential with the sign reversed. But it is clear that in the fictitious world the vacuum state as ordinarily defined is not the state of lowest energy. By creating a large number N of electron-positron pairs, bringing the electrons together in one region of space and the positrons in another separate region, it is easy to construct a "pathological" state in which the negative potential energy of the Coulomb forces is much greater than the total rest energy and kinetic energy of the particles. This can be done without using particularly small regions or high charge densities, so that the validity of the classical Coulomb potential is not in doubt. Suppose that in the fictitious world the state of a system is known at a certain time to be an ordinary physical state with only a few particles present. There is a high potential barrier separating the physical state from the pathological states of equal energy: to overcome the barrier it is necessary to supply the rest-energy for the creation of many particles. Nevertheless, because of the quantum-mechanical tunnel effect, there will always be a finite probability that in any finite time-interval the system will find itself in a pathological state. Thus every physical state is unstable against the spontaneous creation of large numbers of particles. Further, a system once in a pathological state will not remain steady; there will be a rapid creation of more and more particles, an explosive disintegration of the

vacuum by spontaneous polarization. In these circumstances it is impossible that the integration of the equations of motion of the theory over any finite or infinite time interval, starting from a given state of the fictitious world, should lead to well-defined analytic functions. Therefore $F(-e^2)$ cannot be analytic and the series (2) cannot be convergent. (Dyson, 1952b, pp. 631-632)

Almost at the same time as Dyson set forward his argument, C. A. Hurst, working on the so-called φ^3 theory concluded that the perturbative approach was divergent. In particular

He enumerated the number of graphs in field theories with the interaction Hamiltonian of general type and showed that the number of graphs with n vertices increases like $n^{n/2}$ as n increases so that the perturbation expansion cannot converge unless the matrix elements decrease with correspondingly great rapidity as n increases. He studied the case of a three-scalar field interaction $\lambda\varphi^3$ and obtained the conclusion, by evaluating a lower bound for the matrix elements, that in this case the perturbation expansion with respect to λ cannot converge. Hurst remarked that the excellent agreement of QED with experiment would indicate that the series is an asymptotic expansion about the singular point = 0, as Dyson conjectured. (Aramaki, 1989, pp. 91-92)

Dyson's and Hurst's results stimulated W. Thirring to investigate the convergence in the $\lambda\varphi^3$ theory, and he got the same conclusion regarding the series divergence (Aramaki, 1989, p. 92). Also the calculation of A. Petterman and A. Jaffe with particular models supported Dyson's contention that the renormalized perturbation series diverges (Gill & Zachary, 2002, p. 29). More evidence for the perturbation series divergence was found in recent years. According to U. D. Jentschura

A priori, it may seem rather unattractive to assume that the quantum electrodynamics perturbation series may be divergent even after the regularization and the renormalization. However, as shown by explicit nontrivial 30-loop calculations of renormalization group γ functions in a six-dimensional φ^3 theory, and in a Yukawa theory …, we believe that the ultimate divergence of the perturbative expansion can be regarded as a matter-of-fact, clearly demonstrated by explicit high-order calculations. (Jentschura, 2004, pp. 108-109)

For Dyson his 1951 conclusion on the divergence of the S-matrix approach meant the end of his involvement with quantum electrodynamics. According to Dyson

All my efforts up to that point had been directed toward building a complete convergent theory. Finding out that after all the series diverged convinced me that was as far as one could go … That was of course a terrible blow to all my hopes. It really meant that this whole program made no sense. (Quoted in Schweber, 1994, p. 565)

This makes it even more imperative to justify the perturbative approach (which provides excellent agreement with experimental results), and to explain how to get rid of large-order terms of a divergent series that simply would make it impossible to use the theory.

Just from a mathematical perspective the use of only a few terms of a divergent series is difficult to defend, but by considering the input physical assumptions of the theory the justification of throwing away large-order terms will become clear. In part it is related to the weakness of the interaction between the Maxwell and Dirac fields (Mandl & Shaw, 1984, p. 95). *This by itself can explain why a few order terms in a perturbative approach can give so good results*. But it does not by itself justify throwing away terms that should be smaller and smaller but which will ultimately result in a divergent series.

As mentioned, the scattering matrix amplitude S_{AB} can be written as (ψ_B^-, ψ_A^+), where we have $\lim_{t_0 \to -\infty} U(0,t_0)\varphi_A = \psi_A^+$ and $\lim_{t \to +\infty} U(0,t)\varphi_B = \psi_B^-$. Here U is the time displacement unitary operator determined by solving the Schrödinger equation, φ_A and φ_B are the initial and final free states, and the in and out states ψ_A^+ and $\psi_B^-$are taken to be eigenstates of the full interacting Hamiltonian (Schweber, 1961, pp. 317-323). Formally these interacting states can be derived from the (complete) S-matrix. Since the S-matrix series expansion is divergent we can conclude that we cannot obtain these interacting states (Scharf, 1995, pp. 314-318), i.e. it is not possible to find solutions of the coupled non-linear Maxwell-Lorentz and Dirac equations as (infinite) power series expansions in the coefficient *e* (the electric charge). In other words, it is not possible to find a solution for a closed interacting system of an electromagnetic field and charged particles (Dirac field).

Let us recall that the theory was structured around the idea that the interaction between radiation and matter is weak (due to the small coupling constant). We do not quantize the interacting system, but each field separately; i.e. when we speak of weak interaction this has two related aspects: one is that the interaction term in the Lagrangian (or Hamiltonian) is small; the other is that from this we are justified to consider the quantization of radiation and matter *separately* as the quantization of free fields, and to take the interaction term as a perturbative one.[27] As Dyson mentioned, quantum electrodynamics "is in its nature a perturbation theory starting from the non-interacting fields as … unperturbed systems" (Dyson, 1952a, p. 79). Since we are starting from the non-interacting fields, we need to use the adiabatic switching on/off trick to 'connect' the two quantized systems and so to be able to describe their interaction. Now, as we have just seen, if we try to describe within the theory the full weak interaction between radiation and matter (corresponding to determining the eigenstates of the full interacting Hamiltonian) we get into trouble (i.e. we obtain divergent results).

We conclude then that, *in practice* (i.e. in the theory we really have and work with), the notion of weak interaction implies an intrinsic approximate approach, i.e. there is, *in practice*, an unbridgeable gap between the notion of weak interaction and the idea of a full (complete) description of the (weak) interaction (since a full description of the interaction would correspond to obtaining a complete expansion of the S-matrix, which is not possible). Thus the divergence of the S-matrix series expansion implies that we *are unable* to bridge the gap that exists between our starting physical assumption of two independent unperturbed systems and the (*ideal*) closed system of fully interacting radiation and matter; and there is a good reason for this.

As Earman & Fraser showed from a *formal* consideration of fully interacting fields (corresponding to an exact solution that we cannot obtain in the case of quantum electrodynamics), we cannot describe them in terms of the Fock representation for free fields. This means that, *formally*, for a closed system of interacting fields we cannot use all the physical input of quantum electrodynamics associated with the notion of weak interaction of radiation and matter (in particular our starting physical assumption of two non-interacting fields); i.e. the *formal* considerations imply an, *in principle*,

[27] It is important to remember that contrary to what formal presentations of the theory might lead us to think (e.g. Dyson, 1952a, pp. 58-59; Källén, 1972, pp. 75-80), we do not start with a Lagrangian for an interacting system of radiation and matter and then due to practical problems in solving a set of coupled non-linear equations we feel forced to resort to perturbative calculations. On the contrary the theory was pretty much developed along two separate lines – one of them the quantization of the free electromagnetic field (a subject not addressed here) the other the development of a relativistic equation for the electron –, from the start taking into account, implicitly, that we were dealing with two clearly distinct weakly interacting physical entities: (quantized) charged particles and (quantized) electromagnetic field.

incompatibility between the notion of *weak* interaction as implemented in the theory and the (formal) notion of a closed system of fully interacting fields. Also, as we have seen, considering the complete series expansion of the S-matrix would correspond to the description of a closed system of fully interacting fields. *Here the formal results are valid*, i.e. we would have two contradictory mathematical results. This is not the case since the series expansion of the S-matrix is divergent.

We see then that we disregard the large-order terms not simply for pragmatic reasons but for physical reasons. Including these terms would correspond to an improper use of the mathematical structure of the theory beyond its physical content (in a tentative description of a closed system of radiation and matter): in quantum electrodynamics we have the concepts of radiation and matter, and of a weak interaction between them, not of fully interacting fields.[28] At this point *I would like to establish a correspondence between getting meaningful mathematical results and the way we set up the physical concepts in the theory*. In this case, (meaningful) approximate calculations of the *weak* interaction between different physical systems (radiation and matter).

I think that the situation we are facing here can be illuminated by recalling some of Bohr's views related to the Klein paradox and the problem with infinities in the theory (later addressed by renormalization). As we have seen, in the exchange of letters with Dirac in late 1929, Bohr addressed the negative energy problem of Dirac's equation. Bohr called attention to the fact that it arises from not taking into account the elementary unit of electrical charge in the determination of the actual potential barrier, i.e. from not considering the physical concepts inscribed in the theory. According to Bohr, if calculations are made in which this fact and the limits in the determination of the electron's position are not taken into account, we would be facing the

> actual limit of applying the idea of potentials in connection with possible experimental arrangements. In fact, due to the existence of an elementary unit of electrical charge we cannot build up a potential barrier of any height and steepness desired without facing a definite atomic problem. (Quoted in Moyer, 1981, pp. 1057)

In a nutshell, to Bohr the paradox resulted from "an unlimited [mathematical] use of the concept of potentials in relativistic quantum mechanics" (quoted in Moyer, 1981, p. 1058; see also Darrigol, 1991, pp. 154-155).

An analogous situation occurs with the (renormalizable) infinities in the theory. According to Alexander Rueger's presentation of Bohr's ideas,

> only for an [atomic] electron weakly interacting with the electromagnetic field could the radiation reaction, which would render the electron's orbit unstable, be ignored; as Bohr stressed repeatedly, strong interactions would make the idea of approximately stationary states of the electron in the atom impossible. (Rueger, 1992, pp. 317-318)

In these circumstances, Bohr recalls that "the whole attack on atomic problems … is an *essentially approximate procedure*, made possible only by the smallness of [the coupling constant]" (Bohr, 1932a, p. 378). That is, to Bohr

> the attempts to treat the radiation effects on rigorous lines by considering the atoms and the electromagnetic field as a closed quantum-mechanical system led to paradoxes arising from the appearance of an infinite energy of coupling between atoms and field. (Bohr, 1932b, p. 66)

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[28] With this justification for disregarding the large-order terms of the S-matrix series expansion, the excellent empirical results of the theory follow simply – in the perturbative approach – from the weakness of the interaction between the two *separately* quantized fields.

We have then, according to Bohr, that the physical conditions used to set up the theory imply an essentially approximate approach of an electron *weakly* interacting with the electromagnetic field. Like in the case of the Klein paradox if we extend the mathematical structure of the theory beyond its physical content we face a breakdown in the calculations. In my view, this is exactly the situation we are facing with the divergence of the S-matrix series expansion.

When trying to close the gap between two weakly interacting systems (described by an approximate approach) and fully interacting fields (corresponding to obtaining the exact solution for a closed quantized system of interacting fields), we face 'the actual limit of applying the idea' of non-interacting fields that are part of our physical input assumptions.

What we have then is the impossibility of defining within the theory a fully interacting state from the two fields that are defined and quantized as independent entities. Thus, in my view, we have a theory that is able, on an approximate level, to describe (using a few terms in perturbative calculations) the interaction between two separate fields, and not a theory describing as a whole a system of fully interacting fields. From a formal perspective the Haag theorem says that it is not possible to connect the separate fields with (fully) interacting fields when starting from the physical assumptions used to articulate the theory, i.e. from the notion of weak interaction as it is implemented in quantum electrodynamics.

In the theory the consequences of the Haag theorem are circumvented not because we are facing a "canonical framework mathematically ill-defined" (Fraser, 2006, p. 90) but because *we are not even trying to describe a system of (fully) interacting fields* (this eventual possibility is excluded *in practice* due to the divergence in the series expansion of the S-matrix and *in principle,* on formal grounds, by the above mentioned incompatibility between the notion of weak interaction as it is implemented in the theory and the formal results related to interacting fields). We are just trying to describe, by an 'essentially approximate procedure', the weak interaction between radiation and matter as distinct systems.[29] Thus, there is no conflict in quantum electrodynamics with the Haag theorem.

As the divergence in the series expansion of the S-matrix shows, the Lagrangian of quantum electrodynamics does not provide us with the possibility of describing a system of interacting Dirac and Maxwell fields, but with the possibility to describe in an intrinsically approximate way the interaction between the two fields. The descriptions of interactions in the theory are based on the use of the Fock space for each field and the idea of (virtual) quanta exchange. There are no alternatives in quantum electrodynamics. From the start the theory was not developed to treat the question of fully interacting fields, but to treat the question of the interaction between distinct fields that are separately quantized. To consider that "Fock representations are generally

[29] However I agree with Fraser's view that we cannot apply Haag's theorem when working with a "canonical framework mathematically ill-defined" (Fraser, 2006, p. 90). What I do not agree with is Fraser's view that renormalization is the factor that makes it possible to evade the consequences of Haag's theorem enabling the theory to be effective (also, as I mentioned, there are other factors which can be taken to render the theory mathematically ill-defined). That is because, in my view, in quantum electrodynamics, the problem of circumventing the Haag theorem is included in the broader problem of explaining how the theory can give so good results. This involves addressing the divergence of the S-matrix series expansion (necessary to justify the perturbative approach) and circumventing the Haag theorem. But these are not unrelated matters. In reality, as we have seen, when addressing the divergence of the S-matrix series expansion, the consequences of Haag's theorem become irrelevant (independently of the fact that we are considering a mathematically ill-defined approach).

inappropriate for interacting fields" (Earman & Fraser, 2006, p. 330) is, in the context of quantum electrodynamics, to turn upside down the theory as it was developed. The theory is built on top of the physical idea of independent entities whose interaction describes change in nature. When accepting this approach, and its intrinsic limitations, it is difficult to consider inappropriate, at least from an empirical point of view, the results of quantum electrodynamics; and so, contrary to Earman and Fraser's views, we can retain the concept of quanta in the description of interactions.

4 A note regarding the concept of vacuum in quantum electrodynamics

The revision of the role of the Lagrangian of quantum electrodynamics as simply giving rise to an essentially approximate approach has immediate consequences on the interpretation of the mathematical formalism of the theory. According to this view, even if from an abstract point of view we can talk about the Hilbert space of the physical states of the full Hamiltonian of the two fields and their interaction, from a physical point of view we cannot build up these formal states from the individual states corresponding to each field by itself. Since the theory gives rise only to approximate procedures we can only build a physical description of the interaction between the fields with low-order perturbative calculations using the individual states of each field.[30] This

[30] This does not mean that we do not need to take into account for example the renormalization of the electron's mass and charge to get agreement with experimental results. The point is the interpretation given to this. From an experimental point of view it might seem that the so-called physical electron with its 'cloud' of virtual photons (the renormalized quanta of the Dirac field) is the physical concept of particle we have in the theory when considering bound electrons. But recalling again Bohr's ideas we see that that is not the case when making our considerations from the perspective of the physical-mathematical structure of the theory. According to Bohr, "the classically estimated ratio between the radiative reactions on the electron and the nuclear attraction is … of the same order of magnitude as α^3 [where α is the fine structure constant]. It is just this circumstance which affords a justification for the neglect of the radiative reaction in a description of the stationary states including the fine structure" (Bohr, 1932b, p. 66). In this way, according to Bohr, "in the account of the simplest features of the radiation phenomena, we may neglect entirely the radiation reaction in the calculation of the transition probabilities" (Bohr, 1932b, p. 67). But Bohr considers possible "the treatment of such problems as the width of spectral lines and the retardation effects in the interaction of electrons bound in atoms. Still, the condition for such applications is that the effects in question can be treated as small perturbation of the phenomena to be expected if the finite propagation of forces would be neglected" (Bohr, 1932b, p. 67). That is, we *must* consider the electron's self-energy (due to the radiation reaction) as a small perturbation to the 'bare' electron in a central Coulomb potential, in order to justify for example the Lamb shift calculation regarding the energy shift of *stationary states* of the electron in the atom. As Rueger called attention to, "Bohr stressed[ed] repeatedly, [that] strong interactions would make the idea of approximately stationary states of the electron in the atom impossible" (Rueger, 1992, p. 317).

Considering the theory as giving rise only to essentially approximate procedures, *we do not really have a coherent quantum electrodynamical concept of a self-interacting electron*, which would be "always in interaction with the surrounding cloud of virtual particles" (Thirring, 1958, p. 140). Another aspect, related to this is the following: in quantum electrodynamics we describe the physical processes as resulting from the interaction of two clearly distinct fields (which are quantized as free independent fields). Due to the mass renormalization there is a mismatch between the concept of electron as quanta of the Dirac field and the applications where the electron is described by taking into account also the electromagnetic field. When considering the electron's mass, we can no longer make the simple association of the electron to quanta of the Dirac field. In the applications of the theory we must consider the electron's mass as resulting from a contribution from the two fields. It is clear that when we go beyond the lowest-order approximations, and the mass renormalization is needed to render the results finite, we cannot maintain a simple identification of the electrons with quanta of the Dirac field. The observed 'particle' – the electron – is built, in the applications of the theory, from contributions from the two fields (I will came back to this in the next chapter).

means in particular that *there is no physical meaning within quantum electrodynamics to the concept of vacuum (ground state) of the interacting fields*. It is usually thought that the coupled fields vacuum state can be "formally expanded as a superposition of ϕ_0" (Redhead, 1982, p. 86; Schweber, 1961, p. 655), where ϕ_0 are the vacuum states of the free fields. But in the theory we really have, this is a vacuous mathematical statement without any physical counterpart. This does not imply that the concept of vacuum is not relevant in the theory, as we have just seen in the previous chapter.

5 Conclusions

As we have seen, Haag's theorem implies that the perturbative approach used in quantum electrodynamics to treat the interaction between the quantized Maxwell and Dirac fields is not mathematically consistent. This brings up two big questions. How can the way the theory is implemented (giving a prominent role to the concept of quanta in the description of interactions) be justified? And even more importantly, "why perturbation theory works as well as it does" (Earman & Fraser, 2006, p. 307). Earman and Fraser do not provide any answer to this last question as regards quantum electrodynamics. And with respect to the first question, Fraser merely proposes to take shelter in the ill-defined mathematical structure of the theory to justify the inapplicability of the Haag theorem (Fraser, 2006, p. 90). However this argument has no explanatory power. It is an argument based solely on the mathematical structure of the theory (not taking into account its physical content) and it is not providing an explanation of the good results and soundness of the perturbative S-matrix approach.

According to Dyson the series expansion of the S-matrix, used in the description of scattering (and bound state) processes, is divergent. This indicates that the theory only provides a description of interactions using a few lower-order terms (which works well due to the small coupling constant between the fields). This means that the theory can only provide results if we are close to a free field situation. In other words, only when considering the interaction between two different fields as a small perturbation to their individual free states can the theory provide results in agreement with experiments.

We see that one has problems when trying to give a full description of the interaction, which corresponds to treating matter and radiation as one closed system. This would imply to go beyond the initial physical set up of the theory based on the idealization of totally non-interacting fields. In this way I think that quantum electrodynamics can be seen as providing only an approximate approach to the description of the interaction between two fields taken to be different physical systems. Only the lower-order terms of the series expansion can be kept. To take into account the large-order terms would mean to disrupt the physical input assumptions provided by the implementation of the notion of weak interaction (i.e. the possibility of quantization of free fields and the description of their interaction perturbatively, using the adiabatic switching on/off of the interaction). Due to the small coupling constant between the fields, the lower-order terms already provide good results.

From this perspective, how can Earman and Fraser's conundrum be solved while saving the use of quanta in the description of interactions? It is true that we are in an ill-defined mathematical context. However, we do not really need that to make the consequences of the theorem irrelevant in the theory. If we forget about Haag's theorem and set the machinery into motion, we face the situation that we cannot go from a free fields situation to a fully interacting fields situation (exactly as the Haag theorem says). This occurs because we are stretching the physical concepts too much and the

calculations break down, i.e. we have a theory describing the weak interaction between different fields, not a theory describing fully interacting fields. In this way we are outside the scope of Haag's theorem.

Regarding the concept of quanta – which follows naturally from the quantization procedure – this is, as we have seen, a central concept in the quantum electrodynamical description of the weak interactions between the fields (as this description involves free-particle Fock spaces). However we are left with a tension regarding the concept of quanta. The point is that we start with the idealization of non-interacting fields, and, as we have seen, we need the unphysical adiabatic switching on/off trick to set quantum electrodynamics as a perturbation theory into motion. The problem is that when addressing scattering problems, we take the particles (for example electrons) to be far apart before (and after) the scattering, and because of this not interacting (i.e. electrons as quanta of the Dirac field without self-interaction). In this way, we are describing the particles *observed* after the scattering process is over with the idealization of charged particles with a 'disconnected' charge, and this is rather unphysical – since implicit in the possibility of observation of an electron is the possibility of electromagnetic interaction with it.

CHAPTER 6

ASPECTS OF RENORMALIZATION IN QUANTUM ELECTRODYNAMICS

1 Introduction

The appearance of divergent integrals in higher-order calculations in quantum electrodynamics where the so-called radiative corrections are taken into account has been seen as, at least, indicating that the theory fails for high energies. As J. Schwinger stated, "electrodynamics unquestionably requires revision at ultra-relativistic energies" (quoted in Aramaki, 1989, p. 93). Even considering the accuracy of the theory at lower energies, Schwinger considered that the renormalization procedure, that permits avoiding the infinites in the results of calculations, ultimately has to be excluded from physics (Cao & Schweber, 1993, p. 50). Regarding this problem the position of P. Dirac was even less sympathetic: "I am very dissatisfied with the situation, because this so-called "good theory" does involve neglecting infinities which appear in its equations" (quoted in Kragh, 1990, p. 184). In general the position of leading physicists was very critical regarding quantum electrodynamics, and some pinpointed structural problems that go beyond the high-energy behaviour of quantum electrodynamics. For example N. Bohr considered that the whole program only made sense taking into account the weakness of the coupling constant, which means applying the theory only in situations where the electron interacts weakly with the electromagnetic field (Rueger, 1992, p. 317).

In this chapter I will offer a historical account of the renormalization program and recover the views of several physicists that I think permits a more enlightening account of the meaning of renormalization than more recent accounts. In sections 2 and 3 the historical emergence of the problem of infinites in quantum electrodynamics is considered, as well as the 'provisional' solution attained in the late forties with the completion of a renormalization program. The historical approach will enable to recover forgotten aspects of Dirac's subtraction physics and relate them to some of Bohr's views. This will enable a different view regarding renormalization than the one that has become 'standard'. The conceptual motivation behind Dirac's subtraction physics is to be contrasted with the post-war attitude of the physicists that completed a working renormalization approach. We will look in particular into the contributions of Schwinger and Feynman. Feynman's regularization approach is to be contrasted with Dirac's subtraction physics (which technically is similar) in its lack of any conceptual justification for regularization. Looking in detail into Feynman's work will also enable us to follow his first-hand account of his overall space-time approach to the description of interactions. This is an important subject whose conceptual implications will be developed in the next chapters.

Some more technical details of the renormalization program are considered in sections 3 and 4: the calculation of the self-energy of the electron and the photon, and

the role of the cut-off procedure that provides a 'regularization' of the theory, previous to the renormalization proper. We will see that mass renormalization brings with it a mismatch with the presupposition in the theory of two different fields independently quantized. The electrons (and positrons) are taken to be quanta of the Dirac field, characterized in part by what are called the bare mass and bare charge. According to the applications of the theory the bare mass of the electrons has no observational meaning; the observed mass results from a simultaneous contribution from the Dirac and Maxwell fields. In this way we cannot associate the electron exclusively to quanta of the Dirac field. It will also be addressed not only the dubious mathematical procedure related with the calculation of the photon's self-energy, but also the even more dubious – from a physical point of view – procedure of attaching the infinite constant that pops out in the photon self-energy calculation to the charges of the electrons 'connected' by the photon in an interaction process. In particular the charge renormalization procedure is considered in a second-order radiative correction to the Møller scattering amplitude. We will in this case notice limitations regarding the temporal description of physical processes, which are related with the charge renormalization procedure.

2 The emergence of infinites in quantum electrodynamics

When in 1929-30, Heisenberg and Pauli presented in two papers a relativistic quantum theory of the interaction between the quantized Maxwell and Dirac fields, they moved from Heisenberg's first view that the self-energy of the electron did not constitute a problem and the infinite Coulomb self-energy could be neglected, to a more circumspect position recognizing that this problem might even render the theory inapplicable (Darrigol, 1984, pp. 484-486). In the first paper, published in 1929, Heisenberg and Pauli discarded the infinite Coulomb self-energy of the electrons as they did with the zero-point energy of the vacuum, because they considered these divergences to be irrelevant infinite constants that disappear as soon as one evaluates quantities that are observable like the difference between two energy eigenvalues. Also according to Pauli,

> the theory can be called a correspondence theory, insofar as all expressions for the Lagrangian of the field are indeed taken over directly or indirectly from the classical theory … I believe that we have now arrived at the natural limit of range of the correspondence idea on the basis of wave mechanics. Our theory naturally fails at all places where the classical picture fails. (Quoted in Mehra & Rechenberg, 2000, p. 316)

It is well know that in the classical theory of a point-like electron we already have a problem with the electron's self-energy: it is infinite. Even so Pauli had aesthetic reservations regarding the self-energy problem in quantum electrodynamics, and even though he considered that the infinite constants might be removed in practical calculations they represented a 'defect of beauty in principle' (quoted in Mehra & Rechenberg, 2000, p. 316). According to J. Mehra and H. Rechenberg, in the section 8 of their paper, Pauli and Heisenberg

> progressed to a perturbation scheme … under the assumption that the interaction terms could be expanded in a series of small perturbations … The Heisenberg-Pauli solution, however, also contained divergent terms of the form $1/r_{PP}$ (the subscript P referring to the position of the particle), which corresponds to the self-interaction of the charged particle, say, the electron. This additive infinite term occurring in the energy of the total system may simply be neglected (subtracted), so long as the number of electrons does not change. (Mehra & Rechenberg, 2000, p. 325)

By the middle of 1929 Pauli (with whom J. R. Oppenheimer had began to collaborate) was seeking to improve the theory he had developed with Heisenberg. A three-man paper was being planned, where in particular Jordan's criticism regarding gauge invariance would be addressed (Mehra & Rechenberg, 2000, p. 327). By July 1929 Heisenberg still felt that "the catastrophic self-interaction of the electron does not disturb me too much" (Mehra & Rechenberg, 2000, p. 328). Finally Heisenberg and Pauli published a second part of their quantum electrodynamics in 1930, and Oppenheimer published a separate note regarding specifically the self-energy problem. In their paper Heisenberg and Pauli obtained Oppenheimer 's result for the Coulomb self-energy of the electron. Now however they recognized that the infinite self-energy, "in many cases will make application of the theory impossible" (quoted Miller, 1994, p.34). Also, the fact that the self-energy problem could not simply be traced back to a similar situation occurring already in classical electrodynamics was soon revealed by Oppenheimer (1930b) who found out a new (infinite) contribution to the self-energy without any classical counterpart. Using Dirac's second-order perturbation formula

$$H_{fi} = \sum_j \frac{H^1_{fi} H^1_{ji}}{E_i - E_j},$$

and adopting

$$H^1 = -\int \vec{j}\vec{A}^{tr} d\vec{x}, \quad \vec{j} = ie\overline{\psi}\vec{\gamma}\psi$$

for the perturbation term in the Hamiltonian H^1, we can consider the particular case where i = j. This situation represents the perturbation to the energy of the electron's state i arising from the self-interaction of the electron. Considering for simplicity a single free electron (with momentum **p** and energy $E(p) = c(p^2 + m^2c^2)^{1/2}$), the sequence of transitions i → j → i is

$$e \rightarrow e' + \text{photon} \rightarrow e.$$

According to A. Pais the "virtual states [e' + photon] correspond to all momentum-conserving partitions of **p** between e' and the photon. There are infinitely many such states" (Pais, 1986, p. 373). The self-energy of the electron is found to be

$$W(\vec{p}) \sim \frac{e^2\hbar^2c^2}{\hbar cE(p)} \int k\, dk,$$

in addition to smaller terms including the electrostatic (Coulomb) self-energy. What Oppenheimer obtained with this result was that while the classical self-energy diverges linearly (~ 1/r) as we take the electron radius to approach the point-like limit (r → 0), the quantum electrodynamical calculation predicted also a quadratic divergence of the term W(**p**). Also, $W(\mathbf{p}_1) - W(\mathbf{p}_2)$ is not finite (as Heisenberg and Pauli initially expected) but also infinite, which means, "as Oppenheimer stressed, [that] self-energy effects causes infinite displacements of spectral lines" (Pais, 1986, p. 373). A disastrous result for quantum electrodynamics.

The situation of quantum electrodynamics during the thirties did not improve, on the contrary. As we have seen, to solve inconsistencies of his electron theory related to the existence of negative-energy solutions, Dirac proposed his hole theory. From this, a new infinity problem popped out. In Dirac's hole theory we have an infinite sea filled with negative-energy electrons. This made Dirac consider that the electromagnetic field is generated by "the difference in the electric density from its value when the world is in its normal state (i.e. when every state of negative energy and none of positive energy is occupied)" (quoted in Pais, 1986, p. 378). That is, the Maxwell-Lorentz equation for the electric field is given, in Dirac's hole theory, by Div $\mathbf{E} = -4\pi(\rho - \langle\rho\rangle_{vaccum})$.

Going back to chapter 3, we can recall that in his 1930 paper on the hole theory Dirac remarked that "in the general case of an arbitrary varying electromagnetic field we can make no hard-and-fast separation of the solutions of the wave equation into those referring to positive and those to negative kinetic energy" (Dirac, 1930, p. 361). The knowledge of this situation led Dirac to consider in more detail the effect of an 'external' electromagnetic field (that could simply result from the presence of a sole electron above the negative-energy sea) on the definition of the 'normal' state (vacuum state) of the negative-energy sea. According to Dirac

> when applied to space in which there is an electromagnetic field, … one must specify just which distribution of electrons is assumed to produce no field and one must also give some rule for subtracting this distribution from the actually occurring distribution in any particular problem. (Quoted Schweber, 1994, p. 114)

In a letter to Bohr from September 10, 1933, Dirac summarized his findings:

> Peierls and I have been looking into the question of the change in the distribution of negative-energy electrons produced by a static electric field. We find that this changed distribution causes a partial neutralization of the charge producing the field. If it is assumed that the relativistic wave equation is exact, for all energies of the electron, then the neutralisation would be complete and electric charges would never be observable. A more reasonable assumption to make is that the relativistic wave equation fails for energies of the order $137mc^2$. If we neglect altogether the disturbance that the field produces in negative-energy electrons with energies less than $-137mc^2$, then the neutralization of charge produced by the other negative-energy electrons is small and of order 1/137. We then have a picture in which all the charged particles of physics electrons, atomic nuclei, etc. have effective charges slightly less than their real charges, the ratio being about 136/137. The effective charges are what one measures in all low energy experiments, and the experimentally determined value for e must be the effective charge on an electron, the real value being slightly bigger. (Quoted in Schweber, 1994, p. 116)

Dirac presented his results at the seventh Solvay Congress held in October 1933. Due to the fact that in relativistic mechanics the energy is given by $W^2 = m^2c^4 + c^2p^2$, it can take positive and negative values. According to Dirac, "it has not been possible to develop a relativistic quantum theory of the electron in which the transitions from a positive to a negative value of the energy should be excluded" (Dirac, 1934a, p. 136). In particular transitions between the positive and negative energy states are "predicted in general for all processes putting into play exchanges of energy of the order mc^2" (p. 136). Dirac considered that

> it seems there are no reasons of principle against the applicability of the quantum mechanics to similar exchanges of energy. It is true that quantum mechanics does not seem applicable to phenomena which involve distances of the order of the classical radius e^2/mc^2, since the present theory can in no manner discuss the structure of the electron. But such distances, considered as electron wavelengths, correspond to energies of the order $(\hbar c/e^2)(mc^2)$, which are much greater than the changes in question. It seems that the most reasonable solution is to search for a physical meaning for the negative energy states. (pp. 136-137)

Dirac went on to present again his hole theory which gave a physical interpretation for the negative-energy states:

Let us admit that in the universe such as we know it, the states of negative energy are nearly all occupied by electrons, and that the distribution thus obtained is not accessible to our observation on account of its uniformity throughout space. Under these conditions every unoccupied negative energy state represents a break in that uniformity, and must reveal itself as a kind of hole. It is possible to admit that these holes constitute positrons.

This hypothesis resolves the principal difficulties of the interpretation of the states of negative energy … the hole takes exactly the aspect of an ordinary particle, positively electrified. (p. 137)

Dirac then addresses the problem facing his interpretation when an external field is present. As already mentioned when there is no external field it is simple to take into account the infinite negative-energy sea in the Maxwell-Lorentz equation by considering that "the distribution of electrons produces no field in which no state of positive energy is occupied. And that it is the deviations from that distribution which determine the fields" (p. 138). However as Dirac acknowledges, this hypothesis

is completely satisfactory when it is a question of a region of space where there exists no field, and where the distinction between the positive energy states and those of negative energy is cleanly defined; but one must specify when it is a question of a region of space where the electromagnetic field is not zero in order to be able to lead to results free of all ambiguity. We must specify mathematically which distribution of electrons is supposed to produce no field, and also give a rule for subtracting that distribution from the one which exists effectively in each particular problem, in such a way as to obtain a finite difference that can figure into equation [div $\mathbf{E} = -4\pi\rho$], since, in general, the mathematical operation of subtraction between two infinities is ambiguous. (p. 138)

Dirac set out to consider the case of a weak, time-independent electrostatic field using the Hartree-Fock approximation. Dirac defined the density matrix R as

$$(q'|R|q'') = \sum_r \overline{\psi}_r(q')\psi_r(q''),$$

where the ψ's are four-component wave functions that are solutions of Dirac's equation for each individual electron, and the summation runs over all occupied negative energy states. The wave functions are determined in the Hartree-Fock approximation, where each electron is taken to move in an effective field that is the same for all electrons. The equation of motion for R is

$$i\hbar\dot{R} = HR - RH,$$

where $H = c\rho_1(\boldsymbol{\sigma}, \mathbf{p}) + \rho_3 mc^2 - eV$ is the Hamiltonian for an electron moving in the electric field $\mathbf{E} = -\nabla V$; also due to the exclusion principle we must have $R^2 = R$. Dirac assumes that the distribution R_0 that produces no field is given by

$$R_0 = \frac{1}{2}\left(1 - \frac{W}{|W|}\right),$$

where $W = c\rho_1(\boldsymbol{\sigma}, \mathbf{p}) + \rho_3 mc^2$ is the kinetic energy of an electron. Dirac then looks for a "permanent state for which the equation of motion $i\hbar\dot{R} = HR - RH$ reduces to $HR - RH$

= 0" (p. 139). In particular Dirac looks for a solution of the form $R = R_0 + R_1$ where R_1 is a quantity of first order in V. Dirac considers that

the quantity that interests us is the electric density corresponding to the distribution R_1. In order to obtain it we must form the diagonal sum of R_1, with respect to the spin variables, and then take the general diagonal element, multiplied by –e, of the resultant matrix with respect to the position variables x. (p. 140)

Dirac denotes this quantity by $D(R_1)$. Dirac found that when doing the integration of the expression for $D(R_1)$, "the result contains an infinite logarithm" (p. 141). Dirac's reaction was to use a cut off which rendered the result finite. But, according to Dirac there is a physical justification in the use of a cut off:

We could believe, at first sight, that the presence of that infinity renders the theory unacceptable. However, we cannot assume that the theory applies when it is a question of energies greater than the order of $137mc^2$, and the most reasonable way to proceed seems to be to limit arbitrarily the domain of integration to a value of the momentum … corresponding to electron energies of the order indicated. (p. 141)

This is an important point. As we have seen, Dirac had mentioned that

quantum mechanics does not seem applicable to phenomena which involve distances of the order of the classical radius e^2/mc^2, since the present theory can in no manner discuss the structure of the electron … such distances, considered as electron wavelengths, correspond to energies of the order $(\hbar c/e^2)(mc^2)$ [$\cong 137mc^2$]. (pp. 136-137)

This goes along the lines of Bohr's views on quantum electrodynamics. In Bohr's terms an unbound limit of integration would mean to apply the theory not taking into account the physical assumptions used to set up the theory, since we would be disregarding that the theory treats the electron as a point-charge; in it we are always considering distances larger than the electron's 'diameter' (Bohr, 1932b, pp. 63-64). In his Faraday lecture Bohr mentioned that

The scope of the quantum mechanical symbolism is essentially confined, however, to problems where the intrinsic stability of the elementary electrical particles can be left out of consideration in a similar way as in the classical electron theory. In this connexion, *it must not be forgotten that the existence of the electron even in classical theory imposes an essential limitation on the applicability of the mechanical and electromagnetic concepts. Indeed, the finite propagation of electromagnetic forces brings with it the existence of a fundamental length, the so-called "electron diameter" defining a lower limit for the extension of the region where the idealization according to which the electron is considered as a charged material point is justifiable*. Not only would a concentration of the charge of the electron within a smaller space result in an essential modification of its mass, but we even meet here with a limitation of the unambiguous use of the idea of inertial mass. In fact, we lose any simple basis for a sharp separation between ponderomotoric forces and radiative reactions when we consider processes in which the electron undergoes a velocity change of the same order as the velocity of light within a length of path equal to the electron diameter. It is true that such considerations lose their significance to a large extent on account of the existence of the quantum of action which imposes an essential limit to the analysis of motion. *The fertility of quantum mechanics as applied to the problem of atomic stability lies just in the fact that the linear dimensions of the regions ascribed to even the firmest electron-bindings outside the nucleus are still very large compared with the classical electron diameter*. (Bohr, 1932a, pp. 377-378 [my emphases])

Returning to Dirac's take on the logarithmically divergent integral, Dirac considered that

if P is the value of the vector momentum … to which we limit the integration domain, the final result, obtained after a complicated integration, is:

$$-e\left(x\left|D(R_1)\right|x\right)=-\frac{e^2}{\hbar c}\frac{2}{3\pi}\left(\log\frac{2P}{mc}-\frac{5}{6}\right)\rho-\frac{4}{15\pi}\frac{e^2}{\hbar c}\left(\frac{\hbar}{mc}\right)^2\nabla^2\rho\,,$$

where ρ is the electric density producing the potential V, so that

$$\nabla^2 V = -4\pi\rho,$$

and where the terms containing the derivatives of ρ of order greater than second have been neglected. (Dirac, 1934a, p. 141)

Now, Dirac's view was that we could not apply the theory for energies greater than $137mc^2$. This means taking the cut off P to be of order 137mc. For this cut off value the first term in the expression for $-e\left(x\left|D(R_1)\right|x\right)$ is equal to $-(e^2/\hbar c)\,\rho$ (Dirac took the second term not to be an important correction in the present conditions). Dirac's interpretation of this result is as follows:

As a result of the foregoing calculation, it would seem that the electric charges which one ordinarily observes on electrons and protons and the other particles of physics are not the actual charges which these particles carry (appearing in the fundamental equations) but are all slightly smaller, in a ratio of about 136/137. (Quoted in Schweber, 1994, pp. 115-116)

Dirac tried to improve his approach by presenting a more systematic procedure, which, contrary to the previous case (Dirac 1934a), was relativistic and might be applied to the case of external time-dependent fields. In a letter to Bohr of November 10, 1933, Dirac mentioned his new approach:

I have been working at the problem of the polarization of the distribution of negative-energy electrons, from a relativistic point of view. If I have not made a mistake, then there is just one relativistically invariant, gauge invariant treatment, which gets over all the difficulties connected with the infinites, to the accuracy with which the Hartree-Fock method applies … I have not yet seen whether this relativistic treatment leads to any kind of compensation of charge arising from the vacuum polarization. (Quoted in Schweber, 1994, p. 117)

In his development of the density-matrix formalism Dirac again considers the density matrix R; and again it is considered that

each electron moves in a definite electromagnetic field, which is the same for all electrons. This field will consist of a part coming from external causes and a part coming from the electron distribution itself, the precise way in which the latter part depends on the electron distribution being one of the problems we have to consider. (Dirac, 1934b, p. 146)

Dirac's objective was to find "some natural way of removing infinities from $\sum_k \left(xt\left|R\right|xt\right)_{kk}$ and $\sum_k \left(xt\left|\alpha_s R\right|xt\right)_{kk}$ [which is the current density] so as to leave finite remainders" (p. 148).

In the case of no external field, Dirac found that the singularities of $\left(x't'\left|R\right|x''t''\right)_{k'k''}$ all occurred in the light cone (p. 151). In the case of an external field present, Dirac supposed "that the singularities are of the same form as in the case of no field, but have unknown coefficients" (p. 152). Dirac showed that the density matrix could be divided into two parts $R = R_a + R_b$, where R_a contains all the singularities and "the electric and current densities corresponding to R_b are those which are physically

present, arising from the distribution of electrons and positrons. (p. 156). Dirac's idea was that with this division of R in two parts "we can remove the infinities" (p. 156).

Since the singularities were located in the light cone, this means that when $x = x' - x'' \neq 0$ R_a is finite. According to Pais, "Dirac's prescription for extracting finite results was: first subtract these singular terms, then let $x \rightarrow 0$" (Pais, 1986, p. 382). Also, according to A. I. Miller, "the intent, of course, is to propose a counter-term $-R_a$ so that $R - R_a$ and, consequently, the measured charge densities are finite. This will be accomplished by Heisenberg" (Miller, 1994, p. 60).

The uniqueness of Dirac's subtraction method was immediately questioned (Miller, 1994, p. 60; Pais, 1986, p. 383). Heisenberg tried to improve Dirac's method, and in the process, due to his use of a second quantized version of Dirac's formalism in which electron and positrons were treated in a symmetrical way, came up with the existence of an "infinite self-energy of the light-quanta" (Heisenberg, 1934, p. 186). According to Heisenberg, when "compared to Dirac's treatment, [his] paper emphasizes the significance of the conservation laws … and the necessity of formulating the basic equations of the theory in a manner extending beyond the Hartree approximation" (p. 169). In the first part of his paper Heisenberg used the density matrix formalism. Following Dirac's approach Heisenberg considers that "one will have to subtract from the density matrix [R_s] another density matrix [S] which is determined uniquely by the external fields, in order to obtain the 'real' density matrix [r, i.e. a density matrix without singularities]" (p. 171). The problem with Dirac's method is according to Heisenberg that it does not provide a unique specification for S and because of this for the equation of motion of the system (p. 172). Heisenberg's idea is that "by taking into account the conservation laws of charge, energy, and momentum, the possibilities for S can be restricted insofar that a particular value can be distinguished as the simplest assumption" (p. 172). Heisenberg went on to calculate the vacuum polarization, obtaining a corrected second term for the induced charge density (Miller, 1994, p. 64). Like Dirac, Heisenberg took this term as having no physical significance. This is not the case. As shown in 1935 by E. Uehling, this term yields measurable effects. Uehling found for the hydrogen atom the level 2S to be displaced by $\Delta\nu = -27$ megacycles per second (Pais, 1986, p. 383).

In the second part of his paper Heisenberg extended the formalism, treating the Dirac wave function as a quantized Dirac field and also treating the electromagnetic field as a quantized field. In this part Heisenberg gave a symmetrical treatment to electrons and positrons being both treated on equal footing as quanta of the quantized Dirac field (Heisenberg, 1934, p. 183). Adopting Hamiltonian methods, Heisenberg noted that the subtraction of infinites could be done order by order in perturbation theory, noticing nevertheless the presence of self-energy-like terms that the subtraction procedure could not remove (Schweber, 1994, p. 118). According to Heisenberg "the perturbation method can be continued in principle, unless an infinite self-energy causes the method to diverge" (Heisenberg, 1934, p. 184).

This formalism enabled Heisenberg to treat, in particular, the creation and annihilation of electron-positron pairs. Heisenberg found that the process by which a photon creates an electron-positron pair, which subsequently annihilates creating a photon, gives rise to a logarithmically divergent term. Heisenberg interpreted this term (in analogy to the electron's self-energy) as the (infinite) self-energy of the light quanta: "we shall treat the matter density associated with a light quantum and in particular the self-energy of the light quantum derived on the basis of this matter density ... The energy of this matter field becomes infinite, in precise analogy to the infinite self-energy of the electrons" (p. 185).

Regarding the self-energy problems there was not much improvement during the thirties. The only solid result was V. F. Weisskopf's demonstration that the electron self-energy is 'only' logarithmically divergent (Pais, 1986, p. 385). Going back to Oppenheimer's calculation of the electron's self-energy (Oppenheimer, 1930b), Oppenheimer found using single-particle theory (i.e. Dirac's equation as a one-electron equation) a new quantum-mechanical term in the electron's self-energy that diverges quadratically. Weisskopf completed in early 1934 a second-order calculation of the electron's self-energy in hole theory (Weisskopf, 1934, p. 158). Weisskopf divided the electron's electromagnetic field in two parts: a rotation-free part and a divergence-free part. According to Weisskopf the electrostatic self-energy is given by

$$E^S = \frac{1}{2}\int \rho\Phi' \, d\vec{r} \,,$$

and the electrodynamic self-energy is given by

$$E^D = -\frac{1}{2}\int (\vec{i}_{tr}\vec{A}_{tr}) d\vec{r}$$

where $\mathbf{i}_{tr}$ is the divergent-free part of the current density. Expanding the self-energy operators by powers of the electric charge, in the second-order calculation only terms proportional to e^2 are kept. The electrostatic self-energy calculated in the Dirac single-electron theory diverges linearly. Weisskopf made his calculation in hole theory, i.e. considering a multi-electron system where all the states with negative energy are occupied. According to Weisskopf, "to calculate the self-energy of a multi-electron system, it is advantageous to use the method of quantized waves, in which the charge and current densities act as operators on the eigenfunctions, whose variables are the occupation numbers $N^k(\mathbf{p})$ of the stationary states $\mathbf{p}^k$, k=1, …, 4 of the free electron" (p. 160). He then calculated the diagonal element of the self-energy operator E^S for a particular occupation of states. In this way, in the expression for the electrostatic self-energy there is a summation over all the negative-energy states plus the occupied positive-energy state: the electron whose self-energy we want to calculate. Weisskopf found that "the electrostatic self-energy diverges *logarithmically* in the 'hole' theory" (p. 163). In this work Weisskopf made a mistake in the calculation of the electrodynamic part of the self-energy, obtaining initially a quadratic divergence (like in Oppenheimer's calculation). Soon after W. Furry called Weisskopf's attention to his error. In a correction to his first paper, also published in 1934, Weisskopf presented the corrected result. He found like in the case of the electrostatic part of the self-energy that in Dirac's hole theory E^D also had a logarithmic divergence (Miller, 1994, p. 61).[31] Writing to Weisskopf in February 1935, Heisenberg called attention to a shortcoming in Weisskopf's calculation. Heisenberg repeated Weisskopf's calculation and found that

$$E^S = \frac{e^2}{h\sqrt{m^2c^2 + p^2}}(2m^2c^2 + p^2)\int \frac{dk}{k}$$

[31] In 1939 Weisskopf showed that the self-energy of the electron was logarithmically divergent to every approximation in an expansion of the self-energy in powers of the fine structure constant α (Weisskopf, 1939).

$$E^D = \frac{mc}{h\sqrt{m^2c^2 + p^2}}(m^2c^2 - 4/3)p^2 \int \frac{dk}{k}.$$

Heisenberg found these results suspicious because

one must expect on relativistic grounds that

$$E^S + E^D = \text{constant}\,\frac{e^2}{h}\sqrt{m^2c^2 + p^2}\int \frac{dk}{k}.$$ (Quoted in Schweber, 1994, p. 125)

According to Schweber, "the lack of proper relativistic covariance was to plague all self-energy calculations in the prewar period" (Schweber, 1994, p. 125).

3 The submergence of infinites in quantum electrodynamics

Things changed drastically in 1947, with W. Lamb's experimental results on the shift of the $2^2S_{1/2}$ state relative to the $2^2P_{1/2}$ states in the hydrogen atom. H. A. Bethe coming from a conference in Shelter Island, held on 2-4 June 1947, did some calculations on a train going from New York to Schenectady. In the conference W. Lamb presented his recent results on the level shift. Bethe made a nonrelativistic calculation of the Lamb shift, taking into account the suggestion by J. Schwinger, Weisskopf, and Oppenheimer that the self-energy of the electron was responsible for the shift in the energy levels, and Kramers's idea of mass renormalization (Pais, 1986, pp. 455-456; Schweber, 1994, p. 228-231). According to Bethe: "Kramers suggested that what one really ought to do was to renormalize the mass of the electron, taking into account its interaction with its own electromagnetic field. Then only those parts of the self-energy which are not contained in the mass of the particle would be observable" (quoted in Mehra & Rechenberg, 2001, p. 1039). Bethe calculated the self-energy W of a bound electron and subtracted to it the self-energy W_0 of a free electron (with the same average kinetic energy). This corresponds to Kramers's idea of mass renormalization. The difference $W–W_0$ was according to Bethe "the true shift of the levels due to interactions" (quoted in Schweber, 1994, p. 231). This expression is logarithmically divergent. Bethe considered that there should be (in the relativistic theory) a natural cut-off at energies around mc^2 (which is not the case). By taking into account this *ad hoc* cut-off, Bethe was able to obtain a result in good agreement with the observed value.

As seen above, the idea of renormalization, in the case of the electron's charge, was basically present in Dirac's report to the Solvay conference of 1933 (Dirac, 1934a). His ideas are stated more clearly in the letter to N. Bohr written after the preparation of the report:

We then have a picture in which all the charged particles of physics, electrons, atomic nuclei, etc. have effective charges slightly less than their real charges, the ratio being about 136/137. The effective charges are what one measures in *all* low energy experiments, and the experimentally determined value of *e* must be the effective charge of an electron, the real value being slightly bigger. (Quoted in Schweber, 1994, p. 116)[32]

[32] Another statement of the idea of charge renormalization due to the effect of the vacuum polarization can be seen in Weisskopf's paper on vacuum polarization from 1936. According to Weisskopf "the polarizability could in no way be observed, but would only multiply all charges and field strengths by a constant factor" (Weisskopf , 1936, p. 208).

A similar approach regarding the electron self-energy started to emerge in the end of the thirties, in Dirac's own work, and in H. A. Kramers's investigation of the renormalization of the electromagnetic mass at the classical level (as a first step for dealing with the problem at the quantum level). Kramers's intention was to sidestep the problem by obtaining a consistent model for a finite size electron – that avoided the classical self-energy divergence –, considering from the start the experimental mass of the electron (that contained the mechanical mass and the electromagnetic mass). In this way Kramers "tried to present the theory in such a fashion that the questions of the structure and the finite extension of the particles are not explicitly involved and that the quantity that is introduced as the 'particle mass' is from the very beginning the experimental mass" (Kramers, 1938, p. 254). But mass renormalization was only put to use in quantum electrodynamics in 1947, in the quantum-mechanical (non-relativistic) train-ride calculation of Bethe.

A few months after the conference, Schwinger worked on a non-covariant relativistic calculation of the Lamb shift using the mass and charge renormalization recipe, and obtained finite results to order $e^2/\hbar c$. Knowing of G. Breit's suggestion that the electron might have an intrinsic magnetic moment different from the one predicted by the Dirac equation – that explained the discrepancy with the experimental results regarding the hyperfine structure of the hydrogen atom –, Schwinger calculated the so-called anomalous magnetic moment for an electron in an externally applied homogeneous magnetic field, which accounted for the previous hyperfine discrepancies between theory and experiment (Mehra & Rechenberg, 2001, p. 1045). Schwinger published his results in a short note from late December 1947. This note did not include the precise results of his Lamb shift calculations due to discrepancies between the Coulomb (Lamb shift) and the magnetic field (anomalous magnetic moment) calculations, because there existed a difference in the result for the magnetic moment in the case of the electron in an atom and a free electron (Schweber, 1994, p. 319; Mehra, 1994, pp. 238-239). In this brief note Schwinger presented his view on the need for renormalization in quantum electrodynamics. According to Schwinger

> Attempts to evaluate radiative corrections to electron phenomena have heretofore been beset by divergent difficulties, attributable to self-energy and vacuum polarization effects. Electrodynamics unquestionably requires revision at ultra-relativistic energies, but is presumably accurate at moderate relativistic energies. It would be desirable, therefore, to isolate those aspects of the current theory that essentially involve high energies, and are subject to modification by a more satisfactory theory, from aspects that involve only moderate energies and are thus relatively trustworthy. This goal has been achieved by transforming the Hamiltonian of current hole theory electrodynamics to exhibit explicitly the logarithmically divergent self-energy of a free electron, which arises from the virtual emission and absorption of light quanta. The electromagnetic self-energy of a free electron can be ascribed to an electromagnetic mass, which must be added to the mechanical mass of the electron. Indeed, the only meaningful statements of the theory involve this combination of masses, which is the experimental mass of a free electron. It might appear, from this point of view, that the divergence of the electromagnetic mass is unobjectionable, since the individual contributions to the experimental mass are unobservable. However, the transformation of the Hamiltonian is based on the assumption of a weak interaction between matter and radiation, which requires that the electromagnetic mass be a small correction ($\sim(e^2/\hbar c)m_0$) to the mechanical mass m_0 …It is important to notice that the inclusion of the electromagnetic mass with the mechanical mass does not avoid all divergences; the polarization of the vacuum produces a logarithmically divergent term proportional to the interaction energy of the electron in an external field. However, it has long been recognized that such a term is equivalent to altering the value of the electron charge by a constant factor, only the final value being properly identified with the experimental charge. Thus the interaction between matter and radiation produces a renormalization of the electron charge and mass, all divergences being contained in the renormalization factors. (Schwinger, 1948a, p. 416)

The calculations mentioned in the note were done using non-covariant hole-theoretic methods. This is the motive for the discrepancy in the calculations. Afterwards, Schwinger developed a covariant formulation of the Heisenberg and Pauli quantum electrodynamics. Nevertheless, "there were a great many ambiguities in the procedure" (Schweber, 1994, p. 333) of identifying the divergent contributions. Also the calculation method was terribly complicated and threatened to become insurmountable in higher-order calculations.

A key aspect of Schwinger's covariant formulation was the deduction of an equation (later known as Tomonaga-Schwinger equation) that was a manifestly Lorentz covariant generalization of the Schrödinger equation. This was a functional derivative equation that describes the state function ψ as a functional $\psi[\sigma]$ of a general three-dimensional surface σ in space-time:

$$i\hbar c \frac{\delta\psi[\sigma]}{\delta\sigma(x)} = H(x, t)\,\psi[\sigma].$$

According to J. A. Wheeler's notes on Schwinger's presentation of his covariant formulation at the Pocono conference (held from March 30 to April 2, 1948), "these equations contain nothing more than Heisenberg-Pauli formalism and would not be required if one knew how to carry out Heisenberg-Pauli calculations consistently" (quoted in Schweber, 1994, p. 324). Schwinger applied his formalism in the determination of the radiative corrections to the motion of an electron in an external electromagnetic field, i.e. the calculation of the anomalous magnetic moment and the Lamb shift.

At the Ann Arbor summer school (from July 19 to August 7, 1948), Schwinger gave a more detailed presentation of his formalism including an improved treatment of vacuum polarization. The value for the Lamb shift given by Schwinger was

$$\frac{8\alpha^3}{3\pi}\frac{Z^4}{n^3}\left(\ln\frac{mc^2}{\Delta E} - \ln 2 + \frac{3}{8} - \frac{1}{5} + \frac{1}{2}\right) = 1040\,\mathrm{Mc}\,,$$

which includes the 1/5 Uehling term, and where the 1/2-term is the magnetic moment effect (which were not included in the expression Schwinger presented at the Pocono conference).

Schwinger's lectures were based on his paper 'quantum electrodynamics I' (Schwinger 1948b) and a first draft of a sequel where Schwinger applied the formalism to determine the vacuum polarization and the self-energy (Schwinger 1948c).

In the introduction to the first paper Schwinger gave further insights on his views regarding quantum electrodynamics. According to Schwinger

> The unqualified success of quantum electrodynamics in applications involving the lowest order of perturbation theory indicates its essential validity for moderately relativistic particle energies. The objectionable aspects of quantum electrodynamics are encountered in virtual processes involving particles with ultra-relativistic energies. The two basic phenomena of this type are the polarization of the vacuum and the self-energy of the electron.
>
> The phrase "polarization of the vacuum" describes the modification of the properties of an electromagnetic field produced by its interaction with the charge fluctuations of the vacuum. In the language of perturbation theory, the phenomenon considered is the generation of charge and current in the vacuum through the virtual creation and annihilation of electron-positron pairs by the electromagnetic field. If the electromagnetic field is that of a light quantum, the vacuum polarization effects are equivalent to ascribing a proper mass to the photon. Previous calculations have yielded non-vanishing, divergent

expressions for the light quantum proper mass. However, the latter quantity must be zero in a proper gauge invariant theory. The failure to obtain this result from a gauge invariant formulation can be ascribed only to a faulty application of the theory, rather than to an essential deficiency thereof. When the electromagnetic field is that of a given current distribution, one obtains a logarithmically divergent contribution to the vacuum polarization current which is everywhere proportional to the given distribution. This divergent result expresses the possibility, according to the present theory, of creating electron-positron pairs with unlimited energy, a situation that presumably will be corrected in a more satisfactory theory. Thus the physically significant divergence arising from the vacuum polarization phenomenon occurs in a factor that alters the strength of all charges, a uniform renormalization that has no observable consequences other than the conflict with empirical finiteness of charge.

The interaction between the electromagnetic field vacuum fluctuations and an electron, or more exactly, the electron-positron matter field, modifies the properties of the matter field and produces the self-energy of an electron. The mechanism here under discussion is commonly described as the virtual emission and absorption of a light quantum by an otherwise free electron … in a Lorentz invariant theory, self-energy effects for a free electron can only result in the addition of an electromagnetic proper mass to the electron's mechanical proper mass. Calculations performed for a stationary electron have yielded a logarithmically divergent electromagnetic proper mass, a divergence that results from the possibility of emitting light quanta with unlimited energy … the electromagnetic proper mass merely produces a renormalization of the electron mass that has no observable consequences, other than the conflict with the empirical finiteness of mass.

It is evident that these two phenomena are quite analogous and essentially describe the interaction of each field with the vacuum fluctuations of the other field. The effect of these fluctuation interactions is simply to alter the fundamental constants e and m, although by logarithmically divergent factors. However, it may be argued that a future modification of the theory, inhibiting the virtual creation of particles that possess energies many orders of magnitude in excess of mc^2, will ascribe a value to these logarithmic factors not vastly different from unity. The charge and mass renormalization factors will then differ only slightly from unity, as befits a perturbation theory, in consequence of the small coupling constant for the matter and electromagnetic fields, $e^2/4\pi\hbar c = 1/137$. (Schwinger, 1949b, pp. 1439-1440)

It is important to notice that Schwinger considers that the divergences result from 'virtual processes involving particles with ultra-relativistic energies'. These virtual processes came about in perturbative calculations. They are basically the transitory states Dirac found in his second order perturbation theory (see chapter 5; see also chapter 7 for a treatment of virtual quanta). As Schwinger writes, in the 'language of perturbation theory' we have, in what regards the vacuum polarization, the creation and annihilation of transitory (virtual) electron-positron pairs. The most interesting aspect of Schwinger's view is that he considers that a possible future modification of the theory might exclude virtual states with energies 'many orders of magnitude in excess of mc^2'. This is Dirac's subtraction physics with a cut off. The difference is that Schwinger is hoping for a future more elaborated theory with a 'natural' cut off, while Dirac presents the cut off as a necessary 'patch' to maintain the calculation within a mathematical domain where the physical concepts make sense (in this case the abstraction of the electron as a point-like electron; see also chapter 5). To put it simply, Dirac (with Bohr) is seeing a conceptual inconsistency when considering integrals without an energy cut off, where Schwinger (as other renormalization physicists) sees basically a mathematical problem to be solved in a future better theory.

Back in Cornell (from the conference in Shelter Island) in early July 1947, Bethe gave a lecture on his non-relativistic calculation of the Lamb shift, which R. P. Feynman attended. According to Feynman:

He explained that it gets very confusing to figure out exactly which infinite term corresponds to what in trying to make the correction for the infinite change in mass. If there were … any modification whatever at high frequencies, which would make this correction finite, then there would be no problem at all to figuring out how to keep track of everything … if in addition this method were relativistically invariant, then we would be absolutely sure how to do it without destroying [relativistic invariance]. (Feynman, 1965, p. 170)

Feynman considered first the case of determining a relativistic cut-off for classical electrodynamics. Using his path-integral method, Feynman, following Bethe's idea, replaced a delta function appearing in the interaction term of the action by an invariant function dependent on a cut-off parameter that made all results finite; this procedure corresponding to a 'regularization' of the theory. Feynman would then renormalize the mass, putting the bare mass and the now finite electromagnetic mass under the umbrella of the experimental mass.

Feynman did not manage to derive the Dirac equation using his path-integral method. So, by 'guessing' he was able to use an invariant regularization method based on a cut-off with the Dirac theory of the electron (Mehra, 1994, pp. 229-234). Feynman developed his "little theory of electrodynamics in which the interaction is not exact on a delta function" (quoted in Schweber, 1994, p. 427) as if it was different from the conventional electrodynamical theory. In his 1948 paper on the relativistic cut-off, Feynman presented his method as "a model, for which all quantities automatically do come out finite" (Feynman, 1948, p. 1430). This does not mean that Feynman rejected the renormalization method. In his calculations he performed the mass and charge renormalization, but he saw his method as an "attempt to find a consistent modification of quantum electrodynamics" (Feynman, 1949b, p. 778). Because it was inconsistent, the correct physics had to be obtained by making the renormalization of mass and charge, and obtaining expressions independent of the cut-off parameter by making the cut-off parameter go to infinity after renormalization (Feynman, 1962, p. 145).

In between the Shelter Island and the Pocono conferences, Feynman, after developing a relativistic cut off procedure for classical electrodynamics, extended this approach to the case of a spinless relativistic particle, being able to obtain a relativistic generalization of the expression Bethe had used in his calculations. By applying this approach to the Dirac electron (following an intuitive procedure suggested by Bethe), Feynman was able to obtain Weisskopf's expression for the self-energy (now depending logarithmically on Feynmam's cut off parameter). In a letter (from late autumn) written to Bert and Mulaika Corber, Feynman commented on his ongoing work:

> There was so much talk around here about self-energy, that I thought it would be the easiest thing to calculate directly in my form. The result is exactly the same as one gets for ordinary perturbation theory … It therefore also gives infinity. I then altered the delta function in the interaction to be a sum of less sharp function. This corresponds to a kind of finite electron. Then the self-energy of a non-relativistic particle is finite. (Quoted in Schweber, 1994, p. 423)

At the Tenth Washington Conference on Theoretical Physics (held on 13-15 November 1947), Feynman attended a talk by Schwinger. Feynman was interested in a remark made by Schwinger, referring to the fact that, according to Feynman's recollections on the conference, "the discrepancy in the hyperfine structure of the hydrogen noted by Rabi, can be explained on the same basis as that of electromagnetic self-energy, as can the line shift of Lamb" (quoted in Mehra, 1994, p. 236). After the conference Feynman did the calculation of the anomalous magnetic moment using his approach.

In a letter to the Corbers from middle January 1948 we already see an outline of Feynman's regularization approach to the problem of the infinites in quantum electrodynamics:

> I have been working with a theory of electricity in which the delta function interaction is replaced by a less sharp function. Then (in quantum mechanics) the self-energy of an electron including the Dirac hole theory comes out finite … actually, the self-energy comes out finite and invariant and is therefore

representable as a pure mass … thus all mass cannot be represented as electrodynamic unless the cutoff is ridiculously short. The experimental mass is of course the sum of inertial and this electromagnetic correction … I think all the problems of electrodynamics can be unambiguously solved by this process: First compute the answer which is finite (but contains the cutoff logarithm). Then express the result in terms of the experimental mass. The answer still contains the cutoff but this time not logarithmically. Take the limit which now exists, as the cutoff goes to infinity. (Quoted in Schweber, 1994, p. 426)

In the meeting of the American Physical Society that took place at the end of January 1948, Schwinger reported on his results regarding the anomalous magnetic moment of a free electron and his results for the Lamb shift (published on his note from December 1947). In this talk Schwinger mentioned that his results for the anomalous magnetic moment for an electron in a magnetic field did not agree with the value obtained for an electron in a Coulomb field. Feynman mentioned then that he had got things right, i.e. the same result for the magnetic moment of an electron, in both cases of a free or bound electron (Mehra, 1994, pp. 238-239). In his approach Feynman was not working with Dirac's hole theory, but thinking in terms of paths (in space-time) and representing the positrons as electrons going backwards in time (Schweber, 1994, p. 428).

By the time of the Pocono conference Feynman had a working approach that enabled him to calculate the anomalous magnetic moment, Lamb shift and cross sections for diverse processes. What Feynman did not have was a way to deal with the vacuum polarization, which in Feynman's approach was connected with so-called closed loops (i.e. paths that give rise to an infinite polarizability of vacuum). In his presentation Feynman was still hoping that it was possible to get a consistent theory without using loops (Schweber, 1994, p. 443). That was not the case.

After the Pocono conference Feynman decided to write down his work in a set of papers. The first addressed the relativistic cut off for classical electrodynamics. The next an extension of this approach to the case of quantum electrodynamics. In this paper Feynman got the results for the self-energy obtained previously by Weisskopf and Bethe; and it included a discussion of the scattering of an electron by a (classical) potential. In this paper Feynman considered only processes in which the photons appeared only in the intermediate states of the perturbative calculations. Feynman found that he could simply take on equal footing the four polarizations of the photon, transverse, longitudinal, and scalar, in a relativistic and gauge invariant way. All this before the Gupta-Bleuler method. This state of affair was possible because Feynman was considering the case where all the light quanta are virtual. As W. Heitler stresses in his classical book on quantum electrodynamics, "we can compute the transition probability by choosing an initial state without longitudinal and scalar photons, ignoring the Lorentz condition in the meantime, and by calculating only the probabilities of final states which have no longitudinal and scalar photons" (Heitler, 1954, p. 130). In the case of Feynman's calculation we do not even have transverse photons in the initial and final states. In this paper Feynman had still not found a way to deal with the infinites related to the vacuum polarization. We can know about Feynman's progress on the vacuum polarization problem from a letter from late 1948:

In regards to "Q.E.D." as you put it, I don't have a cold dope. I can calculate anything, and everything is finite, but the polarization of the vacuum is not gauge-invariant when calculated. This is because my prescription for making the polarization integral converge is not gauge-invariant. If I threw away the obvious large gauge-dependent term (a procedure which I can not justify legally, but which is practically unambiguous) the result is a charge renormalization plus the usual Uehling term. The amount of charge renormalization depends logarithmically on the cut-off. The Uehling terms are practically independent on the cut-off and give the usual –1/5 in the Lamb shift. (Quoted in Mehra, 1994, p. 265)

By the end of January 1949 Feynman learned about the Pauli-Villars regularization procedure that enables a gauge-invariant regularization of the vacuum polarization. By the spring of 1949 he had all the elements together and published his two most important papers on quantum electrodynamics, where his approach was presented and put to use.

In his 'The theory of positrons', submitted on 8 April 1949, Feynman begins by presenting his idea of positrons as electrons moving backward in time. In the abstract Feynman writes:

> the problem of the behavior of positrons and electrons in given external potentials, neglecting their mutual interaction, is analysed by replacing the theory of holes by a reinterpretation of the solutions of the Dirac equation. It is possible to write down a complete solution of the problem in terms of the boundary conditions on the wave function, and this solution contains automatically all the possibilities of virtual (and real) pair formation and annihilation together with the ordinary scattering processes, including the correct relative signs of the various terms.
>
> In this solution, the "negative energy states" appear in a form which may be pictured (as [done] by Stückelberg) in spacetime as waves travelling away from the external potential backwards in time. (Feynman, 1949a, p. 749)

In here we see Feynman talking about solutions with appropriate boundary conditions, not the equations themselves. In the introduction we start seeing how Feynman thought about physical processes as described in his scheme:

> In the approximation of classical relativity theory the creation of an electron pair (electron A, positron B) might be represented by the start of two world lines from the point of creation, 1. The world lines of the positron will then continue until it annihilates another electron, C, at a world point 2. Between the times t_1 and t_2 there are then three world lines, before and after only one. However, the world lines of C, B, and A together form one continuous line albeit the "positron part" B of this continuous line is directed backwards in time. Following the charge rather than the particles corresponds to considering this continuous world line as a whole rather than breaking it up into its pieces. It is as though a bombardier flying low over a road suddenly see three roads and it is only when two of them come together and disappear again that he realizes that he has simply passed over a long switchback in a single road.
>
> This over-all space-time point of view leads to considerable simplification in many problems. (p. 749)

Feynman then relates his 'over-all space-time view' to his path integral approach to quantum mechanics. Feynman begins by "a brief discussion of the relation of the non-relativistic wave equation to its solution" (p. 750). It goes as follows. Starting with the Schrödinger equation $i\partial\psi/\partial t = H\psi$, if $\psi(x_1, t_1)$ is the solution at x_1 at time t_1, then the wave function for $t_2 > t_1$ is given by

$$\psi(x_2, t_2) = \int K(x_2, t_2; x_1, t_1)\psi(x_1, t_1)d^3x_1 \ ,$$

where the green function K is given by

$$K(2,1) = \sum_n \phi_n(x_2)\phi_n^*(x_1)\exp(-iE_n(t_2 - t_1))$$

(E_n and ϕ_n are the eigenvalues and eigenfunctions of the operator H in the case of a free particle). Feynman calls "K(2, 1) the total amplitude for arrival at x_2, t_2 starting from x_1, t_1. (It results from adding an amplitude, exp(iS), for each space time path between these points, where S is the action along the path)" (p. 750).

In the case of a particle in a weak external potential U (x, t), differing from zero for t between t_1 and t_2, we can expand K in increasing powers of U:

$$K(2, 1) = K_0(2, 1) + K^{(1)}(2, 1) + K^{(2)}(2, 1) + \cdots.$$

To zero order in U, K is that for a free particle: $K_0(2, 1)$. In first order of perturbation theory $K^{(1)}(2, 1)$ results from the action of the potential U at some time t_3 (between t_1 and t_2). From t_1 to t_3, and from t_3 to t_2 the particle is free. In this way it can be shown that $K^{(1)}(2, 1)$ is given by

$$K^{(1)}(2,1) = -i\int K_0(2,3)U(3)K_0(3,1)d\tau_3 .$$

In Feynman's explanation of the meaning of these formulas we see how his over-all space-time approach goes:

We can imagine that a particle travels as a free particle from point to point, but is scattered by the potential U. Thus the total amplitude for arrival at 2 from 1 can be considered as the sum of the amplitudes for various alternative routes. It may go directly from 1 to 2 (amplitude $k_0(2, 1)$) … or it may go from 1 to 3 (amplitude $k_0(3, 1)$), get scattered there by the potential (scattering amplitude –iU(3) per unit volume and time) and then go from 3 to 2 (amplitude $k_0(2, 3)$). This may occur for any point 3 … Again it may be scattered twice by the potential … It goes from 1 to 3 ($k_0(1, 3)$), gets scattered there (–iU(3)) then proceeds to some other point, 4, in space time (amplitude $k_0(4, 3)$) is scattered again (–iU(4)) and then proceeds to 2 ($k_0(2, 4)$). Summing over all possible places and times for 3, 4 find that the second order contribution to the total amplitude $k^{(2)}(2, 1)$ is

$$(-i)^2\int\int K_0(2,4)U(4)K_0(4,3)U(3)K_0(3,1)d\tau_3 d\tau_4 .$$ (p. 751)

After presenting his approach in the case of non-relativistic quantum mechanics Feynman addresses the relativistic case. Starting with Dirac's equation $(i\nabla - m)\psi = A\psi$, for a particle of mass m in an external potential A, the equation determining the propagation of a free particle is $(i\nabla_2 - m)\, K_+(2, 1) = i\delta(2, 1)$. In analogy to the non-relativistic case, the first order and second order corrections to $K_+(2, 1)$ are given by

$$K_+^{(1)}(2,1) = -i\int K_+(2,3)A(3)K_+(3,1)d\tau_3$$

$$K_+^{(2)}(2,1) = -\int\int K_+(2,4)A(4)K_+(4,3)A(3)K_+(3,1)d\tau_3 d\tau_4 .$$

The core part of this paper is the selection of the admissible solutions according to Dirac's hole theory (related to his 'positrons as electrons moving backward in time' view):

We would now expect to choose for the special solution of [the equation for $K_+(2, 1)$], $K_+ = K_0$ where $K_0(2, 1)$ vanishes for $t_2 < t_1$ and for $t_2 > t_1$ is given by [the equation for K(2,1)] where ϕ_n and E_n are the eigenfunctions and energy values of a particle satisfying Dirac's equation … The formulas arising from this choice, however, suffer from the drawback that they apply to the one electron theory of Dirac rather than to the hole theory of the positron … the choice K+ = K_0 is unsatisfactory. But there are other solutions of [the equation for $K_+(2, 1)$]. We shall choose the solution defining $K_+(2, 1)$ so that $K_+(2, 1)$ for $t_2 > t_1$ *is the sum of [the equation for K(2, 1)] over positive energy states only*. … With this choice of [$K_+(2, 1)$] our equations such as [the previous one for $K_+^{(1)}(2, 1)$] and [the previous one for $K_+^{(2)}(2, 1)$] will now give results equivalent to those of the positron theory. (p. 752)

In this paper Feynman only considered the case of several non-interacting particles, leaving the problem of interacting particles to his next paper.

In "Space-Time Approach to Quantum Electrodynamics", sent to publication on 9 May 1949, Feynman put forward the regularization procedure he had been developing within his over-all space-time view. Feynman addressed first the case of particles interacting instantaneously, which could then be easily generalized to the case of delayed interactions. As in the case of the previous paper Feynman considers

> the solutions of equations rather than the time differential equations from which they come. We shall discover that the solutions, because of the over-all space-time view that they permit, are as easy to understand when interactions are delayed as when they are instantaneous. (Feynman, 1949b, p. 771)

Using the methods of the previous paper, Feynman addresses the case of two interacting particles, considering first the non-relativistic case described by the Schrödinger equation. In the case of two free particles the amplitude is given by

$$K(x_a, x_b, t; x_a', x_b', t') = K_{0a}(x_a, t; x_a', t')K_{0b}(x_b, t; x_b', t')$$

where x_a' and x_b' are the positions of the particles at time t', and x_a and x_b the positions of the particles at a later time t. We can also define the amplitude

$$K_0(3, 4; 1, 2) = K_{0a}(3, 1)K_{0b}(4, 2)$$

that the particle a goes from x_1 at t_1 to x_3 at t_3 and that particle b goes from x_2 at t_2 to x_4 at t_4. According to Feynman

> When the particles do interact, one can only define the quantity K(3, 4; 1, 2) precisely if the interaction vanishes between t_1 and t_2 and also between t_3 and t_4. In a real physical system such is not the case. There is such an enormous advantage, however, to the concept that we shall continue to use it, imagining that we can neglect the effect of interactions between t_1 and t_2 and between t_3 and t_4. For practical problems this means choosing such long time intervals $t_3 - t_1$ and $t_4 - t_2$ that the extra interactions near the end points have small relative effects. As an example, in a scattering problem it may well be that the particles are so well separated initially and finally that the interaction at these times is negligible. Again energy values can be defined by the average rate of change of phase over such long time intervals that errors initially and finally can be neglected. Inasmuch as any physical problem can be defined in terms of scattering processes we do not lose much in a general theoretical sense by this approximation. (p. 771)

Feynman first gives an example of this approach in the case of an instantaneous Coulomb interaction, and then shows how it can be extended to the case of a delayed interaction. Considering a Coulomb potential e^2/r (where r is the distance between the particles), which is 'active' for only a short time interval Δt_0 at time t_0, the first order correction to the amplitude is given by

$$K^{(1)}(3, 4; 1, 2) = -ie^2 \iint K_{0a}(3, 5)K_{0b}(4, 6)r_{56}^{-1} \times K_{0a}(5, 1)K_{0b}(6, 2)d^3x_5 d^3x_6 \Delta t_0 ,$$

where $t_5 = t_6 = t_0$. Considering now the potential to be active all the time, according to Feynman, "the first-order effect is obtained by integrating on t_0, which we can write as an integral over both t_5 and t_6 if we include a delta-function $\delta(t_5 - t_6)$ to insure contribution only when $t_5 = t_6$" (p. 772). In this case the first order correction to the amplitude is given by

$$K^{(1)}(3,4;1,2) = -ie^2 \iint K_{0a}(3,5)K_{0b}(4,6)r_{56}^{-1} \times \delta(t_{56})K_{0a}(5,1)K_{0b}(6,2)d\tau_5 d\tau_6$$

where $d\tau = d^3xdt$. In the case of a delayed interaction the story goes as follows. Since "the Coulomb potential does not act instantaneously, but is delayed by a time r_{56}, taking the speed of light as unity. This suggests simply replacing $r_{56}^{-1}\delta(t_{56})$ in [the expression for $K^{(1)}(3, 4;1, 2)$] by something like $r_{56}^{-1}\delta(t_{56} - r_{56})$ to represent the delay in the effect of b on a."(p. 772). According to Feynman things are not that easy because "when this interaction is represented by photons they must be of only positive energy, while the Fourier transform of $\delta(t_{56} - r_{56})$ contains frequencies of both signs" (p. 773). Because of this, Feynman uses instead the expression

$$\delta_+(x) = \int_0^\infty e^{-i\omega x} d\omega/\pi = \delta(x) + (\pi i x)^{-1}.$$

This is not the whole story. After taking into account the contribution due to the case when $t_5 < t_6$ (which corresponds to a emitting the quantum that b receives), generalizing to an interaction described also by the vector potential, and adapting the formalism to the case of electrons described by the Dirac equation, Feynman arrives at the expression

$$(1 - \alpha_a \cdot \alpha_b)\delta_+(s_{56}^2) = \beta_a\beta_b\gamma_{a\mu}\gamma_{b\mu}\delta_+(s_{56}^2).$$

In this way, in the case of electrons interacting through an electromagnetic field, the amplitude is given by

$$K^{(1)}(3,4;1,2) = -ie^2 \iint K_{+a}(3,5)K_{+b}(4,6)\gamma_{a\mu}\gamma_{b\mu} \times \delta(s_{56}^2)K_{+a}(5,1)K_{+b}(6,2)d\tau_5 d\tau_6 .$$

Feynman calls it his fundamental equation for quantum electrodynamics. According to Feynman it "describes the effect of exchange of one quantum (therefore first order in e^2) between two electrons. It will serve as a prototype enabling us to write down the corresponding quantities involving the exchange of two or more quanta between two electrons or the interaction of an electron with itself" (p. 772). Feynman then gives a description of the meaning of the equation presenting a graphical support to his interpretation: a Feynman diagram. It goes as follows:

> It can be understood (see Fig. 1) as saying that the amplitude for "a" to go from 1 to 3 and "b" to go from 2 to 4 is altered to first order because they can exchange a quantum. Thus, "a" can go to 5 (amplitude ($K_+(5, 1)$) emit a quantum (longitudinal, transverse, or scalar $\gamma_{a\mu}$) and then proceed to 3 ($K_+(3, 5)$). Meantime "b" goes to 6 ($K_+(6, 2)$), absorbs the quantum ($\gamma_{b\mu}$) and proceeds to 4 ($K_+(4, 6)$). The quantum meanwhile proceeds from 5 to 6, which it does with amplitude $\delta_+(s_{56}^2)$. We must sum over all the possible quantum polarizations it and positions and times of emission 5, and of absorption 6. Actually if $t_5 > t_6$ it would be better to say that "a" absorbs and "b" emits but no attention need be paid to these matters, as all such alternatives are automatically contained in [the fundamental equation]. (pp. 772-773)

Feynman first applied his technique to the case of the electron's self-energy. Since the calculations turn out to be easier in the momentum-energy space, Feynman presented rules to calculate the amplitude working with momentum and energy variables. Feynman then shows how his regularization scheme works. In this paper Feynman also addresses the problem of vacuum polarization making use of the gauge invariant regularization procedure developed by Pauli and Villars.

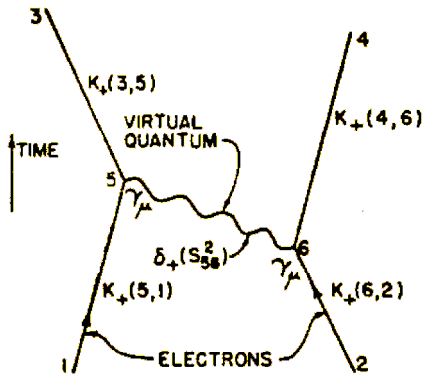

Figure 1: The fundamental interaction (described by Feynman's fundamental equation). Exchange of one quantum between two electrons.

To see regularization at work I will look into the problems of the electron's self-energy and photon's self-energy. In the case of the electron's self-energy, Feynman's 'fundamental formula' reduces to

$$K^{(1)}(2,1) = -ie^2 \int\int K_+(2,4)\gamma_\mu K_+(4,3)\gamma_\mu K_+(3,1)d\tau_3 d\tau_4 \delta_+(s_{43}{}^2)\,.$$

According to Feynman, this first order correction to the amplitude $K_+(2, 1)$, "arises because the electron instead of going from 1 directly to 2, may go (Fig. 2) first to 3, ($K_+(3, 1)$), emit a quantum (γ_μ), proceed to 4, ($K_+(4, 3)$), absorb it (γ_μ), and finally arrive at 2 ($K+(2, 4)$). The quantum must go from 3 to 4 $\delta_+(s_{43}{}^2)$)" (p. 773). Feynman shows how this expression is related with the self-energy of an electron, which turn out to be

$$\Delta E = e^2 \int (\bar{u}\gamma_\mu K_+(4,3)\gamma_\mu u)\exp(ip\cdot x_{43})\delta_+(s_{43}{}^2)d\tau_4\,.$$

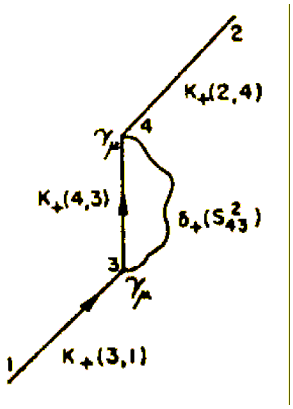

Figure 2: Interaction of an electron with itself

As mentioned, for easiness in the calculations Feynman works in the momentum-energy space. In this case the self-energy is the matrix element between $\bar{u}$ and u (taken from the plane wave solution for a free Dirac electron: u exp(−px)) of the matrix

$$(e^2/\pi i)\int \gamma_\mu (p-k-m)^{-1}\gamma_\mu k^{-2} d^4k\,.$$

According to Feynman:

The equation can be understood by imagining (Fig. 3) that the electron of momentum p emits (γ_μ) a quantum of momentum k, and makes its way now with momentum p − k to the next event (factor $(p - k - m)^{-1}$) which is to absorb the quantum (another γ_μ). The amplitude of propagation of quanta is k^{-2}. (There is a factor $e^2/\pi i$ for each virtual quantum). One integrates over all quanta. The reason an electron of momentum p propagates as $1/(p - m)$ is that this operator is the reciprocal of the Dirac equation operator, and we are simply solving this equation. Likewise light goes as $1/k^2$, for this is the reciprocal D'Alembertian operator of the wave equation of light. The first γ_μ represents the current which generates the vector potential, while the second is the velocity operator by which this potential is multiplied in the Dirac equation when an external field acts on an electron. (p. 775)

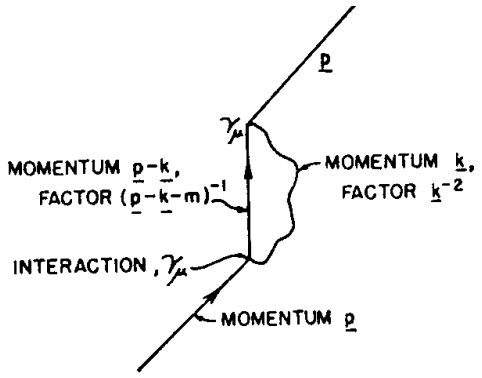

Figure 3: Interaction of an electron with itself. Momentum-energy space.

Up to this point, things are moving smoothly. However if we calculate the integral to obtain the self-energy it turns out, as already mentioned, to be infinite. Using contemporary notation, the problems in the calculation of the electron self-energy are all concentrated in this apparently harmless integral (Mandl & Shaw, 1984, p. 187):

$$ie_0^2\,\Sigma(p) = \frac{e_0^2}{(2\pi)^4}\int d^4k \frac{1}{k^2 + i\varepsilon}\frac{2\not{p} - 2\not{k} - 4m_0}{(p-k)^2 - m_0^2 + i\varepsilon}\,.$$

As it stands this integral is divergent. From Lorentz invariance Σ(p) can be put in the form

$$\Sigma(p) = A + (\not{p} - m)B + (\not{p} - m)\Sigma_c(p)\,,$$

where m is the electron's (experimental) mass, and, in particular, A = Σ(p) when $\gamma^\mu p_\mu = m$ (Mandl & Shaw, 1984, p. 189). This term provides a correction $\delta m = -e_0^2 A$ of electromagnetic origin to the bare mass m_0 of the electron, which can be seen as resulting from the interaction of the electron with its own field. In this way, at the level of quantum electrodynamical applications, the electron's mass that is experimentally measured corresponds to a renormalized mass where the electron's self-energy is taken into account.

For $k \to \infty$ the previous integral is logarithmically divergent (this is the famous ultra-violet divergence). A way out is to make a "change in the fundamental laws"

(Feynman, 1961, p. 137): the photon propagator $1/k^2$ is multiplied by a relativistically invariant convergence factor, assumed by Feynman to be $c(k^2) = -\lambda^2/(k^2 - \lambda^2)$. This change has to be seen as a formal calculational device, a mathematical trick to get rid of the logarithmic divergence in the integral. If we try to see it as a new theory distinct from the one derived from classical electrodynamics we obtain a non-hermitian interaction Lagrangian that implies that probability is not conserved. Also from a physical point of view the use of this convergence factor is equivalent to considering "an additional interaction of the electron-positron field with a vector field whose quanta have mass λ and whose propagators are $-(k^2 - \lambda^2)^{-1}$" (Schweber, 1961, p. 519). With this prescription it is possible to calculate the integral. With this regularization procedure we have

$$A = -\frac{3m}{8\pi^2} \ln \frac{\Lambda}{m},$$

where Λ is a cut-off parameter (Mandl & Shaw, 1984, 191). It turns out that the only contribution from the self-energy which is not renormalized is the finite integral $\Sigma_c(p)$. From this term the radiative correction (due to the electron self-energy) to the lowest-order calculations is obtained. If we stopped here, we would have an experimentally measurable radiative correction dependent on an arbitrary cut-off parameter Λ.[33] To get things right, after the renormalization we have to make the cut-off parameter go to infinity, so that the radiative correction term "remains well-defined and finite in this limit and independent of the details of the regularization procedure" (Mandl & Shaw, 1984, p. 191). This method to overturn the problem of infinites in quantum electrodynamics was summarized by Feynman in one of his quantum electrodynamical rules: "(1) Put in an arbitrary cutoff factor $c(k^2) = -[\lambda^2/(k^2 - \lambda^2)]$ for each propagator $1/k^2$. (2) Express everything in $m_{exp} = m - \delta m$. (3) Take the limit as $\lambda \to \infty$ and keep m_{exp} fixed." (Feynman, 1962, p. 143).

4 Different views on renormalization

It is usually held that the divergence problem in quantum electrodynamics is due to a failure of the theory at ultra-relativistic energies, that is, to the fact that there is no upper bound to the energy of the virtual quanta that are exchanged during interactions. This might lead to the idea that the cut-off parameter serves like a "boundary line separating the knowable region from the unknowable" (Cao & Schweber, 1993, p. 52). But since there is no indication on where to put this cut-off, it seems that "we cover our ignorance by calculating only quantities which are independent of the exact value of the cut-off" (Teller, 1988, p. 87). This procedure results in a change from the approximative regularized version of the theory to a recovered quantum electrodynamics with renormalized mass and charge. This means changing "the status of the cutoff from a tentative, and tantalizing, threshold energy to a purely formalistic device" (Cao & Schweber, 1993, p. 53). Even if Feynman was trying to achieve a consistent regularized theory, and published his method as a provisional one while searching for a "correct

[33] This problem does not arise with δm because we consider it to be 'absorbed' in the experimental measurable mass $m_{exp} = m_0 + \delta m$, which is seen as an amalgamation of the bare mass and the electromagnetic mass, and whose magnitude – as a phenomenological parameter – is determined not by the theory but from experiments.

form of f_+ [the function that substitutes the delta function appearing in the interaction term] which will guarantee energy conservation" (Feynman, 1949b, p. 778), it seems that it ended up being what Bethe had envisaged from the beginning: a mathematical calculational device designed to overcome the divergence problems in some integrals. Also, as previously mentioned, from a physical point of view the regularized theory is completely different from quantum electrodynamics. It does not have a divergence problem because of the presence of an auxiliary vector field. This field can be seen as a formal mathematical device if, and only if, after the renormalization we recover a cut-off independent theory. If we tried to maintain the regularized theory, so that we did not have to deal with the problem of infinites in the calculations, we would be working not with quantum electrodynamics but with another (inconsistent) field theory.

We see in the case of Feynman (like previously with Schwinger) a lack of understanding of the possible implications at a conceptual level of the regularization scheme and renormalization. As we have seen Feynman as looking for a consistent modification of quantum electrodynamics. Contrary to Dirac (with Bohr), Feynman does not relate the regularization to structural aspects of the theory (i.e. to the adoption in Dirac's equation of a point-like electron) that might imply (even if in an inconsistent way) an upper bond to the possible energy exchanges.

Contrary to a common view I think that the divergence of the integrals and the use of the cut-off trick do not reveal where the theory stops being good and a 'true' theory should come into play. It reveals structural problems in the construction of the theory, that are impossible to ignore when we have some integrals, that should (from a physical point of view) provide small radiative corrections to lower-order calculations, and end up blowing apart in a proliferation of infinites. In quantum electrodynamics the description of the interaction between 'particles' (like photons and electrons) as quanta of the Maxwell and the Dirac fields is given by the perturbative expansion of the scattering matrix that describes the interaction (and it is in the terms of the S-matrix that the divergent integrals appear). Considering the second-order term of the scattering matrix $S_2(x_1, x_2)$ in configuration space, the mathematical expression of the terms related with the divergent part of the electron's self-energy are dependent on $\delta(x_1 - x_2)$. This means that "all the divergences in $S_2(x_1, x_2)$ come from terms proportional to $\delta(x_1 - x_2)$ and to its derivatives which differ from zero only in the infinitesimal neighbourhood of the point $x_1 = x_2$" (Bogoliubov & Shirkov, 1959, p. 299). The divergence problem does not arise solely from the fact that there is in the theory no upper bound to the energy of the virtual quanta. It results from the 'coincidence' in the theory of the inexistence of a natural limit to the energy of virtual quanta and from the local character of the interaction between the fields in quantum electrodynamics.

One other aspect of the mass renormalization procedure is that when we go beyond the lowest-order approximations, and the mass renormalization is needed, there is a mismatch between the conceptual basis of the theory and its description of matter: conceptually quantum electrodynamics is developed from the idea of two independently quantized fields – one of them describing matter – that interact. The electrons (and positrons) are described in quantum electrodynamics as quanta of the quantized Dirac field, having a (bare) mass associated with them. At the same time the higher-order calculations require considering the mass of the electron as having a non detachable contribution from the Maxwell field. The observed or experimental mass of the electron results in the applications of the theory from a simultaneous contribution from the bare mass of quanta of the Dirac field and the self-energy of these quanta due to the interaction of the Dirac and Maxwell fields.

That the divergence in the calculation of the electron's self-energy reveals structural problems related to distinct aspects of the theory does not mean that the theory does not have other less noticed limitations, also related to the divergence of integrals. This can be seen on a closer look at the second-order calculation of the photon self-energy. Again we have a divergent integral and again a regularization scheme is used and a renormalization is made.

The (second-order) photon self-energy leads to a modification of the photon propagator: $D_{\mu\nu}'(k)= g_{\mu\nu}D(k)+ D(k)\Pi_{\mu\nu}(k)D(k)$, where $\Pi_{\mu\nu}(k)$ is a quadratically divergent integral and D(k) is the bare photon propagator. Considering the requirement of Lorentz and gauge invariance, the second-order tensor $\Pi_{\mu\nu}(k)$ must have the form $(g_{\mu\nu}k^2 - k_\mu k_\nu)\Pi(k^2)$ (Jauch & Rohrlich, 1976, p. 189). As it stands, for $k^2 = 0$ we have $\Pi_\mu^{\ \mu}(0) \neq 0$. This would mean that the propagator we obtain taking into account this second-order correction is not the propagator for a zero mass photon but the propagator for a massive neutral vector boson (Sakurai, 1967, p. 275). To recover our photon we must recall that $\Pi_{\mu\nu}(k)$ must be gauge invariant. Imposing this condition, we must have $\Pi_{\mu\nu}(k)k^\nu = 0$. From this we obtain the ambiguous result that the quadratically divergent integral

$$\Pi_\mu^{\ \mu}(0) = -\frac{2\alpha}{\pi}\frac{1}{i\pi^2}\int \frac{p^2+2m^2}{(p^2+m^2)^2}d^4p,$$

must be identically zero (Jauch & Rohrlich, 1976, p. 190). The only way to circumvent this situation is to consider that "the integral is, strictly speaking, meaningless, since it is divergent" (Schweber, 1961, p. 552).

The pragmatic view is that we need a 'functioning' theory that is gauge invariant and provides a zero mass for the photon in the lower terms of the perturbation expansion of the S-matrix that are used in practice. This, when evaluating $\Pi_{\mu\nu}(k)$, can be done by taking into account the divergent integral $\Pi_\mu^{\ \mu}(0)$ and subtracting it from $\Pi(k^2)$, which leads to a logarithmically divergent integral. Using a gauge invariant regularization scheme we have $\Pi(k^2)= C + k^2\Pi^f(k^2)$, where $\Pi^f(k^2)$ is a finite correction term that as $\Lambda\rightarrow \infty$ "tends to a well-defined finite limit which is independent of the detailed form of the regularization procedure" (Mandl & Shaw, 1984, p. 187), and C is logarithmically divergent as $\Lambda\rightarrow \infty$ (Sakurai, 1967, p. 277). With this procedure we obtain a regularized photon propagator that includes second-order photon self-energy effects.

The next step is to incorporate the regularized constant C in a parameter of the theory whose value is experimentally determined, so that we can take the cut-off limit to infinity and recover quantum electrodynamics from the regularized 'theory'. Considering, for example, the second-order correction to the electron-electron or Møller scattering[34] due to the self-energy of the photon, the change in the Møller scattering amplitude amounts to

$$\frac{e^2(\bar{u}_1'\gamma_\mu u_1)(\bar{u}_2'\gamma_\mu u_2)}{ik^2}\rightarrow$$

[34] I will look into some general aspects of the Møller scattering in the next chapter.

$$e^2(1-C)\frac{e^2(\bar{u}_1'\gamma_\mu u_1)(\bar{u}_2'\gamma_\mu u_2)}{ik^2}+ie^2\Pi^f(k^2)(\bar{u}_1'\gamma_\mu u_1)(\bar{u}_2'\gamma_\mu u_2)\text{ . (Sakurai, 1967, p. 278)}$$

The trick is to consider the (infinite) constant 1 – C not as a correction factor related to the photon propagator itself, but, as can be seen more clearly in the limit $k^2 \rightarrow 0$, as a correction to the charges of the electrons which interact via the photon. In this way we relate this (infinite) correction to the coupling constant. In the limit $k^2 \rightarrow 0$ the modified photon propagator is given by $D'_F(k) = (1 - C)\, D_F(k)$. We renormalize the theory considering that $(1 - C)^{1/2}$ is a correction to the unobservable electron bare charge e_{bare}, so that what is observed is $e_{obs} = (1 - C)^{1/2}\, e_{bare}$. The distinctive flavour of this renormalization procedure when compared with the mass renormalization is that we are, so to speak, transferring the problems of the photon to the electrons.

Looking closely at the second-order self-energy correction to the Møller scattering, the infinity arising in the photon propagator is absorbed by the charges of the electrons 'located' at both 'vertices' of the interaction. This is possible because the description of the scattering by an S-matrix perturbative approach is done in a way that what appears in between the initial and final asymptotic states is not described as a process occurring in time, but the situation is such that "the S-matrix describes the scattering in the operational spirit of Heisenberg's matrix mechanics. It gives transition probabilities which correspond to measurable relative frequencies. But it treats the scattering itself as a black box" (Falkenburg, 2007, p. 131). Implicit in the procedure is a notion of time lapse between the initial and final asymptotic states (formally taken to be infinitely apart). What we do not have is a classical-like description of the photon propagation as something taking time to happen: in the renormalization procedure there is no possibility for the photon propagation to be seen as related to a causal temporal order connecting the electrons evolved in the scattering. In the applications of the theory, the Minkowski space-time loses any possible operational meaning related to space and time measurements, and becomes a sort of configurational space that is part of the machinery that enables to calculate energy-momentum cross-sections. There is, as I said, an idea implicit of temporal order in the scattering (also present in the ordering of operators in the terms of the S-matrix) but no temporal description of the process as something related to the exchange of a 'signal' propagating at light speed. All these are pretty much well-known aspects of quantum electrodynamics. But I think that the full implication of this situation has not been considered previously. The charge renormalization is possible only by not requiring a temporal description of the processes in the applications of quantum electrodynamics. But if a temporal description was (somehow) intended, it is clear that it would be incompatible with the charge renormalization procedure, because we can only have charge renormalization in an overall temporal description of the interaction going on inside an unobservable 'black box' (in the next chapters I will explore this situation a bit more).

Up to this point, I have been considering lowest order radiative corrections and the necessary mass and charge renormalization. This is not the whole story. I have not mentioned how Feynman's approach relates to the S-matrix calculations, the renormalization to all orders of the S-matrix, and what to make of Dyson's 1952 result about the divergence of the series expansion of the S-matrix; in the process of doing so I will return to the views that several physicists have had regarding renormalization.

Dyson gave a more formal structure to Feynman's approach. Considering the perturbative solution of the Tomonaga-Schwinger equation in terms of a unitary operator, Dyson realized that when taking the limits for an initial state in the infinite past and a final state in the infinite future, Schwinger's unitary operator was identical to

the Heisenberg S-matrix. Following Feynman's symmetrical approach between past and future, Dyson used a chronological operator P( ) that enabled him to present the S-matrix in the form

$$S(\infty) = \sum_{n=0}^{\infty} (-i/\hbar c)^n [1/n!] \int_{-\infty}^{+\infty} dx_1 \ldots \int_{-\infty}^{+\infty} dx_n P(H^I(x_1), \ldots, H^I(x_n)),$$

where $H^I(x)$ is the term in the Hamiltonian corresponding to the interaction between the Maxwell and Dirac fields (Dyson, 1948, p. 492). In the case of electron-electron scattering, the second-order term of this expansion is given by Feynman's fundamental equation (taking into account Pauli's exclusion principle).[35]

This Dyson did after the summer of 1948, having already talked substantially with Feynman and assisting in particular Schwinger's lectures at Ann Arbor in that summer. On arriving at the Institute for Advanced Study in Princeton in early September 1948, Dyson wrote home that

> on the third day of the journey a remarkable thing happened; going into a sort of semi-stupor as one does after 48 hours of bus-riding, I began to think very hard about physics, and particularly about the rival radiation theories of Schwinger and Feynman. Gradually my thoughts grew more coherent, and before I knew where I was, I had solved the problem that had been in the back of my mind all this year, which was to prove the equivalence of the two theories. Moreover, since each of the two theories is superior in certain features, the proof of the equivalence furnished incidentally a new form of the Schwinger theory which combines the advantages of both. (Quoted in Schweber, 1994, p. 505)

Afterwards Dyson confronted the question of whether the perturbative approach could be made finite to every order. Dyson was able to show inductively that if all divergences had been removed in a particular order n then they could be removed in order n + 1. Since this was the case in lowest order by using renormalization procedures, this would also be the case to whatever order we actually achieved when making a calculation. In this way the perturbative expansion of the S-matrix is renormalizable to all orders (Dyson, 1949). However as we have already seen, the perturbative expansion of the S-matrix is divergent. What to make of this with respect to renormalization?

First I will look again into Schwinger's view on the renormalization. Schwinger considered that the infinites meant that the theory breaks down at ultra-relativistic energies. Under this view, to Schwinger

> [renormalization] is the clear separation of what we don't know–but which affects our experiments in a clear limited way–from what we do know and where we can calculate in detail. In fact, I insist that all

[35] The S-matrix program was originally developed by W. Heisenberg as an alternative to quantum field theory. His idea was to sidestep the problem of divergences in quantum field theory – in his view due to the point-like interaction between fields – by considering only what he saw as measurable quantities (Miller, 1994, p. 97). Heisenberg's idea was to retain only the basic elements of quantum field theory, like the conservation laws, relativistic invariance, unitarity, and others, and to make the S-matrix the central element of a new theory (Pais, 1986, p. 498). This was not done because in practise it was not possible to define an S-matrix without a specific use of the theory it was intended to avoid (Cushing, 1986, p. 118). The S-matrix later reappeared in mainstream physics with Dyson's use of it as a calculational tool. In Dyson's view the "Feynman theory will provide a complete fulfilment of Heisenberg's S-matrix program. The Feynman theory is essentially nothing more than a method of calculating the S-matrix for any physical system from the usual equations of electrodynamics" (quoted in Cushing, 1986, p. 122).

theories are like this. –People may not want to face up to it, there is always an area beyond where the theory either breaks down or where other phenomena come into play that you don't know about. They do not upset everything in the area you can control, and you isolate that from it: That's what renormalization is really about. Not sweeping infinities away but isolating the unknown part and recognizing its limited influence.

I am not sure that I was at all interested in the mathematical question of convergence to all order. I don't think that is a physical question. I have a feeling even then that I did not take renormalization too seriously. If in fact the theory had been not renormalizable at the 27th stage or whatever have you, I would have said "O.K. That's good" because here is a place where what we don't know, namely what happens at very large energies, enters the theory and will learn something. It wasn't essential to me that the theory be renormalizable to all orders. That was nice to get the theory going to lowest order. What would be even more interesting is if it didn't work. I wasn't very caught up in all these all order questions. (Quoted in Schweber, 1994, p. 366)

We see that for Schwinger it was not problematic that the series expansion of the S-matrix is divergent (even if he does not mention it explicitly, I think this agrees with the view he presents). However, we see that there is not in Schwinger a connection between the mathematical problems facing the theory and a limitation on its applicability in a way to be consistent with the underlying concepts (like the idea of a point-like electron), as we can see in Dirac's subtraction physics.

My view is that Dyson's 1952 new divergence does not change much whatever view we decide to have on renormalization. We can still think that there is a breakdown at high energies or/and problems in the type of description of the interaction between the fields adopted in quantum electrodynamics. Depending on what we make of Dyson's divergence we can see it related, or not, to the renormalized infinites. I tend to see a relation, because, in my view, both are related with limitations in the description of the interactions in quantum electrodynamics, and both are manifestations of an improper use of the mathematics beyond the physical content of the theory.

In the previous chapter I defended that we can relate the divergence of the S-matrix series expansion with a tentative application of the theory beyond the possibilities provided by the input physical assumptions used to set up the theory as a perturbative approach. Now I put together the elements for the equivalent point in the case of renormalization. For this I will return to Dirac's subtraction physics and to Bohr's views on the problem of infinities in quantum electrodynamics. In a nutshell Dirac concluded that an external electromagnetic field had an effect of polarization of the distribution of negative-energy electrons. The calculation of the density matrix of the sea electrons, in the simple case of an external electrostatic field, gave a logarithmically divergent result. Dirac considered that we cannot assume that the theory applies when it is a question of energies greater than the order of $137mc^2$. So, he used a cut-off to render the results finite. With the finite result in his hands, Dirac concluded that there is no induced electric density except at the places where the electric density producing the field is situated, and at these places the induced electric density cancels a fraction of 1/137 of the electric density producing the field. This means that the electron's charge that is measured is smaller than the real charge.

For me the crucial aspect can be found in Dirac's argument for the need of a cut off. He says that

quantum mechanics does not seem applicable to phenomena which involve distances of the order of the classical radius e^2/mc^2, since the present theory can in no manner discuss the structure of the electron … such distances, considered as electron wavelengths, correspond to energies of the order $(\hbar c/e^2)(mc^2)$ [$\cong 137mc^2$]. (Dirac, 1934a, pp. 136-137)

As already mentioned, this can be seen as a Bohrian sentence, in the sense of taking into account the input physical assumptions in the theory of a point-like electron to justify disregarding energies greater than the order of $137mc^2$. To appreciate properly this point let us look again into Bohr's views on quantum electrodynamics:

> The foundations of the present treatment of atomic phenomena are the discoveries of the ultimate electrical particles and the elementary quantum of action, which rely upon quite separate lines of experimental evidence and at the present stage of atomic theory are introduced in essentially different and independent ways.… The possibility of treating the elementary particles and the quantum of action as independent foundations of the theory of the electronic constitution of atoms rests essentially upon the fact that the atomic dimensions, as deduced from quantum-mechanics and symbolized by the "radius" of the hydrogen atom $a = h^2/4\pi^2e^2m$ [(2)], are very large compared with the electron diameter given by [$d = e^2/mc^2$ (1)]. Obviously, *this is a necessary condition for considering the electron as a charged material point in the fundamental mechanical equations*…. Notwithstanding its fertility, the attack on atomic problems in which the particle idea and the quantum of action are considered as independent foundations is of *an essentially approximative character* … The possibility of treating radiation phenomena and other effects of the finite propagation of forces to a considerable extent rests entirely on the smallness of the two dimensionless constants of atomic theory, the fine structure constant $\alpha = 2\pi e^2/hc$ and the ratio between the masses of the electron and the proton $\beta = m / M$. Thus as will be seen from (1) and (2), it is the small value of α which is responsible for the smallness of the ratio between d and a, which is just equal to α^2. It is just this circumstance which affords a justification for the neglect of the radiative reaction in a description of the stationary states including the fine structure ... *the attempts to treat the radiation effects on rigorous lines by considering the atoms and the electromagnetic field as a closed quantum-mechanical system led to paradoxes arising from the appearance of an infinite energy of coupling between atoms and field*. The solution of these difficulties will certainly claim a formalism in which the elementary particles and the quantum of action appear as inseparable features…. It is important, however, to examine more closely to what extent the present theory offers a reliable guidance for the analysis of the phenomena ... In this procedure, in which the radiation field is not considered as part of the system under investigation ... By a proper application of the quantum mechanical formalism it has been possible … the treatment of such problems as the width of spectral lines and the retardation effects in the interaction of electrons bound in atoms. Still, *the condition for such applications is that the effects in question can be treated as small perturbations* of the phenomena to be expected if the finite propagation of forces would be neglected. *Due to the smallness of the constant α, mentioned above, this condition is widely fulfilled in problems of atomic constitution, since even for the electrons most firmly bound in atoms of high nuclear charge, "orbital" dimensions and spectral wave-lengths are very large compared with the classical electron diameter*. (Bohr, 1932b, p. 62-67 [my emphases])

Contrary to others that look into the renormalizable infinites in quantum electrodynamics from the perspective of a putative better theory, Bohr looks from within quantum electrodynamics. As we have seen, for example in the case of the Klein paradox, to Bohr it is not that the negative-energy solutions are non-physical or some other thing. It is simply that we cannot disregard the atomicity of matter, and when we do that, by considering mathematically possible potentials that are physically impossible when taking into account part of the conceptual basis of the theory (i.e. the atomicity of matter), we get into trouble. We obtain strange mathematical results without any clear physical meaning. The same holds in the case of the renormalizable infinities. In the structure of the theory we have a point-like description of the electron. This means we can not consider distances were we might have in some way to talk about the internal structure of the electron (whatever this might mean). When considering high-energy interactions we would be so to speak poking into the electron, i.e. going beyond the conceptual basis of the theory. The infinities show not where a better theory is needed but where we are stretching the mathematics beyond the physical basis of the theory. In quantum electrodynamics, according to Bohr, it only makes sense to consider distances larger than the so-called "electron diameter", which implies taking a limited range for

the energy in interactions. This in practice corresponds to using a Dirac type cut off in the necessary expressions (i.e. Feynman's regularization), even if it turns out to be a mathematically inconsistent procedure (as others in the theory).

5 Conclusions

The objective in this chapter was twofold. One of them was to address renormalization from the perspective of the spacio-temporal description of physical processes in quantum electrodynamics. As we have seen implicit in the charge renormalization procedure is the fact that we are considering an overall space-time description. In practice this means that we are not really describing the physical processes in time. The charge renormalization is possible exactly because of this. We implement a view of the physical processes as if from outside space-time and we move around infinities that should be related to the electromagnetic mediation between charged particles, i.e. related to delayed interactions, and 'by hand' put the infinities where it is more convenient. In this case the infinity due to the photon self-energy is attributed to the charge of the particles and 'renormalized'.

The other objective of this chapter was to dig into the history of renormalization to see if from an encounter with the original moments where the developments were being made it was possible to find a 'new' perspective on renormalization that might not be part of the contemporary philosophical views on renormalization; the objective was not to present a detailed study of the different contemporary views.[36]

The view regarding renormalization presented here is based on Bohr's ideas. As we have seen, according to Bohr

> the existence of the electron even in classical theory imposes an essential limitation on the applicability of the mechanical and electromagnetic concepts. Indeed, the finite propagation of electromagnetic forces brings with it the existence of a fundamental length, the so-called "electron diameter" defining a lower limit for the extension of the region where the idealization according to which the electron is considered as a charged material point is justifiable. (Bohr, 1932a, p. 377)

We must recall that in the structure of quantum electrodynamics is inscribed, through the Dirac equation, a point-like description of the electron (see chapter 3). This idealization of the electron as a point-like particle implies according to Bohr limitations to quantum electrodynamics:

> the difficulties inherent in any symbolism resting on the idealization of the electron as a charged material point appear also most instructively in the recent attempt of Heisenberg and Pauli to build up a theory of electromagnetic fields on the lines of quantum mechanics. (Bohr, 1932a, p. 378)

I regard Dirac's 'subtraction physics' as an example of a procedure that identifies and overcomes in an imperfect way one of these difficulties.[37] As we have seen, according to Dirac

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[36] In particular I do not address the renormalization group approach (on this subject see e.g. Huggett and Weingard, 1995).

[37] To Bohr the difficulties of quantum electrodynamics were, in particular, "Dirac's unobservable negative energies, the ambiguity of force indicated by the Klein paradox, the unmeasurable magnetic moment of the electron, the uninterpretable spin, and the unresolved infinities" (Moyer, 1981, p. 1061).

quantum mechanics does not seem applicable to phenomena which involve distances of the order of the classical radius e^2/mc^2, since the present theory can in no manner discuss the structure of the electron … such distances, considered as electron wavelengths, correspond to energies of the order $(\hbar c/e^2)(mc^2)$ [$\cong 137mc^2$]. (Dirac, 1934a, pp. 136-137)

In this way Dirac made use of a cut-off in the applications of the theory, corresponding to a maximum value of the energy of the order $137mc^2$:

we cannot assume that the theory applies when it is a question of energies greater than the order of $137mc^2$, and the most reasonable way to proceed seems to be to limit arbitrarily the domain of integration to a value of the momentum … corresponding to electron energies of the order indicated. (Dirac, 1934a, p. 141)

With this procedure we would be avoiding a conflict between one of the input physical assumptions of the theory (the point-like electron) and applications not taking into account this physical assumption.

Does this means that the theory sets from the inside its experimental domain of application? It seems that this was Bohr's view. According to a letter of Dirac from 1931,

Bohr is at present trying to convince everyone that the places where relativistic quantum theory fails are just those where one would expect it to fail from general philosophical consideration. (quoted in Moyer, 1981, p. 1060)

This is not the view being defended here. To clarify this point let us consider for example Newton's theory of gravitation. As it is well known, Newton's theory predicts a particular numerical value in relation to the drift of the perihelion of mercury, which, contrary to Einstein's gravitation theory, is not in good agreement with observation. However from the internal perspective of Newton's theory there is nothing strange about this result: it is physically meaningful (i.e. it goes along the line of different results provided by the theory). What is happening is that we are facing a limit of application of the theory in what regards 'saving the phenomena'. The situation with the renormalizable infinities is different; it is not related to the experimental/observational domain of applicability of quantum electrodynamics (i.e. it is not related with 'saving the phenomena'). In my view it represents a locus of 'divergence' between the physical assumptions of the theory and its mathematical applications; contrary to the view that Dirac attributes to Bohr (I think correctly), the limitations in the application of physical concepts do not affect or enable to define clearly the experimental/observational domain of applicability of the theory. When addressing appropriately the problem of infinities by the renormalization procedure it does not affect the domain of application of the theory.

How do we identify situations where a mismatch occurs between for example the physical idealization of a point-like electron and applications that go beyond this idealization? In my view when we obtain results that are not physically meaningful (without taking into account any comparison with observations). This is particularly clear when for example we expect on *physical grounds* to calculate a very small correction to the electron mass due to its self-energy and it turns out that the result is divergent. This does not imply that in all theories we must take a divergent result as a sign of a mismatch between the physical input assumptions and the mathematical applications of the theory. I have no general argument pointing to this, and I do not even explore this possibility. As mentioned, in this work the objective is only to look into a

few conceptual-mathematical problems of quantum electrodynamics not related to ‘saving the phenomena’.

CHAPTER 7

THE FEYNMAN DIAGRAMS AND VIRTUAL QUANTA

1. Introduction

As we have seen, during the development of quantum electrodynamics in the 1930s and most of the 1940s, the calculations beyond the lowest order of perturbation theory gave infinite corrections to the results, before the renormalization program eventually succeeded in "sweeping the dirt under the rug" (Feynman 1962, 137). It might seem that the lowest order applications of the theory, where there are no infinites to struggle with, are free from problems, and that in particular Feynman's space-time approach to quantum electrodynamics might provide consistent means of representation and visualization of the lowest order processes in quantum electrodynamics. In this chapter, however, I shall argue that things are not quite that simple. In particular, I will focus on the role played by photons in the description of electron-electron interactions. I will analyse the relevance of virtual and real photons in making possible a description of the interaction as a delayed interaction, as it is possible in classical electrodynamics.

In section 2 the derivation of Møller's semi-classical formula for electron-electron scattering is considered, by a full quantum electrodynamical treatment using the so-called Feynman fundamental formula (related to the second-order term of the S-matrix expansion). The electron-electron interaction is described in this case as an exchange of a virtual photon between the electrons. In section 3 the lowest order calculation of the electron-electron scattering that permits the derivation of the Møller formula is used to analyse the type of description of interaction provided by quantum electrodynamics and its limitations. It turns out that it is not possible to give a description of the electron-electron interaction as a process occurring in time, i.e. as a delayed interaction. To better understand this limitation in relation to the classical description, in section 4 I will consider a quantum model for the interaction between two bound electrons. In this case, contrary to the previous, the photon responsible for the interaction can be taken to be a real photon. In this circumstance we regain a delayed interaction as in the classical case. The problem is that we are not truly working with an application of quantum electrodynamics, but with a heuristic construction of a quantum model of the interaction between two bound electrons patching together different elements.

2 The Møller scattering and Feynman's fundamental equation

In the early 1930s, the relativistic electron-electron scattering was treated using a semi-classical approach in the lowest order of perturbation theory. C. Møller used in the Maxwell equations the charge and current densities associated with the state transition of an electron from an initial to a final free state as described by the Dirac equation. The

effect of the retarded potentials determined in this way on a second electron results in a state transition of the electron. With this scheme Møller obtained a symmetrical expression for the matrix elements for the scattering of two electrons interacting via classical retarded potentials (Møller, 1931; see also Heitler, 1954, p. 233). Around the years 1932-33, the use of correspondence methods by Møller lost part of its appeal, due to Bethe and Fermi's demonstration that the formula could be derived within quantum electrodynamics, and also due to Bohr's confidence in the logical consistency of the theory (Kragh, 1992, pp. 323-324), even if, as Bohr recognized, the divergence problems in the theory were still not solved, and physics was "confronted with the necessity of a still more radical departure from accustomed modes of description of natural phenomena" (quoted in Schweber, 1994, p. 84). In any case, Møller's scattering formula did not attract much attention during the thirties and forties, until it revealed itself as an almost immediate application of the new formulation of quantum electrodynamics (Roqué, 1992, p. 256).

Briefly Møller's method goes as follows. Møller considers that when a particle makes a transition (during an interaction) from an initial state i to a final state f, it can be associated with charge and current densities given by

$$\rho = -e\psi_f^* \psi_i$$

$$j = e\psi_f^* \alpha \psi_i$$

Møller then makes use of Klein's 'correspondence approach', where we consider at the same time the one-electron Dirac equation and the classical Maxwell-Lorentz equations. In Klein's approach the expressions for the charge and current densities provided by quantum theory are used in the classical Maxwell-Lorentz equations to determine the field emitted in a transition (Kragh, 1992, p. 310). According to Klein

> As we try here to connect wave mechanics directly with the electromagnetic field equations, we will assume, that the electromagnetic phenomena corresponding to the magnitudes [of the charge density] and [the current density] give, in the sense of Bohr's correspondence principle, a quantitative expression of the observable actions related to the presence of an atom in a certain stationary state. (Quoted in Roqué, 1992, p. 202)

Møller considers now that the charge and current densities resulting from a quantum transition give rise to a classical potential given by the equations

$$\Delta\phi - \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = -4\pi\rho$$

$$\Delta A - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} = -\frac{4\pi}{c} j,$$

whose solutions are

$$\phi = -\frac{h^2 e}{\pi}\frac{\psi_f^* \psi_i}{(p_i - p_f)^2}$$

$$A = \frac{h^2 e}{\pi} \frac{\psi_f^* \alpha^{(1)} \psi_i}{(p_i - p_f)^2},$$

where p = (E/c, **p**) is the four-momentum of the electron. This potential is taken to be a perturbation to a second particle described by Dirac's equation:

$$\left(i\hbar \frac{\partial}{\partial t} - ic\hbar \alpha^{(2)} \cdot \vec{\nabla} + \beta m_2 c^2 \right) \psi^{(2)} = -e(\phi + \alpha^{(2)} \cdot \vec{A}) \psi^{(2)}$$

Møller uses the (spatial part) of the classical perturbing potential, and by considering the particles to be described by plane waves (i.e. the particles are described as free particles), arrives at the interaction matrix element

$$H_{fi} = e^2 \int \psi_f^{(2)*} \psi_f^{(1)*} (1 - \alpha^{(1)} \cdot \alpha^{(2)}) \frac{e^{ikR}}{R} \psi_i^{(2)} \psi_i^{(1)} d\tau_1 d\tau_2,$$

which is symmetric in the two particles, and can be taken to describe the interaction between the particles (even if its derivation was made in an unsymmetrical way by taking the potential arising from the first particle to perturb the second particle). By a straightforward procedure it is possible to calculate the formula for the scattering cross section, which is then used to compare with experimental results. This is, in a nutshell, Møller's semi-classical treatment – in first order of perturbation theory, and using the 'correspondence approach' of Klein – of the electron-electron scattering.

Should we consider this semi-classical approach when addressing the description of interactions in quantum electrodynamics as giving some sort of valuable different perspective? Taking into account the views of E. T. Jaynes, accepted here, the answer is no. According to Jaynes

What I will call Semiclassical A (SCA) was the original method of incorporating the electromagnetic field into quantum theory, antedating QED. SCA is what we were all taught in our first course in quantum mechanics, defined for our present purposes (which are served adequately by the model of a single nonrelativistic spinless hydrogen atom) by the Schrödinger equation

$$i\hbar \dot{\psi} = \left[\frac{(p - e/c\, A)^2}{2m} + e\phi \right] \psi$$

in which the electromagnetic potentials A, ϕ are considered given. This equation determines the effect of the field on the atom; from it we obtain the quantum theory of the Zeeman and Stark effects, the Einstein B-coefficients of black-body radiation theory, the Rutherford scattering law, the photoelectric cross-section, and with appropriate generalization, very much more.

SCA is incomplete in that it fails to give the effect of the atom on the field. To supply this, so that one could describe emission and scattering of radiation, there arose the "Klein Vorschrift" … Closely related to this was the "transition current method" (TCM) which is still very much in the use today … In TCM, one specifies initial ψ_i and final states ψ_f, for the electrons, and sandwiches an operator representing current, dipole moment, etc. between them, making the "transition current"

$$j_{fi}(x,t) = \frac{e}{mc} \psi_f^* (p - e/c\, A) \psi_i$$

or the "transition dipole current", etc. Then we switch to classical electromagnetic theory, and calculate the fields that would be produced by such a current or dipole moment. In this way, surprisingly,

we obtain the correct Einstein A-coefficients for spontaneous emission. TCM also yields many other useful results, such as the Møller e-e scattering formula.

TCM can hardly be considered as a well-motivated physical theory in its own right, because it mixes up the initial and final states in a way that defies any rational physical interpretation. Note, however, that if

$$\psi = \sum_i a_i \psi_i$$

is a linear combination of stationary states, the quantity

$$j(x,t) = \frac{e}{mc} \mathrm{Re}\left[\psi_f^* (p - e/c\, A)\psi_i\right]$$

usually called the "probability current", will be interpreted by neoclassical theory as actual current (or, at least, its divergence will equal the divergence of the actual current). Using the expansion (3), we see that the current (4) contains all the transition currents with amplitude $a_i^* a_j$:

$$j(x,t) = \sum_{ij} j_{ij}(x,t) a_i^* a_j$$

Because of the above difficulty of interpretation, and because both the Klein vorschrift and TCM received an *a posteriori* justification from QED, I would consider that they do not represent parts of any semi-classical theory, but should be regarded as convenient short-cut algorithms contained in QED. (Jaynes, 1973, pp. 38-40)

We will then turn our attention to the quantum electrodynamical treatment of electron-electron scattering.

Following J. A. Wheeler's view that all physical phenomena could be seen as scattering processes (Schweber, 1994, p. 379), Feynman considered the mutual interaction of two electrons as a fundamental interaction described by his fundamental equation for quantum electrodynamics (Feynman, 1949b, p. 772; see chapter 6 for details on Feynman's 'fundamental equation'). The Møller scattering formula is obtained directly from this equation when Pauli's exclusion principle is taken into account (Feynman, 1949b, p. 773).

As already mentioned, in 1948, Dyson proved the equivalence of the theories of Feynman and Schwinger (and Tomonaga). The main contribution of Dyson was to show that the two so seemingly different approaches could be put together by resort to the S-matrix approach. In the abstract of his paper, sent to publication in October 6, 1948, Dyson states his primary aim:

A unified development of the subject of quantum electrodynamics is outlined, embodying the main features both of the Tomonaga-Schwinger and the Feynman radiation theory … The chief results obtained are (a) a demonstration of the equivalence of the Feynman and Schwinger theories, and (b) a considerable simplification of the procedure involved in applying the Schwinger theory to particular problems. (Dyson, 1948, p. 486)

In his paper Dyson gives an outline of the derivation of the Tomonaga-Schwinger equation:

$$i\hbar c \frac{\delta \psi[\sigma]}{\delta \sigma(x_0)} = H_1(x_0)\, \psi[\sigma],$$

where H_1 gives the interaction between the quantized fields. Taking for the general solution of the equation a wave function $\psi(\sigma) = U(\sigma)\psi_0$, a perturbative solution can be given in powers of H_1:

$$U(\sigma,-\infty) = 1 - \frac{i}{\hbar c}\int_{-\infty}^{\sigma} H_1(x_1)dx_1 + \left(-\frac{i}{\hbar c}\right)^2 \int_{-\infty}^{\sigma} dx_1 \int_{-\infty}^{\sigma_1} dx_2 H_1(x_1)H_1(x_2) + \ldots$$

According to Dyson, $U(\infty,-\infty)$ "is identical with the Heisenberg S matrix" (p. 489). After redefining the Hamiltonian term corresponding to the two independently quantized fields in a way to incorporate the electromagnetic mass, Dyson considers the perturbative solution of the equation for the unitary operator $S(\sigma,-\infty)$, which is the same as that of $U(\sigma,-\infty)$ in the absence of an external field.

In the presence of an external field, the state vector defined by $\psi(\sigma) = S(\sigma)\Omega(\sigma)$, obeys the equation $i\hbar c[\partial\Omega/\partial\sigma(x_0)] = (S(\sigma))^{-1}H_e(x_0)S(\sigma)\Omega = H_T(x_0)\,\Omega$, where $H_e(x_0)$ gives the external field. The substitution of the previous series into this equation gives

$$H_T(x_0) = \sum_{n=0}^{\infty}\left(\frac{i}{\hbar c}\right)^n \int_{-\infty}^{\sigma_0} dx_1 \int_{-\infty}^{\sigma_1} dx_2 \ldots \int_{-\infty}^{\sigma_{(n-1)}} dx_n \left[H_1(x_n),[\ldots[H_1(x_2)[H_1(x_1),H^e(x_0)]\,]\ldots\,]\,\right]$$

According to Dyson, "the repeated commutators in this formula are characteristic of the Schwinger theory, and their evaluation gives rise to long and rather difficult analysis" (p. 491). Dyson turns then to Feynman's approach:

> In the Feynman theory the basic principle is to preserve symmetry between past and future. Therefore, the matrix elements of the operator H_T are evaluated in a "mixed representation"; the matrix elements are calculated between an initial state specified by its state vector Ω_1 and a final state specified by its state vector Ω_2'. The matrix element of H_T between two such states in the Schwinger representation is ${\Omega_2}^* H_T\,\Omega_1 = {\Omega_2}'^* S(\infty)H_T\,\Omega_1$, and therefore the operator which replaces H_T in the mixed representation is $H_F(x_0) = S(\infty)H_T(x_0) = S(\infty)(S(\sigma))^{-1}\,H^e(x_0)\,S(\sigma)$. (p. 491)

Dyson then shows how to derive what he calls Feynman's fundamental formula (which can be simply related, in second-order, to Feynman's 'fundamental equation'). First, Dyson defines a chronological operator: " If $F_1(x_1)$, …, $F_n(x_n)$ are any operators defined, respectively, at the points x_1, … , x_n of space-time, then P() will denote the product of these operators, taken in order, reading from right to left, in which the surfaces $\sigma(x_1)$, ..., $\sigma(x_n)$ occur in time" (p. 492).

By substituting the series for H_T into the expression for H_F, and by taking advantage that the integrand in the expression for H_F "is a symmetrical function of the points x_1, … , x_n" (p. 492), Dyson obtains

$$H_F(x_0) = \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar c}\right)^n [1/n!]\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \ldots \int_{-\infty}^{\infty} dx_n \times P(H^e(x_0), H_1(x_1),\ldots,H_1(x_n))\,.$$

In the case where there is no external field present the previous expression simplifies to

$$S(\infty) = \sum_{n=0}^{\infty}(-i/\hbar c)^n[1/n!]\int_{-\infty}^{+\infty} dx_1 \ldots \int_{-\infty}^{+\infty} dx_n P(H^I(x_1),\ldots,H^I(x_n))\,.$$

According to Dyson, "the further development of the Feynman theory is mainly concerned with the calculation of matrix elements of [the previous expression] between various initial and final states" (p. 492). Dyson then derives the Feynman rules, for problems with an initial (and final) charged particle (electron or positron) and with no photons in the initial and final states. Accordingly Dyson aims to

> obtain a set of rules by which the matrix element of [H_F] between two given states may be written down in a form suitable for numerical evaluation, immediately and automatically. The fact that such a set of rules exists is the basis of the Feynman radiation theory; the derivation in this section of the same rules from what is fundamentally the Tomonaga-Schwinger theory constitutes the proof of equivalence of the two theories. (pp. 492-493)

Dyson considers the contribution of the nth order term of the transition matrix (S-matrix) element, which is a sum of terms of the form

$$M = \varepsilon' \prod_{i \neq k} \frac{1}{2} S_F(x_i - x_{r_i}) \prod_{i \neq k} \frac{1}{2} \hbar c D_F(x_{s_j} - x_{t_j}) \psi^*(x_k) \psi(x_{r_k}),$$

where D_F and S_F are the Feynman propagators for an electron and a photon, and $\psi(x)$ is the electron-positron field operator and $\psi^*(x)$ its adjoint operator. Following Feynman, Dyson calls attention to the fact that to each term in the matrix element can be associated a graph (a Feynman diagram) and that there is "a one-to-one correspondence between types of matrix elements and graphs" (p. 495). Also Dyson mentions too that "in Feynman's theory the graph corresponding to a particular matrix element is regarded, not merely as an aid to calculation, but as a picture of the physical process which gives rise to that matrix element" (p. 496). This is an important point to which I will return soon.

As mentioned, the Møller formula for electron-electron scattering can be derived as a direct application of quantum electrodynamics through the fundamental equation. This is the simplest description of an electron-electron interaction, based on the exchange of one virtual quantum between two electrons. We can of course consider improved calculations using higher-order corrections (Feynman, 1949b, p. 787), but these terms are corrections to the lower-order terms being used. They do not change the overall space-time description of interaction processes as already present in the lower-order calculations. For this reason I will only consider the overall space-time description of scattering processes in quantum electrodynamics as given by its lower-order applications.

3 The description of interactions as space-time processes resulting from the exchange of virtual quanta

In the second-order expansion of the S-matrix the electron-electron interaction results from a photon exchange (see Fig. 1). In the overall space-time approach of Feynman we are considering virtual photon propagation (exchange) between all the Minkowski space-time points. The Feynman photon propagator is given by

$$\langle 0 | T\{A^\mu(x) A^\nu(x`)\} | 0 \rangle = i\hbar c D_F^{\mu\nu}(x - x') \quad \text{(Mandl \& Shaw, 1984, p. 86).}$$

This expression means that we are considering a photon 'created' at one space-time location and 'annihilated' at another. The use of the time-ordered product T{ } means that in this covariant expression we are already considering, depending on the time order, a propagation from one electron to the other or vice versa, since $T\{A^{\mu}(x)A^{\nu}(x')\} = A^{\mu}(x)A^{\nu}(x')$ if $t > t'$, and $T\{A^{\mu}(x)A^{\nu}(x')\} = A^{\nu}(x')A^{\mu}(x)$ if $t' > t$. Loosely speaking, we have contributions in which the 'emitter' and 'receiver' change roles.

The transition amplitude for Møller scattering in the second-order expansion of the S-matrix (the simplest for this process) results from a contribution of all possible localized interactions of Dirac and Maxwell fields 'connected' by a photon propagator (Mandl & Shaw, 1984, p. 113):

$$S^{(2)}(2e^{-} \rightarrow 2e^{-}) = \frac{-e^2}{2!}\int d^4x_1 d^4x_2 N\left[(\overline{\psi}^{-}\gamma^{\alpha}\psi^{+})_{x_1}(\overline{\psi}^{-}\gamma^{\beta}\psi^{+})_{x_2}\right] iD_{F\alpha\beta}(x_1 - x_2).$$

This means that the overall process we call 'interaction' results from the contribution of photon propagation from one electron to the other and vice versa: it is a two-way process in all space-time.

The label 'virtual' attached to the photon is related to two things. In the space-time points where the photon is created or annihilated we have conservation of energy and momentum between the photon and the electrons. But the energy-momentum relation for the virtual photon is not $k^2 = (k^0)^2 - \mathbf{k}^2 = 0$ corresponding to a zero mass photon, it is different from zero due to the fact that in the expression for the propagator $\mathbf{k}$ and k^0 are independent of each other (Mandl & Shaw, 1984, p. 86). In a certain sense it is as if the 'dynamics' of the virtual photon are all messed up (the same occurs with the electron when it is in the role of a virtual quanta), because it is as if it has a mass during the virtual process. At the same time the 'kinematics' come out wrong also, because the propagator is nonvanishing at space-like separations (Björken & Drell, 1965, pp. 388-389). The second point is that this virtual quanta is supposed by definition not to be observable – it is part of the internal machinery of the application. In the case of the photon in the electron-electron scattering it seems impossible to avoid this situation, as the idea that this is the most elemental process possible is implicit in the theory.

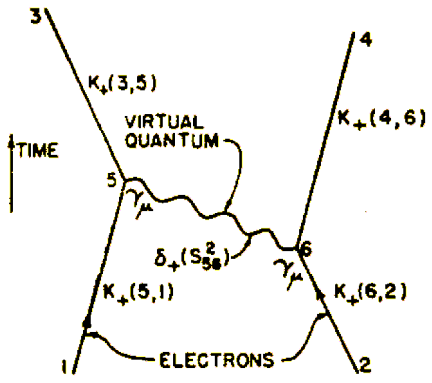

Figure 1: Electron-electron scattering in second order, resulting from a virtual photon exchange (direct diagram).

The question arises: are the virtual particles simply the result of the perturbative treatment of interaction, i.e. simply mathematical terms, or do they convey as Dyson

remarks, "a picture of the physical process which gives rise to that matrix element" (Dyson, 1948, p. 496). The contemporary view in philosophy of physics is that they do not. According to Tobias Fox, the virtual particles serve "to symbolise the interaction" (Fox, 2008, p. 35), and they "are merely pictorical descriptions of a mathematical approximation method" (p. 35). Reviewing the arguments of several authors[38] Fox centers on what he considers the argument that proves the status of virtual particles, "as only pictorical symbols for mathematical terms" (p. 36). This so-called argument of superposition rests on the (wrong) idea that in the S-matrix description of interactions we have to use an infinite expansion of the S-matrix that results in "the infinite superposition of Feynman diagrams of higher and higher order" (p. 38), even if according to Fox, "due to practical reasons–the perturbation progression is stopped sooner or later" (p. 37).

One among several variants of this argument was set forward by Robert Weingard. If, when calculating, say, the amplitude for electron-electron scattering, the complete S-matrix was (somehow) considered, then there would be an infinite number of terms corresponding to an infinite number of combinations of different quanta. One could say that in this case the quanta "type and number are not sharp" (Weingard, 1988, p. 46). The quanta description of interactions, as quanta exchange, would then appear to be a mathematical fiction due to the use of perturbation theory in the calculation of the scattering amplitude. However, when considering the scattering as described in the theory, we can only use a few terms of the S-matrix expansion. There simply is no possibility of considering the (unexisting) exact S-matrix, only the asymptotic S-matrix.[39]

On similar lines, but with important differences in relevant details, Brigitte Falkenburg considers the virtual particles as "formal calculational tools" (Falkenburg, 2007, p. 223). According to Falkenburg the virtual particles come into play within time-dependent perturbation theory:

> the propagators of the virtual field quanta are mathematically components of a quantum theoretical superposition. Operationally, it is by no means possible to resolve them into single particle contributions. They are nothing but the mathematical contributions to an approximation procedure: like the harmonics of the oscillators of a mechanical string, the Fourier components of a classical electromagnetic field, or the cycles and epicycles in Ptolemy's planetary system. (p. 234)

However Falkenburg, after concluding that "virtual field quanta are nothing but formal tools in the calculation of the interactions of quantum fields" (p. 237), calls attention to the fact that "this does not mean, however, that the perturbation expansion of the S-matrix in terms of virtual particles is *completely* fictitious" (p. 237). According to Falkenburg,

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[38] For example, Mario Bunge takes the virtual quanta (and interaction processes described as exchange of virtual quanta) to be "fictions and as such have no rightful place in a physical theory" (Bunge, 1970, p. 508); Paul Teller's view is that "a Feynman diagram is only a component in a much larger superposition" (Teller, 1995, p. 139); and Fritz Rohrlich considers that "virtual particles are an artifact of the perturbation expansion into free particle states" (Cao, 1999, p. 363).

[39] There might appear to be ways of sidestepping this type of approach by considering the Feynman path integral approach (Weingard, 1988, p. 54). But again, when considering the specific applications of the theory there is no infinite expansion of the transition amplitudes. In the mathematical expression for the transition amplitudes there are quanta propagators, and the interpretation of the propagators relating them to quanta cannot be overturned in a (finite expansion) application based on path integrals.

The virtual processes described in terms of the emission and absorption of virtual particles contribute to a scattering amplitude or transition probability. Hence, *infinitely many* virtual particles, *together* may be considered to cause a *real collective effect*. In *this* sense, they obviously *have* operational meaning. What is measured is an S-matrix element or the probability of a transition between certain real incoming and outgoing particles. The transition probability stems from *all* virtual field quanta involved in the superpositions of the relevant lowest and higher order Feynman diagrams.

In the low energy domain, it is sometimes even possible to single out the contribution of one single Feynman diagram to the perturbation expansion. There are even several well-known high precision measurements to which mainly one Feynman diagram or the propagator of a virtual particle corresponds. This is demonstrated in particular by the best high precision tests of quantum electrodynamics, the measurement of the hydrogen Lamb shift and the $(g - 2)/2$ measurement of the gyromagnetic factor g of the electron or muon. Dirac theory alone incorrectly predicts the fine structure of the hydrogen spectrum (no splitting of the levels $S_{1/2}$ and $P_{1/2}$ for $n = 2$) and a gyromagnetic factor $g = 2$ for the electron or muon. Measurements reveal the Lamb shift of the hydrogen fine structure and the anomalous magnetic moment of the electron.

The anomalous difference $(g - 2)/2$ between the prediction of the Dirac theory and the actual magnetic moment was measured with high precision from the spin precession of a charged particle in a homogeneous magnetic field. The next order quantum electrodynamic correction stems from a single Feynman diagram which describes electron self-interaction. Here, theory and experiment agree at the level of 1 in 10^8, with a tiny discrepancy between theory and experiment in the eighth digit. In such a case, the experiments are *for all practical purposes* capable of singling out the real effect of a single Feynman diagram (or virtual field quantum). The case of the Lamb shift is similar. Here the next order perturbation theory gives a correction based on two Feynman diagrams, namely for vacuum polarization and electron self-interaction. The correction shows that only 97% of the observed Lamb shift can be explained without the vacuum polarization term. A textbook on experimental particle physics tells us therefore that the missing 3% are "a clear demonstration of the actual existence of the vacuum polarization term". Any philosopher should counter that this is *not really* the case. The virtual field quanta involved in this term cannot be *exactly* singled out.

Hence, the above conclusions remain. Virtual particles are formal tools of the perturbation expansion of quantum field theory. They do not exist on their own. Nevertheless they are not fictitious but rather produce collective effects which can be calculated and measured with high precision. (pp. 237-238)

In this way even if Falkenburg recognizes that the virtual quanta can have operational meaning, due to the superposition argument she maintains the view that virtual quanta are formal tools. My point regarding this view is that the superposition argument does not hold in quantum electrodynamics; we do not have an infinite expansion of the S-matrix, what we have are applications of the theory resting on an approximate scheme of description of the interaction between two fields that cannot be taken beyond a few order calculations (see chapter 5). We do not 'stop the perturbation progression for practical reasons'; we only really have a few lower order terms to count on.

Returning to the operational meaning of the virtual quanta it is important to notice that "[i]n the low energy domain, it is sometimes even possible to single out the contribution of one single Feynman diagram to the perturbation expansion" (Falkenburg 2007, 237). Knowing that we can only count on a finite number of Feynman diagrams (and its corresponding virtual quanta), in some cases it is possible experimentally to single out the contribution of a few or even just one Feynman diagram. That is, it is not that "the experiments are *for all practical purposes* capable of singling out the real effect of a single Feynman diagram" (Falkenburg 2007, 237–238), on the contrary, the experiments are in some cases even capable of singling out the 'real' effect of a single Feynman diagram, i.e. there are experiments in which we can give operational meaning to a virtual quantum exchange (more generally we can give operational meaning to all finite superpositions of Feynman diagrams and corresponding virtual quanta). The operational relevance of virtual quanta does not by itself imply that they can be given a realistic interpretation. In particular, as we will see, a simplistic view of virtual quanta

as some sort of quantum entities – the bearers of the quantum interaction – existing in space-time is not feasible.

According to David Kaiser, referring to the S-matrix theory developed in the 1950s and 1960s in particular by Geoffrey Chew, there was an "association of 'realism' with Feynman diagrams … based on their simple similarity to 'real' photographs of 'real' particles" (Kaiser 2000, 75). This resulted from a misinterpretation of lowest-order Feynman diagrams as depictions, as a sort of Minkowski diagrams, representing a schematic reconstruction of bubble chamber photographs; according to Kaiser

> the Feynman and Feynman-like diagrams that were taken over into S-matrix theory *were* not the high-order loop corrections … but rather *lowest-order* and, most frequently, *single-particle exchange* diagrams. And what were the 'visual ingredients' of these particular classes of Feynman diagrams? Nothing but vertices and propagation lines. (Kaiser 2000, 74; see also Kaiser 2005, 362-373)

This is not the view being proposed here. Letitia Meynell called attention to the fact that in Feynman's work a 'bubble chamber view' of the Feynman diagrams is not enforced. Meynell asked the question if "Feynman diagrams prescribe imaginings of definite trajectories through and positions in space-time?" (Meynell 2008, 53). Now, Feynman presented his approach to quantum electrodynamics in two papers from 1949 that are strongly interrelated. According to Meynell, "the quintessential Feynman diagram pictured in the second paper drew on the physical interpretations and visual schemata of the first" (Meynell 2008, 53). In this first paper, Feynman illustrates the scattering of an electron with two equivalent pictures (that Meynell calls pre-Feynman diagrams). In one case Feynman gives a wave description of the electron scattering and in the other a particle description (Feynman 1949a). Thus, According to Meynell, Feynman was not trying to enforce a reading of the diagram as representing a trajectory in space-time. In fact Feynman called his approach an overall space-time approach (Feynman 1949b, 769). To see what we can make of Feynman's overall space-time description of physical processes and the role of Feynman's diagrams and virtual quanta within this approach I will now return to the analysis of the description of the electron-electron scattering in quantum electrodynamics.

The crucial aspect of the description of scattering in quantum electrodynamics is that there really is no description *in time* of the interaction. This is due to the fact that in the application of the S-matrix method we are always considering a free particle initial state (at $t = -\infty$) and a free particle final state (at $t = +\infty$) while disregarding the detailed description of the intervening times. In this sense we have an overall temporal description of the scattering processes. Feynman did not consider this as a limitation; on the contrary, his view was that "the temporal order of events during the scattering … is irrelevant" (Feynman 1949a, 749).

To see how Feynman's overall space-time approach works out let us consider a counterfactual realistic picture of 'virtual processes in space-time', involved in the calculation of the S-matrix. When considering the interaction between two electrons, the S-matrix element is constructed with an underlying idea of an elapsing time. A (virtual) photon is emitted by one electron, which means that due to the localized interaction of the Dirac and Maxwell fields it is created at a specific space-time point. This photon propagates and is luckily absorbed by an electron expecting it. We have a sort of effect 'next': the quantum 'knows' what is going to happen and behaves accordingly so that we have a smooth adjustment between the electrons and the photon. In reality the sequence of creation and absorption of the photon is adjusted '*ab initio*' in a mathematical expression – the S-matrix – that provides an overall temporal (and spatial) description of what we consider to be an *in time* temporal phenomenon. In a certain

sense the problem does not lie in the adjustment of the creation and annihilation of the photon but in the use of temporal language in an overall description of the interaction in quantum electrodynamics; like when Feynman considered a situation where it was supposed that "one electron was created in a pair with a positron destined to annihilate the other electron" (Feynman 1949b, 773).

Exploring a little more the counterfactual realistic picture of virtual 'processes' 'really' occurring in space-time, if we try to maintain an *in time* temporal perspective considering, in contradiction to the usual interpretation of quantum theories, a submicroscopic 'observer'– say Alice –, then the cat – our propagator – will reveal peculiar behaviours. The fact is that the propagator does not vanish for a space-like separation. This means that we would have an interaction between space-time points not connectable with a classical electromagnetic wave. However in this quantum world the photons and electrons (or positrons) being propagated between two points are not restricted by the usual energy-momentum relations, so we are beyond any classical dynamical description of the 'propagation', and, as mentioned previously, we refer to these quanta as 'virtual' (while using the ontologically charged word 'real' for the quanta whose energy-momentum relations are $k^2 = 0$ in the case of the photon and $p^2 = m^2$ in the case of fermions). For a submicroscopic 'observer' located in the space-time point where a quantum is emitted we can imagine that an objective notion of present (emission) and future (absorption) exists. The problem is that for a space-like separation, a moving 'observer' – Alice – might see the absorption before the emission. In the case of electron propagation this would imply seeing a positron. The cat would be changing its form. Considering Einstein's kinematical interpretation of relativity (Einstein 1905, 48; see also Smith 1995), from the perspective of a moving 'observer' – Alice – (which we imagine to make her 'observations' using a 'submicroscopic' classical electromagnetic wave, i.e. 'respecting' Einstein's relativity), in the situation described above it would seem as if there is an interchange of the creation and annihilation points. In the case of photon propagation, this only makes her think that the direction of propagation is the opposite. In the case of electron propagation it will seem as if the (unobserved) quantum is now a positron. But even Alice, taking into account relativity theory, can only see the points of interaction between the fields, not the propagation 'process' itself. In this way the 'true' virtual electron only appears to be a virtual positron due to 'kinematical' relativity, but it is 'really' a virtual electron.

When considering the *overall* amplitude the problem fades away. The point is that the S-matrix is covariant. So, different 'observers' will obtain the same result for the scattering amplitude, with their identical submicroscopic experimental devices, when considering the propagation between all space-time points (a 'real' observer cannot make these space-time experiments to determine the scattering amplitude, she can only obtain experimental cross-sections). We can express the covariant S-matrix in two alternative forms (Sakurai 1967, 204):

$$S_a^{(2)} = (-i)^2 \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{t_1} dt_2 H_I(t_1) H_I(t_2) \text{, and } S_b^{(2)} = (-i)^2 \int_{-\infty}^{\infty} dt_1 \int_{t_1}^{\infty} dt_2 H_I(t_2) H_I(t_1) .$$

To see the content of these formulas let us consider localized 'observers' of 'processes in space-time' that can be described by S_a. In this case we are considering 'processes' where $t_2 < t_1$. Now, a passer-by might think, in relation to a spacelike propagation, that she is seeing a 'process' where $t_1 < t_2$ as described in S_b. But she will also think that another 'process', which for the localized 'observer' is from S_b, is described in S_a. The

overall result will be the same for both 'observers'. The possible time inversion problem does not occurs as it is swept under the covariance of the S-matrix:

$$S^{(2)} = (-i/2)^2 \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \{H_I(t_1)H_I(t_2)\theta(t_1 - t_2) + H_I(t_2)H_I(t_1)\theta(t_2 - t_1)\},$$

where $\theta(t) = 1$ if $t > 0$, and $\theta(t) = 0$ if $t < 0$ (Sakurai 1967, 204).

Going back to real observers, the fact is that we do not have a submicroscopic experimental access to the theoretical point-like interaction between the fields (this is one of the reasons I call a description of the quanta exchange in terms of space-time processes counterfactual; the other is that we are calculating probability amplitudes and describing them in terms of classical-like processes in space-time not taking into account the interpretation of the formalism). In the case of scattering processes we *only* have experimental access to cross-sections calculated from the S-matrix (Jauch and Rohrlich 1976, 163–167). The point is that with the (experimentally accessible) cross-section calculated from the S-matrix – the only possible theoretical approach to scattering processes within quantum electrodynamics – we are not considering time as it goes by, but an overall temporal (and spatial) calculation of the interaction processes: all of the past and future is put into it. We see then that the Feynman diagrams must be seen as a representation of an *overall* space-time description of scattering processes (as an exchange of quanta) in which "the scattering process itself is a *black box*" (Falkenburg 2007, 234). We do not have an in space and *in* (*through)* time description of the interactions. In this way a realistic interpretation of virtual quanta as the bearers of the quantum interactions in space-time seems to be inappropriate.

For some it might yet seem that mine is a straw-man position. The fact that I am using Dyson's result against the superposition argument might seem not enough according to some views on this argument. It is correct that we cannot consider any more that the virtual quanta "type and number are not sharp" (Weingard 1988, 46). However it might be the case that there are versions of the superposition argument where the fact that we may still consider several Feynman diagrams in the description of the interactions is enough to relegate the diagrams and virtual quanta to the role of accessory tools not giving in any sense a physical description of the interactions. I think that Teller's argumentation can be seen as an example of this 'finite' superposition argument. The part of Teller's argumentation not depending explicitly on *classical analogies* is sustained on the following points:

1) As we have already seen, in the description of the electron-electron interaction, when considering one Feynman diagram (in second order) we

> have x_1 and x_2 as free variables, which must be integrated before we get the diagram's final contribution to the scattering amplitude. The processes allegedly described by the diagram [(which I referred to as 'processes')] must be superimposed for all values of x_1 and x_2 before we get a description of what is still only a contribution of a quantum-mechanical amplitude for a real scattering process. (Teller 1995, 142)

Now, the point is that, as I mentioned, we have only one global process described by this one Feynman diagram, corresponding to the black box calculation of localized 'processes', which are mathematical artifacts resulting from the point-like description of the interaction between the quantum fields (which has no operational meaning). This does not entail that the exchange of quanta cannot be regarded (in some way) as a physical process, simply that it is not a physical process in the classical sense of space-time processes that we have in classical theories. Teller recognizes this much, since he mentions that, in his view, "in quantum theories the components represent potentially

but not actually existing states" (Teller 1995, 141). I will not discuss Teller's interpretation of quantum field theories, but simply recall that we are not dealing with 'classical pictures' of physical processes occurring in space and *in* time. Reversing the order of arguments, we can take the intricate description of one Feynman diagram (representing, in the case being considered, the exchange of one virtual quantum) as the physical description of interactions in quantum electrodynamics, giving at the same time the only available physical-mathematical meaning to what we understand by the term 'exchange of quanta'. We cannot have implicit in our argumentation classical analogies when interpreting the physical-mathematical description of interactions in quantum electrodynamics (in this part Teller's point is dependent on a supposed superposition of different 'processes' occurring in different points of space-time).

2) Even if we cannot count on an infinite series expansion of the S-matrix we still have a superposition of several terms (related to different Feynman diagrams). According to Teller, "the full scattering amplitude, is, in principle, given only when the results from second order are further superimposed with contributions from all even higher orders" (Teller 1995, 142). Now, we do not have a *full* scattering amplitude that is, in principle, given by further superimposing *all* higher order terms. However it is in general necessary to consider higher order contributions to the S-matrix to get a good agreement with experimental results (Falkenburg 2007, 237-238). Again, my view is that we must not fall into the trap of classical analogies when addressing a quantum electrodynamical description of the interaction of radiation and matter (described within the theory as quantum fields). The fact that we can (and sometimes have to) describe the scattering by considering simultaneously several Feynman diagrams (corresponding each to a particular type of exchange, where the quanta type and number *are* sharp) does not imply that we must see them as simply abstract mathematical tools. My view is that we can see the virtual quanta as an explanatory nexus – through an extension of the concept of quanta – of the quantized exchange of energy and momentum between real particles; this is so even if it turns out to be an *intricate one* (i.e. resulting from the contribution of different Feynman diagrams), in which there is no place for an account relying on classical-like analogies, i.e. it is not like we have two tennis players playing with several sets of balls at the same time, as Fox refers to (Fox 2008, 42). It is important to have in mind that for example in the electron-electron scattering the interaction between the particles is *mediated* by the quantized electromagnetic field, and that the core interaction described in quantum electrodynamics is not (contrary to Feynman's views) a scattering process but the interaction between radiation and matter. This interaction occurs according to conservation principles and as a quantized exchange of energy and momentum between radiation and matter. When transposed to the perturbative description of scattering processes (the only one available in quantum electrodynamics) the mediation role (guaranteeing the conservation of energy and momentum) is taken by virtual quanta of the quantized electromagnetic field, which, as has been seen have operational meaning as a finite collective effect.

The point I am making about virtual quanta as mediators of the quantized exchange of energy and momentum in the scattering of 'real' particles has some similarities with Harré's views. According to Harré the Feynman diagrams have 'epistemic power'. This is in part due to the fact that the concept of virtual quanta "is legitimated via its explanatory power in the tidy accounting of energy budgets" (Harré 1988, 69) in the interactions.

In resume: I have defended that the main argument for taking virtual quanta as formal tools – the superposition argument cannot be sustained in quantum electrodynamics. In this way by a reconsideration/reformulation of Falkenburg's

argument 'against' virtual quanta, I have defended that we can in some experiments single out the lowest-order Feynman diagram and give operational meaning to the virtual quantum exchange. It is true that we usually need to consider further terms of the S-matrix series expansion as *corrections* to this (in Feynman's words) 'fundamental interaction', but since the series expansion of the S-matrix is at best asymptotic we know that this is a finite correction of the main term describing the interaction. For example in the electron-electron scattering simultaneously with the photon exchange we can consider a finite number of higher order processes involving other virtual quanta, and the finite collective effect of the superpositions of the virtual quanta exchanges has operational meaning. Besides this operational dimension, the concept of virtual quanta has an epistemic dimension. As mentioned, in the description of scattering processes it is the virtual quanta that implement the quantized exchange of energy and momentum. Harré attributes epistemological relevance to this fact since the virtual quanta enable to explain/characterize for example the electron-electron scattering through a conserved exchange of energy and momentum between the two particles. In this way at an 'epistemic level' we can consider the virtual quanta to be more than simply mathematical tools since they convey a relevant physical description/explanation of the quantum interaction in terms of providing the link for a quantized exchange of energy and momentum between the real particles. The epistemic dimension by itself does not entail an ontological reading of the virtual quanta concept, but taken toghether with the operational dimension they are strong evidence for taking the virtual quanta to be more than formal tools (implying that the Feynman diagrams are more than simply mnemonic aids to calculations).

4 A quantum model of the delayed interaction between two bound electrons

To try to recover a temporal description of processes we have to build a model of interaction that approaches somewhat the ones provided by classical electrodynamics. Let us consider two well-separated hydrogen atoms (see e.g. Fierz, 1950). Considering the interaction between the bound electrons, we do not have to consider all space-time. The photon is emitted in a certain region, where we can consider one of the atoms to be located, and is absorbed in another region by the other atom (i.e. the electron bound in a static external field). For clearly separated atoms we can get a notion of temporality from the sole propagation of a photon from one atom to the other. But with this kind of model we disregard the two-way character of the interaction, and approach the more classical description of radiation emission.

Suppose that the emission from one atom takes place at a certain region V_y of space-time, meaning that the atom is in a certain location of space and that a photon with energy ω_0 is emitted during a period of time T. This photon is absorbed in the region V_x by another atom. We are going to take for granted for the moment that if the emission takes a time T then there will be an uncertainty $\Delta\omega$ in the energy ω_0 of the photon, so that we have $T\Delta\omega > 1$. At the same time we will consider only a situation where $\Delta\omega$ is much smaller that ω_0, which means that the sign of the energy is defined, and so it is clear that the energy is flowing out of the atom in V_y. We thus suppose we can adjust T so that $\Delta\omega \ll \omega_0$. From all this we have that $\omega_0 T \gg 1$. With this condition, considering "the part of S-matrix which is due to transitions in V_x and V_y" (Pauli, 1973, p. 134) and using explicitly the form of the wave functions of the bound electrons, every instant of time in the space-time region V_x is greater than every instant of time in V_y. In this particular model we can from the S-matrix obtain a description of emission and

absorption of a photon consistent with a notion of temporal order associated with the process, but this temporal order is imposed independently of the S-matrix calculation. What the calculation provides are definitions of the time relations involved and the spatial separation of the two regions that were from the start considered bound and separated in space-time. The result is that the two bounded regions do not overlap, so that we can say that "if the energy of the charged particles in V_x increases … and if the energy in V_y decreases, then V_x is later in time than V_y" (Pauli, 1973, p. 133). Also, the second region must be on the (diffuse) light cone of the first. For this reason, besides an uncertainty $\pm T$ resulting from "the uncertainty in the time of the emission process" (Thirring, 1958, p. 146), we only have contributions in the S-matrix from space-time points in regions that can be connect by photons propagating at light speed. This also means that for the distance r between the two atoms we have $r\omega_0 \gg 1$: the second atom must be in the wave zone of the first (roughly speaking a region where r is much bigger than the wavelength of the emitted photon: $r \gg \lambda$).

Maybe the most interesting aspect of this model is that in the wave zone we see that the contribution from the propagator comes from the poles, corresponding to a process with a real photon (Thirring, 1958, p. 146). As Feynman remarked "in a sense every real photon is actually virtual if one looks over sufficiently long times scales. It is always absorbed somewhere in the universe. What characterizes a real photon is that $k \to 0$" (Feynman, 1962, p. 95). *We see that the distinction between virtual and real can depend on the separation between the atoms: in the near zone ($r \ll \lambda$) the photons are virtual and on the wave zone they are real* (Thirring, 1958, p. 146).

One point is clear from the previous case. To approach an idea of 'temporality' (i.e. temporal order in the physical processes) in models of interaction, using as a fundamental part quantum electrodynamics, we need structures in the models – like the atoms in our case – that permit the appearance of real photons, which approach a more classical electrodynamical type of interaction (emission and posterior absorption of light). Also for a consistent outcome from this model it is necessary that $\omega_0 T \gg 1$ and this is not provided by the theory directly, because there is no time-energy uncertainty relation in quantum theories in the same sense as in non-relativistic quantum mechanics where there is an uncertainty relation between the position and momentum operators (Hilgevoord, 1996, p. 1451). We have somehow to impose it from the outside.

In the Maxwell-Lorentz classical theory we have a relation between $\Delta\omega$ – the line width – and the lifetime T of the radiation emission process. Considering "a linear harmonic oscillator as a simple model for a light source" (Heitler, 1954, p. 32), and taking into account the effect of the field produced by the charge on the charge itself (the self-force), the (emission) intensity distribution is given by

$$I(\nu) = I_0 \frac{\gamma}{2\pi} \frac{1}{(\nu - \nu_0)^2 + \gamma^2/4}$$ (Heitler, 1954, p. 33),

where ν_0 is the frequency of the undamped oscillator, and γ is the width at half of the maximum intensity and is equal to the reciprocal of the lifetime of the oscillator (due to the damping of the self-force the oscillator radiates during a period of time until it comes to rest). Under the assumption that the reaction force is small we have that the lifetime is long when compared with the period of the oscillator, so that we have $\gamma \ll \nu_0$, that is, $\omega_0 T \gg 1$. Following the same approach when describing the decay of an excited state of an atom in quantum theory, again it is assumed that "the lifetime is large compared with the frequency of the atom" (Heitler, 1954, p. 183), that is $\omega_0 T \gg 1$, and

we obtain the same expression for the intensity distribution of the emission (now as a probability function). In this way, we do not use any 'uncertainty' relation to obtain the result $\omega_0 T \gg 1$ which is needed to obtain a model for the interaction between the atoms that appears to give a consistent spatio-temporal description of the interaction. Thus, the model is dependent on results that can be also derived in a classical treatment of the emission of radiation by an atom.

There is a huge difference between the quantum treatment of a two-atom system and the quantum electrodynamical description of scattering processes. In the model we obtain the desired result by patching together different parts while the S-matrix calculation of scattering amplitudes is a direct application developed from the Lagrangian of interacting Dirac and Maxwell fields.

By a heuristic procedure, taking into account the relation $\omega_0 T \gg 1$ and the corresponding emission line, a specific form is given to the bilinear density $\overline{\psi}\gamma^{\mu}\psi$ in the second order term of the S-matrix used in this model. In this way the – classically derivable – spectral line curve is a fundamental aspect of this model (Fierz, 1950, pp. 734-735; Pauli, 1973, pp. 134-135). This means that this model could be seen as a semi-classical one. Then an adjustment is made of the distance between the atoms so that the second atom lies in the wave zone of the first. The point is that, as mentioned before, in the near zone the photon behaves as a virtual one, while in the wave zone we have (as a limit) the energy-momentum relation for a 'real' photon. This means that in the last leg of the model development, depending on how we choose the distance between the atoms, we can have a situation where we can associate a causal temporal order to the emission and absorption process of a 'real' photon, or a situation where it is not possible to associate a causal temporal order to the emission and absorption of a 'virtual' photon. Another difference between this model and the S-matrix calculations of scattering processes is that in the second case we obtain results that can be compared to experiments (Falkenburg, 2007, pp. 105-107) while in the first case we can only associate with the model a thought experiment (Buchholz & Yngvason, 1994, p. 613). In this way the model patched from the theory gives the impression of a solid verifiable consequence which it really is not. This does not seem to be a solid procedure we can use to defend that we can retain within a quantum treatment the possibility of a temporal description of processes that we have in classical electrodynamics.

5 Conclusions

It is clear that we only have access to a temporal description of interactions using the S-matrix when developing models that approach more classical situations. The problem is that in a full quantum electrodynamical S-matrix calculation we really do not have a representation of scattering processes in space-time (we face this same situation for bound-state problems, which can be treated by using basically the same S-matrix approach). We have an overall space-time description, and from this, the incorrect idea that we have a description of processes in time. What we really have is a mathematical construction using as a basic structure the Minkowski space-time that enables us to obtain the cross-section for a particular scattering. But this theoretical cross-section is determined from the contribution of the Feynman diagrams in energy-momentum space, and ultimately it is this energy-momentum cross-section that is compared with experimental results (Falkenburg, 2007, p. 131).

We do have (in a limited sense) a description of the interaction in terms of virtual quanta exchange between our observed 'particles'. What we do not have is a description

of this exchange in space and through time. We have a quantum electrodynamical application based on a computational device – the propagator – and a calculation based on a configurational space constituted by the Minkowski space-time points. In the case of scattering experiments we have no 'insider' making observations, we have the initial state corresponding to a determined preparation of the system and the final calculated state that will enable us to make comparisons with the experimental results (Peres, 1984, p. 647). To have a path in space-time we cannot consider the elemental interactions, because we cannot observe the configurational space where the interaction 'occurs' through the mathematical device of the propagator. Let us recall Heisenberg's description of an α-particle in a Wilson cloud chamber. Heisenberg considers that each successive ionisation of molecules of the medium is "accompanied by an observation of the position" (Heisenberg, 1930, p. 69). This sequence of observations reveals a 'path' in space. However, in between each ionisation, the particle is described by a wave function. There is no quantum mechanically described microscopic trajectory. Each observation corresponds to a state preparation for the next one. It is the sequence of observations controlled by us that gives the impression of a trajectory in space-time. In the case of Møller scattering we do not have that. It is a unique and global process associated with a single experiment. It is not possible to visualize this process as something that is going on as we speak. Minkowski space-time has to be seen, when used in the context of S-matrix calculations, as a configurational space, where mathematical objects like the propagators are used as calculation tools. If we consider the scattering process as a 'black box' (Falkenburg, 2007, p. 234), it is the space-time itself that is this black box. When considering an overall space-time approach we take the observer to be outside this space-time, and there is not much we can say about the temporal order of the phenomena as described by the theory.

CHAPTER 8

THE RELATION BETWEEN CLASSICAL AND QUANTUM ELECTRODYNAMICS

1. Introduction

In the wonder world of physics it is often thought that the relation between the classical and quantum theory is unproblematic and that by a more or less clear procedure we can regard the classical theory as some sort of limit of the quantum theory. Usually these considerations are done in the realm of non-relativistic quantum theory and not much is said about the relation between quantum electrodynamics and classical electrodynamics. Be it the relativistic or non-relativistic theory, we are in the paradoxical situation, which is usually presented as non-paradoxical and natural, that the quantum theory is supposed to contain the classical theory but at the same time needs it for its own foundation (Landau, 1974, p. 13).

In the following I will try to present the idea that classical electrodynamics and quantum electrodynamics form a not fully coherent theoretical framework in which the quantum part has to be seen as an extension of the classical part but not as containing the classical theory. In this way quantum electrodynamics cannot be regarded as an independent and more fundamental theory of physics than its classical counterpart.[40]

First, section 2 will present the current classical framework provided by classical electrodynamics and the theory of relativity,[41] and address the question of the possible inconsistency of classical electrodynamics and the possible meaning of this. Then, in section 3, after looking again briefly into the development of quantum electrodynamics from the quantization of the classical Maxwell field and the classical Dirac field, I will address the possibility of a classical limit. Taking into account the limitation of quantum electrodynamics in the temporal description of scattering processes I will defend that properly speaking we cannot reduce classical electrodynamics to quantum electrodynamics.

[40] In this work, I am not taking into account different interpretations of quantum theory and different approaches to the quantum theory of measurement (in particular decoherence). I am solely developing my argument within an ensemble interpretation (e.g. Isham 1995, pp. 80-81) that gives a natural connection between the calculations done using quantum electrodynamics and the results from the experimental procedures followed (e.g. Falkenburg 2007, pp. 106 and 207).

[41] I am here taking the theory of relativity to be part of classical physics. This is the view usually adopted, in which, for example, Einstein's theory of gravitation is taken to be a classical field theory (e.g. Landau and Lifshitz 1971).

2 Classical electrodynamics

Classical electromagnetism as presented nowadays is not the theory as developed by J. C. Maxwell. In his more mature work, published in 1873, Maxwell used the Lagrangian formalism to avoid any specific mechanical model of the medium that causes the electric and magnetic phenomena (Harman, 1982, p. 118). His approach was centered on the description of this medium – the ether. The electric current was described as a variation of the polarization – seen as a more fundamental concept – in a material medium (dielectric or conductor); and in this line, the electric charge was considered 'simply' as a spatial discontinuity in the polarization (Darrigol, 2003, p. 164). In practice Maxwell considered the ether and matter as a single medium existing in absolute space (Harman, 1982, p. 120), more exactly, he treated matter "as if it were merely a modification of the ether" (Whittaker, 1910, p. 288). This was a macroscopic theory of the electromagnetic medium that did not make a clear-cut distinction between matter and ether.

In 1892, what can be considered as a new microscopical classical version of electrodynamics was developed by H. A. Lorentz. Adopting the view of microscopical charged particles used in action-at-a-distance theories, Lorentz combined it with the Maxwell theory of the ether in a way that enabled him to explain Fresnel's results regarding the propagation of light in moving bodies. The positive and negative charged material particles would move in the ether without dragging it and only interacting with each other through the mediation of the ether that filled all space: they had a delayed interaction (Whittaker, 1910, p. 420).

Lorentz presented the fundamental equations of his theory as a generalization of the results provided by electromagnetic experiments (Lorentz, 1909, p. 14). This means that he made an extension of Maxwell's macroscopic field equations to a microscopic level taking into account his consideration of the charge as a density distribution attached to a microscopic solid body. With this microscopic and atomistic turn, the field equations are in Lorentz electrodynamics given by:

$$\operatorname{div} \mathbf{d} = \rho, \qquad \operatorname{div} \mathbf{h} = 0,$$

$$\operatorname{rot} \mathbf{h} = 1/c\,(\dot{\mathbf{d}} + \rho\mathbf{v}), \qquad \text{and } \operatorname{rot} \mathbf{d} = -1/c\,\dot{\mathbf{h}},$$

where **d** is the dielectric displacement, **h** is the magnetic force, ρ is the charge density, and **v** is the absolute velocity of the microscopic body (Lorentz, 1909, p. 12).

Lorentz considered that the ether pervades all space including the 'interior' of the solid bodies, but as being always at rest in relation to absolute space. The law that dictates the influence of the electromagnetic fields, as a manifestation of the internal state of the ether, on the charged bodies, can be seen, as in the previous cases, as an extension of the experimental results represented in the force laws of Coulomb and Biot-Savart, and is given by $\mathbf{f} = \mathbf{d} + 1/c\,[\mathbf{v} \times \mathbf{h}]$. These five equations with their underlying assumptions can be considered the core of Lorentz's electrodynamics (McCormmach, 1970).

With Lorentz's electrodynamics the conceptual distinction between matter and ether is clearer than in the Maxwell theory. We have a more precise physical characterization of matter, ether, and their interaction, and the scope of application of the theory is extended. In this way we can consider Lorentz's electrodynamics as more fundamental than Maxwell's. But it appears to have a weak spot, which is maintained even after considering A. Einstein's contribution to classical electrodynamics bringing with it the

downfall of the concepts of ether and absolute space and the rethinking of electrodynamics within the more general theory of relativity.

When in his first works on the subject Lorentz considered the existence of charged corpuscles, he associated them with the ions of electrolysis. P. Zeeman's experimental results that the charge to mass ratio of the particles was one thousand times smaller than supposed indicated that these particles were not the ions of electrolysis. This conceptual distinction led Lorentz to consider the existence of sub-atomic corpuscles (with positive or negative charge), adopting as others the term 'electrons' (Arabatzis, 1996, pp. 421-424). Lorentz considered the electron as a charged rigid body, giving to it a "certain degree of substantiality" (Lorentz, 1909, p. 14), to which the laws of motion apply. He modelled the electron as a sphere with a uniformly distributed surface charge. He considered the electron when in motion in relation to the ether (at rest in absolute space) to take the form of an elongated ellipsoid. Considering a very small departure from uniform motion and applying expressions obtained in that case, Lorentz determined "the force on the electron due to its own electromagnetic field" (Lorentz, 1909, p. 38). He found that this effect corresponded to the existence of a mass of electromagnetic origin and was led to the idea of an effective mass composed of the mechanical mass and the electromagnetic mass. Due to Kaufmann's experiments, and considering the mechanical mass not from the point of view of the not yet developed theory of relativity but from Newtonian mechanics, Lorentz even considered the possibility that the electron's mass was all of electromagnetic origin. Lorentz's work was critically examined by H. Poincaré who concluded that a non-electromagnetic internal pression was needed, so that the electron was stable under the electrostatic repulsion between its elements of charge (Poincaré, 1905).

From the point of view of the theory of relativity it is clear that the mass of the electron cannot be solely of electromagnetic origin. The electron's momentum and energy generated by its own field do not form a four-vector. In relativistic mechanics we can consider a particle to be defined by having a determined energy-momentum four-vector (Jammer, 1961, p.164). This definition can be justified without taking into consideration any aspect of electrodynamics, as G. N. Lewis and R. C. Tolman have done: we can determine the relativistic expression for the particle's mass by considering the collision between the particles and postulating a conservation law of momentum and using the relativistic law of addition of velocities (Pauli, 1958, p. 118). From this it can immediately be seen that the momentum and the energy of the particle behave under Lorentz transformation as the components of a four-vector. This result can be checked experimentally again without any explicit use of electrodynamics, as was done in the early thirties by F. C. Champion, who studied the scattering of β-particles with electrons at rest in a Wilson chamber (Zhang, 1997, p. 234). This means that the experimental and conceptual framework of relativistic mechanics can be developed and verified on its own, detached from any electrodynamical considerations. This point is crucial in the analysis of the difficulties that relate to classical models of the electron.

When considering a point-like model of the electron, the self-energy is infinite. In 1938, P. Dirac proposed a clear covariant procedure to separate the finite and infinite contributions to the self-energy (Dirac, 1938). The infinite contribution to the electron's mass is taken care of by a renormalization procedure in which the observed mass encloses the mechanical mass and the (infinite) electromagnetic mass. The finite effect is a reaction force depending on the derivative of the acceleration. So, when considering the electron's self-energy we have a departure from the Lorentz force equation and obtain an equation – the Lorentz-Dirac equation – in which besides the external force we have present the radiation reaction from the electron's field. This equation has very

unphysical solutions. In the absence of any external force the equation admits solutions where the radiation reaction provides a self-acceleration to the charged particle. Choosing appropriate asymptotic conditions this type of solution is avoidable. Nevertheless a problem still remains. When considering the case of a particle subject to an external force, the motion of the particle is affected by the force even "before the action of the force" (Barut, 1964, p. 198): we have a pre-acceleration of the electron before the action of the external force. It seems that the point-like electron is not a classically acceptable model. The pre-acceleration solution, where we have a non-zero acceleration before the external force is applied, appears to be avoidable with a classical extended electron model.

Let us consider a classical extended electron model consisting in "a charge *e* uniformly distributed on the surface of an insulator which remains spherical with constant radius *a* in its proper inertial frame of reference" (Yaghjian, 1992, p. 31). Taking into account the finite velocity of propagation of an electromagnetic disturbance across the 'electron', in the derivation of the solution to the equation of motion of this 'electron', no pre-acceleration solutions occur.

This result has been challenged, and it might be the case that even this model does not resolve the problem of pre-acceleration (Frisch, 2005, p. 62). In this way there seems to be no conceptually unproblematic way to overcome the inconsistency we have in the actual applications of classical electrodynamics where, when considering a particle-field system, the Lorentz laws are applied taking into account energy-momentum conservation while ignoring the self-field of the particle. According to M. Frisch

> the standard way of modeling phenomena involving the interaction between discrete charged particles and electromagnetic fields relies on inconsistent assumptions ... the equation of motion for discrete charges that is used in all applications of classical electrodynamics, which ignores the self-fields of the charge, is inconsistent with the Maxwell equations and the standard principle of energy momentum conservation. (Frisch, 2007, p. 2)

Also, in Frisch's view

> there are a host of conceptual problems that arise when one tries to develop a fully coherent and complete classical theory of charged particles interacting with electromagnetic fields–a theory that does not simply ignore self-interaction effects. (Frisch, 2007, pp. 3-4)

In this way the conceptual problems would be forcing upon us an inconsistent approach.

I think that rather than some sort of inconsistency we are here facing interesting and revealing aspects of classical electrodynamics. I think one thing that we can conclude from the analysis that led to the inconsistency claim by M. Frisch, is that we have a limited description of matter within classical theory. As has been noted regarding classical electrodynamics,

> the main problem with taking this theory to be the fundamental theory of the interaction of classical charges and fields is that it is in an important sense incomplete. Without substantive additional assumptions concerning how charged particles are to be modelled, the theory cannot be understood as describing the behaviour of the particle-field system. (Frisch, 2005, p. 47)

Basically we only have general rules from relativistic mechanics that give an overall prescription about what general laws matter must 'obey'; like the definition of the concept of particle by considering that it must have a certain energy-momentum four-vector, which is independent of any particular model of the particle and the possible

inconsistency of any derived force law (as I mentioned earlier, the experimental and conceptual framework of relativistic mechanics can be developed and verified on its own, detached from any electrodynamic considerations). We really do not have any elaborated theory of matter. From this I would say that the classical theory is incomplete, in the sense that part of its conceptual framework – the one related with the description of matter – shows severe limitations. But, contrary to the view expressed by Frisch (2007), I find it difficult to regard (in some sense) a theory that we have strong reasons to consider incomplete as being inconsistent.

Another aspect, related to the previous, is that the theory was designed by considering two clearly distinct entities: the field and the particles, and in the usual applications of the theory "electric charges are treated *either* as being affected by fields *or* as sources of fields, but not both" (Frisch, 2004, p. 529). In trying to overcome this approximate approach, the development of the theory faces clear difficulties that within the classical realm seem to have no easy solution (Frisch, 2007, p. 11). In this way, recalling the case of quantum electrodynamics, it seems that we might be facing the intrinsically approximate character of the description of the interaction of radiation and matter also at the classical level, which seems inevitable in the present approach developed by considering radiation and matter as two clearly distinct phenomena. If it turns out to be so, we are really facing something else than 'simply' a problem of incompleteness of the classical theory.[42]

3 The relation between classical and quantum electrodynamics

In this part I will defend the idea that quantum electrodynamics cannot be seen as a more fundamental theory than its classical counterpart, in the sense that we could recover the classical theory from some sort of limit of the quantum theory. Instead I will propose to see the quantization procedure as a literal 'upgrading' procedure in which we build the quantum part from the classical one in such a way that the quantum part is dependent of the underlying classical structure.

I will start, in the first subsection, by considering the quantization procedure. I will then consider briefly the literature addressing the so-called classical limit in quantum electrodynamics. While in the case of quantum mechanics there is a vast literature about this subject, it seems that physics and philosophy have not taken the question of the relation between classical electrodynamics and quantum electrodynamics too much into account. What we find is basically the usual idea of the Planck's constant 'limit' ($h \to 0$) transposed to the case of quantum electrodynamics.

In the second subsection I present part of the argument against the previous simplified view of the relation between the two theories. As we know the application of quantum electrodynamics to the description of bound-state or scattering problems is made by resorting to perturbative approaches (in particular the S-matrix approach). The point is that in the perturbative approach we are calculating integrals that go from $t = -\infty$ to $t = +\infty$. This overall temporal description makes it impossible to associate a particular

[42] As we have seen, according to Bohr's views this is also the situation in quantum electrodynamics (Bohr 1932a, p. 378; Bohr 1932b, p. 66; see also Rueger 1992, pp. 317-318). That we might be facing similar problems in the two theories can be expected according to the view being proposed here on the relation between the two 'theories'; another example is the renormalization of the electron's mass in the two 'theories'; see e.g. Barut (1964, pp.190-191) and Schweber (1961, pp. 524-530).

time interval (duration) to the physical processes described by the theory.[43] The problem is then to see how the duration of physical processes which are found at the macroscopic level (as described by classical theories) could emerge from the quantum realm since the theory is unable to provide any indication of a temporal duration of the processes that are supposed to be occurring at the microscopic level and constituting the macroscopic level where our perception of time is taking place.

Now if we take classicality as emerging from the 'quantum world', the physical processes that at a macroscopic level we see taking place during finite time intervals should emerge from some, even if 'diffuse', assignment at the quantum level of a 'duration' to the physical processes ('constituting' the macroscopic ones). As mentioned, at the level of the usual applications of quantum electrodynamics this is not possible: we just have an overall temporal description. In subsection 3.3 I will consider whether it might be possible within quantum electrodynamics to recover a more classical type of association of a time interval to physical processes. To this purpose I will consider Fierz's (1950) take on Fermi's two-atom system (see e.g. Fermi, 1932). It turns out that the description, using in part the formalism of quantum electrodynamics, of the interaction between two bound electrons cannot be seen as a direct application (or consequence) of the theory. It is more like a piecemeal model that can be seen to include a classical input. It is exactly this classical input (or quantum input at the correspondence level where by design the quantum theory provides results equivalent to those of the classical theory) that makes it possible to associate a temporal time interval – duration – to the process of emission and subsequent absorption of a photon between two bound electrons. In this way it seems that the type of temporal description of physical processes we have at the classical level cannot be regarded as emerging from the quantum level of description.

3.1 The quantization procedure and the so-called classical limit

Within quantum electrodynamics the starting point are classical fields like the Maxwell field and the Dirac spinor field defined on a Minkowski space-time. We can see the quantization scheme as a set of physical rules that enable an extension of the applicability of the classical concepts to phenomena that while categorized as related to matter, radiation and their interaction are beyond the classical sphere of description.

As we have seen in chapter 4, considering the usual quantization procedure, in the case of a free Maxwell field the vector potential can be expanded as

$$A^{\mu}(x)=\sum_{r\mathbf{k}}\left(\hbar c^2/2V\omega_{\mathbf{k}}\right)^{1/2}\left(\varepsilon_r^{\mu}(\mathbf{k})a_r(\mathbf{k})e^{-ikx}+\varepsilon_r^{\mu}(\mathbf{k})a_r^{*}(\mathbf{k})e^{ikx}\right)$$ (Mandl & Shaw, 1984, p. 84).

In order for $A^{\mu}(x)$ to be related to the Maxwell equations, a subsidiary condition is imposed, the so-called Lorentz subsidiary condition, which, as mentioned, at a quantum level has to be changed. In this case the connections between the classical equations and concepts and their quantum upgrades are very direct. Under the quantization scheme $A^{\mu}(x)$ is now a field operator, and the Fourier expansion coefficients are now, as

[43] In quantum electrodynamics, interaction processes are described as exchange of virtual quanta, and it is impossible to associate to the exchange of virtual quanta finite time intervals in opposition to the case of real quanta where this is possible (see main text; see also chapter 7).

operators, conditioned by the commutation relations $[A^{\mu}(x), A^{\nu}(x')] = 0$, $[A'^{\mu}(x), A'^{\nu}(x')] = 0$, and $[A^{\mu}(x), A'^{\nu}(x')] = -i\hbar c^2 g^{\mu\nu}(\mathbf{x} - \mathbf{x}')$ (Mandl & Shaw, 1984, p. 86).

In the case of the Dirac equation, as we have seen in chapter 3, we can consider the equation as a classical equation of an electron-wave, that can have its properties explored in experiments like the diffraction experiment of Davisson and Germer (Tomonaga, 1962, p. 10, Vol. 2). Following Jordan, we can consider the quantization of this classical spinor field, using in this case anticommutation relations, and obtaining, by a procedure even more simple than the quantization of Maxwell field, the Dirac field operators

$$\psi(x) = \sum_{r\mathbf{p}} (mc^2/VE_{\mathbf{p}})^{1/2} \left(c_r(\mathbf{p}) u_r(\mathbf{p}) e^{-ipx/\hbar} + d_r^*(\mathbf{p}) v_r(\mathbf{p}) e^{ipx/\hbar} \right),$$

$$\overline{\psi}(x) = \sum_{r\mathbf{p}} (mc^2/VE_{\mathbf{p}})^{1/2} \left(d_r(\mathbf{p}) \overline{v}_r(\mathbf{p}) e^{-ipx/\hbar} + c_r^*(\mathbf{p}) \overline{u}_r(\mathbf{p}) e^{ipx/\hbar} \right),$$

where c_r^*, d_r^*, c_r and d_r obey the anticommutation relations $[c_r(\mathbf{p}), c_r^*(\mathbf{p})] = [d_r(\mathbf{p}), d_r^*(\mathbf{p})] = \delta_{rs}\, \delta_{\mathbf{pp}'}$, with all other anticommutation relations vanishing (Mandl & Shaw, 1984, p. 68).

As mentioned, we can see Dirac's equation as a classical-level description of matter from a wave perspective, but in agreement with the laws of relativistic mechanics. In particular, the relativistic Hamiltonian $H = c(m^2c^2 + p_1^2 + p_2^2 + p_3^2)^{1/2}$ can be seen as fundamental in the derivation of Dirac's equation (e.g. Dirac, 1958, p. 255): in his 1928 paper on the relativistic one-electron wave equation, Dirac considered that the relativistic wave equation of the electron should be linear in $p_0 = i\hbar\, \partial/(c\partial t)$ and $p_r = -i\hbar\, \partial/(c\partial x_r)$ with r = 1, 2, 3. In this way it had the form $(p_0 + \alpha_1 p_1 + \alpha_2 p_2 + \alpha_3 p_3 + \beta)\psi = 0$. The matrices α_1, α_2, α_3 and β, are determined by the relativistically invariant equation $(p_0^2 - m^2c^2 - p_1^2 - p_2^2 - p_3^2)\,\psi = 0$ defined using the relativistic Hamiltonian (Dirac, 1928).

The previous quantization scheme enables the construction of the quantum structure from the underlying classical structure. According to C. J. Isham, "the need for such a tentative approach is rather unsatisfactory, and suggests that the whole idea of 'quantizing' a given classical system is suspect even though, in practice, the procedure does generate many quantum systems of considerable importance … A more logical process would be to start from a quantum system that is given in some intrinsic way, and then to ask about its classical limit" (Isham 1995, p. 94). The problem is that "there is no clear understanding of what it means to specify a quantum system in an 'intrinsic way'" (Isham 1995, p. 94). This situation does not prevent taking the quantum theories to be broader than their classical counterparts that are supposed to be recovered from them by some sort of limiting procedure, i.e. it is usually considered that classicality emerges from the quantum realm (see e.g. Landsman 2006, p. 38).

A definition of a limiting procedure in which classical theory appears as some sort of limit of quantum theory presents mathematical and conceptual problems, which have not received an unequivocal answer (Ballentine 1998, p. 388; see also Landsman 2006). In general the idea of a classical limit is that we might define a sort of mathematical limit that corresponds to a succession of quantum mechanical theories that would take us from quantum to classical physics (Rowe 1991, p. 1111). In this way "an explicit algorithm may then be used to construct the classical phase space, define a consistent Poisson bracket, and find a classical Hamiltonian, such that the resulting classical dynamics agrees with the limiting form of the original quantum dynamics." (Yaffe

1982, p. 408) The key point is that the 'original' quantum dynamics is constructed by a quantization procedure from the classical description, as was done by Dirac using classical Hamiltonians and the Poisson brackets (see e.g. Kragh 1990, p. 19). To develop a sort of mathematical procedure to go the other way around can be seen as a consistency check, independently of the interpretation of this procedure as an emergency of classicality.[44] The point of all this is that there is an ambiguity in the interpretation of this procedure. For some it can be seen simply as a consistency check and for others as a limiting procedure. It is only after the argument being presented next (about limitations in the temporal description of physical processes) that I have an independent argument to claim that the so-called limiting procedure is just a consistency check.

To present classical electrodynamics as a limit of quantum electrodynamics is a tricky business, but with the usual long mathematical manipulations we might recover expressions that look like some expressions of classical electrodynamics from quantum electrodynamics, and with this have the impression of obtaining a classical limit of quantum electrodynamics. However in the journey through this mathematical jungle we are loosing sight of the physical interpretation of the formalism of quantum electrodynamics – we only recover some uninterpreted mathematical expressions that resemble expressions from classical electrodynamics but which have not been given a physical interpretation according to the quantum theory they belong to. We can see examples of this, for example, in the work by Stehle and DeBaryshe (1966) and Dente (1975). In the case of Dente the classical limit is supposed to emerge, in the simple case of a particle interacting with an oscillator, by considering the expression for the transition amplitude where the photon coordinates are 'eliminated'. According to Dente the expression for the transition amplitude, "is just the expression which should arise in a classical electrodynamical calculation" (Dente, 1975, p. 1737). The problem is that this is a quantum-electrodynamical expression and should be interpreted accordingly; also this result can be 'read' as a consistency check, i.e. (1) we start from classical physics, (2) we implement a quantization procedure, and (3) we present a 'mathematical' procedure to 'recover' classical-like expressions.[45]

Regarding Stehle and DeBaryshe they call attention to the fact that even the expected 'correspondence' under particular circumstances (according to the authors the high-intensity limit) between quantum-electrodynamical and classical-electrodynamical calculations faces difficulties. They consider in particular the case of the scattering of light by light that has no classical counterpart. According to Stehle and DeBaryshe, "it is not clear that even a low-frequency limit will lead to Maxwell theory" (Stehle & DeBaryshe, 1966, p. 1136). However in the case of the scattering of light by free electrons it is possible to obtain from the quantum-electrodynamical calculation a cross-section equivalent to the classical one (see also Schweber, 1961, pp. 638-640). This result does not have to be seen as a mathematical derivation of the classical limit. It can be seen as a consequence of the correspondence principle, which entails, in particular circumstances, 'identical' predictions from both theories (for details on the correspondence principle see e.g. Bokulich, 2009; Darrigol, 1997).

That the so-called 'limiting procedure' does not deliver what it promises can be seen by considering the temporal description of physical processes within quantum electrodynamics as compared to the description we have at the level of classical

[44] I thank Henrik Zinkernagel for calling my attention to this possibility. This view is also presented by Bohm (1951, p. 626).

[45] That we should be careful with this type of naïve identification of a 'classical limit' can be seen already in the case of quantum mechanics; see e.g. Ballentine, Yang, and Zibin (1994).

electrodynamics. In fact, if classical electrodynamics could be seen as a sort of 'mathematical limit' of quantum electrodynamics, the description of processes in the classical theory should also be in some way a limit of an 'underlying' quantum description of the processes. As I will show next, that is not the case.

3.2 The overall temporal description of physical processes in quantum electrodynamics

The retardation due to the finite velocity of propagation of the electromagnetic interaction should also be revealed in a quantum electrodynamical treatment by looking at the quantum description of the electromagnetic interaction between charged particles. This would guarantee that it is in principle possible to associate a finite time interval to a particular physical process described at the quantum level. The problem is that quantum electrodynamics does not provide an '*in* time' description of scattering processes (i.e. we cannot associate a finite time interval corresponding to the retardation in the interaction to a physical process like an electron-electron scattering); on the contrary the theory only provides transition probabilities which correspond to measurable relative frequencies, and, as emphasized by B. Falkenburg, "it treats the scattering itself as a black box" (Falkenburg, 2007, p. 131).[46]

The system constituted by the Dirac and Maxwell fields in interaction is described by a set of coupled non-linear equations. It is not possible to find exact solutions of these field equations and the use of perturbative calculations becomes mandatory to the point that, according to Dyson, quantum electrodynamics "is in its nature a perturbation theory starting from the non-interacting fields as an unperturbed system" (Dyson, 1952a, p. 79). To be able to use free fields in the description of scattering processes two things are necessary: (1) to consider that the initial and final states of the system are eigenstates of the Hamiltonian for the non-interacting fields (intuitively meaning that since the particles are far apart their interaction is negligible), and (2) that the interaction occurs in a short (undefined) period of time when compared to the time it takes the particles to arrive at the 'interaction region' and their posterior observation (which is taken to occur much later when the particles are not interacting anymore).

This rather vague picture of a scattering process is given a more formal structure within the theory by considering that the interaction between particles in a scattering process is adiabatically switched on from the remote past and adiabatically switched off in the remote future (Lippmann & Schwinger, 1950, p. 473; see also Bogoliubov & Shirkov, 1959, p. 197). This is achieved by considering an initial state at $t = -\infty$ corresponding to free particles and a final state at $t = +\infty$ also corresponding to free particles. This will imply that in this approach, when calculating the so-called S-matrix, we are always considering integrations between $-\infty$ and $+\infty$ in the temporal variable (the same occurs with the spatial variables), while disregarding the detailed description of the intervening times. In this sense we have an *overall* temporal description of the scattering processes, but there really is no description *in time* of the interaction (we are unable to associate a finite time interval to a physical process). From an experimental point of view, things make sense as they are because in scattering processes we only have experimental access to cross-sections. In quantum electrodynamics the scattering cross-section is calculated from the transition probability per unit space-time volume, which is related to the S-matrix in a simple way (for details see e.g. Jauch & Rohrlich, 1976, pp. 163-167). According to Falkenburg,

[46] For more details regarding the content of this section see chapters 5 and 7

the effective cross-section is the physical magnitude with which the current field theories come down to earth. As a *theoretical quantity*, the cross-section is calculated from the S-matrix of quantum mechanics … as an *empirical quantity*, it is the measured relative frequency of scattering events of a given type. (Falkenburg, 2007, p. 107)

We might think that this 'black box' description results from a particular method and is not a general feature of the theory; but the case is that, even if this formalism is particularly tailor-made for the description of scattering processes, it is also applicable to bound-state problems (see e.g. Veltman, 1994, pp. 62-67). That is, all the calculations made within quantum electrodynamics, giving an excellent agreement with experimental results, can be seen as S-matrix type perturbative calculations (see e.g. Berestetskii, Lifshitz & Pitaevskii, 1982, p. 554).

3.3 A tentative quantum electrodynamical model providing a temporal description of physical processes

Even if the theory shows severe limitations in assigning a temporal duration to physical processes, we might hope that there are still some other applications of quantum electrodynamics approaching more classical situations where this 'black box' type of description (characterized by an overall space-time approach) does not arise. At first sight, it could seem that a simple treatment of the interaction between two atoms might provide just that (Fierz, 1950): when an atom initially in an excited state decays emitting a photon, it will only be absorbed by a second atom (initially in ground state) after roughly the time r/c (where r is the distance between the atoms and c is the velocity of light). In this way, it would be possible to associate a clear (finite) time interval to the interaction process (i.e. we do not have an overall temporal description of the physical process but an *in time* description like in the classical case).

There is a huge difference between this treatment of a two-atom system and the description of scattering processes. As I have mentioned in the previous chapter, in the model we obtain the desired result by patching together different elements. It is not a purely quantum electrodynamical derivation. In the model, first we obtain a wave function associated with the electron bound in an atom by solving the Dirac equation as a relativistic one-electron equation and by using the equation in a way that is known not to have a consistent interpretation (Schweber, 1961, p. 99), and then defining field operators using the (one-electron) solutions to the equation. In this way in the field operators that are associated with the electrons we have contributions that from a quantum field theory point of view are related also to positrons (see chapter 3). These operators are used within the S-matrix formalism which from a mathematical point of view can be done and is the usual procedure followed (Jauch & Rohrlich, 1976, pp. 318-319), but which does not corresponds to a full quantum field theory calculation; properly speaking it is a semi-classical calculation due to the use of an unquantized external field.[47] In any case in the model development we only need very general characteristics of these field operators (Pauli, 1973, p. 133).

[47] Usually the term semi-classical is used when considering some heuristic approach with both classical and quantum components. One example is Møller's original derivation of an electron-electron scattering formula based on the correspondence principle (Kragh, 1992, pp. 310-312), but whose rigorous justification is only possible when deriving it from quantum electrodynamics (Jaynes, 1973, p.40). Here I am also using the term semi-classical when we seem to have a classical potential in a quantum electrodynamical equation (see footnote 14, chapter 3).

As we have seen, to arrive at the intended result the relation $\omega_0 T \gg 1$ between the time of the emission process T and the energy of the emitted photon ω_0 is fundamental. This relation can be seen as resulting from the classical theory of the natural line breadth. It can also be made plausible in a quantum theory calculation (Heitler, 1954, pp. 181-184); and it can be seen simply as following from considering Bohr's correspondence principle. Taking into account this relation and the corresponding emission line, a specific form is given to the bilinear density $\overline{\psi}\gamma^{\mu}\psi$ in the second order term of the S-matrix used in this model:

$$\text{const} \int_{V_x} d^4x \int_{V_y} d^4y (\overline{\psi}(x)\gamma^{\mu}\psi(x)) D_c(x-y) (\overline{\psi}(y)\gamma^{\mu}\psi(y)) ,$$

with $\overline{\psi}\gamma^{\mu}\psi \sim a_1 a_2^{*} \rho_{\mu}(x) \exp [i\omega_0 t - t^2/T^2]$, where $\omega_0 > 0$.[48]

We have then in the 'core' expression of the model a term derived in the correspondence limit, i.e. a term that can be derived either by classical electrodynamics or quantum mechanics.

In simple terms what I mean by 'correspondence limit' is the asymptotic agreement between the predictions of quantum and classical mechanics. According to Bohr the correspondence principle can be seen as a law of quantum theory (see e.g. Bokulich, 2009). His view is that "the correspondence principle expresses the tendency to utilise in the systematic development of the quantum theory every feature of the classical theories in a rational transcription appropriate to the fundamental contrast between the [quantum] postulates and the classical theories" (quoted in Bokulich, 2009, p. 18). In Heisenberg's and Bohr's view matrix mechanics embodies the correspondence ideas by a 'symbolic' translation of the Fourier components of the motion to *corresponding* quantum amplitudes. According to Darrigol in this last formulation of the 'correspondence principle' as part of quantum theory we have a 'symbolic translation' of classical concepts (i.e. we obtain the corresponding quantum concepts by the quantization procedure) and maintain the (statistical) asymptotic agreement between the quantum and the classical theories (Darrigol, 1997). It is important to notice that this asymptotic agreement (correspondence limit) is built into the theory and it is not related to any eventual 'mathematical limiting procedure' that recovers the classical theory from the quantum theory.

The implication of all this is that the model must be seen as a semi-classical one. Thus when using this model we are then at the 'interface' of contact between the classical and quantum theories. We are not 'diving' into the quantum world, which is supposed to be underlying the classical mode of description. What I am interested in is the (*in* time) temporal description (if any) of physical processes in this 'quantum world', i.e. the description given in a full quantum electrodynamical calculation. Before returning to this point let us return to the model under consideration.

The final ingredient in the development of the model is an adjustment by hand of the distance between the atoms so that the second atom lies in the wave zone of the first. In this way we can take the photon to be real, and we find that it is possible to associate a causal temporal order to the emission and absorption process of the 'real' photon. In

[48] We see that a Gaussian function is being used. The expected function according to classical theory (or its quantum counterpart) is a Lorentzian function. The Gaussian can be obtained when considering the broadening due to the Doppler effect occurring in a 'gas' of atoms at temperature T (Major, 1998, pp. 142-149). That is, the expression being used is not valid in the case of one single atomic system, which is the case being considered in this model.

summary, we are using a model that describes a thought-experiment; it makes reference to general aspects of the electron's wave function that result from using Dirac's equation not as a classical wave equation (from which a quantum field is derived by a quantization procedure), but as a semi-classical one-electron equation (Schweber, 1961, p. 100). Ultimately the main input that determines the form of the bilinear density is not provided by the Dirac equation computation but by a heuristic use of what can be seen as a classical result for the radiation emission of a bound electron and an adjustment by hand of the distance between the atoms to make it possible to obtain the desired temporal behaviour. This cannot be seen as an application of the quantum electrodynamical formalism. More properly it is a heuristic semi-classical model, which, as mentioned, works at the correspondence level of description (since part of its elements are described by classical physics).

I think that to arrive at any conclusive results, we have always to stick to the physical interpretation of quantum theory and consider clear applications of quantum electrodynamics related with feasible experiments. Here we have seen that the theory only provides 'black box' descriptions of physical processes, corresponding to an overall space-time approach. In this way from what has been presented *one cannot consider that from the quantum level of description it is possible to recover the temporal description of processes that we have at a classical level*.

4 Conclusions

Considering the results presented here, there seems to be no smooth and physically unproblematic way to connect quantum electrodynamics with classical electrodynamics. Thus the status of quantum electrodynamics has to be reconsidered. Quantum electrodynamics cannot be seen as an independent theory that "contains [classical] electrodynamics as a special case" (Stehle & DeBaryshe, 1966, p. 1135). It seems more adequate to regard quantum electrodynamics as a physical-mathematical upgrade of classical theory (electrodynamics and the theory of relativity), which permits an extension of the domain of application of the classical theory in the description of natural phenomena, but which does not constitute a reduction of the classical theory. This conception of quantum electrodynamics as something constructed on top of classical physics fits well with Darrigol's idea of a modular structure of physical theories. According to Darrigol

> The practice and the history of physics show that physical theories are not homogenous wholes, and that a given physical theory is usually used in conjunction with other theories … I introduce the notion that any non-trivial theory has essential components, or *modules*, which are themselves theories with different domains of application. (Darrigol, 2008, pp. 195-196)

Thus quantum electrodynamics can be seen as part of a broader theoretical modular structure that is expected to describe –with both its classical and quantum parts– what we consider to be the phenomena of matter, radiation and their interaction. Quantum electrodynamics works as an extension (or upgrade module) of the classical theory into 'regions' where previously this failed completely. But since it has been developed from classical concepts, and its probabilistic interpretation puts clear constraints on the applicability of the theory, we cannot expect to recover the classical part of the description of the phenomena from the quantum part by some limiting procedure. In

particular, it is not possible to recover fully, from quantum electrodynamics, the kind of temporal description of physical processes that we have with the classical theory. [49]

[49] From a different perspective, not taking into account the relation between classical and quantum electrodynamics, Teller (1999) argues against taking quantum electrodynamics to be a fundamental theory.

CAPÍTULO 9

COMENTARIOS FINALES

Como conclusión de este estudio histórico-filosófico de anomalías en la electrodinámica cuántica cabe precisar un poco lo que tiene o no de filosófico este trabajo. Haciendo una analogía con la cuestión de la teoría de perturbaciones tratada en este trabajo se puede decir que aquí se presenta un análisis filosófico de primer orden sin adentrarme en cuestiones más complejas. Esta es una opción consciente que resulta de lo intrincado de los problemas filosóficos implícitos en este trabajo.

Los debates filosóficos desde la filosofía de la física enfocando la teoría cuántica de campos van desde perspectivas defendiendo que la teoría cuántica de campos no aporta ningún elemento autónomo que no se encuentre ya en la mecánica cuántica (Cushing, 1988) a la perspectiva de que existen temas filosóficos propios a la teoría cuántica de campos (Cao, 1999). Un ejemplo es el caso 'clásico' de la cuestión del estatus ontológico de los cuantos en la teoría: la llamada cuestión de la 'interpretación' (ontológica) en términos de cuantos o campos.

Por lo general los problemas tratados me parecen bastante más vastos e intrincados que los estudios filosóficos especializados permiten suponer. En particular con la idea propuesta aquí de que no se puede analizar la teoría cuántica sin tener también en cuenta la teoría clásica surgen dudas respecto a la 'validez' y 'generalidad' de muchos análisis 'filosóficos' disponibles en el mercado académico. Esto es en parte el motivo de presentar 'estudios separados de primer orden' sin buscar una integración clara de los distintos elementos.

¿Cómo se podría hacer una filosofía de 'orden' superior? En primer lugar resulta evidente la cuestión de usar la estructura más general clásico-cuántica. Pero no es sólo eso. Queda evidenciado en este trabajo que existe una cuestión de adecuación entre la matemática y la física. Ésta se tiene que tratar en un ámbito más amplio que el de la electrodinámica (clásico-cuántica). También la cuestión de la consistencia del formalismo físico-matemático con la experimentación. Aquí creo posible un tratamiento centrado en la electrodinámica pero un enfoque más global puede resultar más interesante. A lo largo del trabajo queda clara la importancia que doy al aspecto de comparar/relacionar el formalismo con la experimentación (lección aprendida con el trabajo clásico de Bohr y Rosenfeld (1933) que no abordo de forma directa en este trabajo), pero esto es, en si mismo, un trabajo que va bastante más allá de lo que busqué realizar aquí. La cuestión de la adecuación entre la estructura matemática y los conceptos físicos implementados en la teoría, es a mi entender una cuestión que también Bohr enfocó sin denominarla así. Es uno de los elementos que exploro en este trabajo para tratar de dar una interpretación clara del formalismo que haga consistente la práctica de los físicos y la estructura conceptual de la teoría (y así evitar la aceptación meramente pragmática de tener que recurrir a un método aparentemente ad hoc que era lo que estaba pasando en la teoría). Lo que no hago es ir más allá de esta cuestión más

específica e intentar desarrollar una 'visión' filosófica del papel de la matemática en la física. Esto es una cuestión mucho más amplia, que creo no poder tratar solamente teniendo en cuenta una teoría en particular. Pese a no desarrollar filosóficamente estos temas, ellos están presentes en este trabajo, y junto con la cuestión del espacio-tiempo (para la cual también es necesaria una perspectiva más amplia) constituyen el hilo conductor que 'conecta' los distintos capítulos. Así, aunque no presento el desarrollo filosófico más amplio en el que se podría encuadrar mi trabajo, presento ejemplos claros e interconectados (por resultar de la misma teoría) de la importancia de las mencionadas cuestiones filosóficas de orden superior.

Así, por ejemplo, al tratar la cuestión del vacío del campo electromagnético enfoqué la cuestión de la consistencia entre la interpretación del formalismo físico-matemático de la teoría y los resultados experimentales que se pueden considerar como una 'manifestación' del vacío electromagnético. Resulta que son consistentes, pero hay un problema a nivel de la teorización física respecto a la descripción de la interacción entre la radiación y materia. Eso no parece posible de evitar en la electrodinámica cuántica que resulta ser un método intrínsecamente aproximativo, que no permite tratar la radiación y la materia como un sistema cerrado en el cual se da una descripción exacta de la interacción. Incluso parece que ésta es la situación en la electrodinámica clásica. Resultaría extraño si no fuera así ya que la estructura de la electrodinámica cuántica se construye partiendo de la de la electrodinámica clásica. Resulta así esencial tratar la cuestión de la relación entre la estructura matemática y conceptual en la teoría para interpretar el formalismo y sus aplicaciones. Así, al contrario de la visión más usual en la filosofía de la física, podemos ver la necesidad de la renormalización como una indicación del ajuste 'fino' que hay entre la estructura matemática y conceptual. Los infinitos resultan en este caso de aplicarse la teoría sin tener en cuenta la estructura atómica de la materia que es una componente esencial de la formalización matemática del concepto físico de electrón en la ecuación de Dirac. Del mismo modo la divergencia de la expansión en serie de la matriz-S se puede ver como resultado de una aplicación ilimitada del formalismo matemático sin tener en cuenta la definición limitada de interacción con que se parte en la teoría. Como Bohr y Rosenfeld precisaron, en la electrodinámica cuántica se describe la interacción evanescente (vanishing) entre radiación y materia nada más (Bohr & Rosenfeld, 1950, p. 794). Resulta entonces que los resultados divergentes con que nos enfrentamos en la teoría tienen origen en un uso ilimitado del formalismo matemático. Queda por saber si eso es una característica general en la física-matemática o si hay teorías 'avanzadas' en que tal situación no ocurre. También las cuestiones filosóficas relacionadas con la teoría de perturbaciones van más allá del caso particular aquí tratado, por lo que no se pueden obtener conclusiones generales de este caso particular.

La cuestión de la adecuación físico-matemática tiene incidencia en la interpretación de los términos de la expansión en serie de la matriz S, en particular en lo que respecta al estatus de los cuantos virtuales. Pero esto no afecta el aspecto de la descripción espacio-temporal global tal como la tenemos en la electrodinámica cuántica. Como comenté en la introducción el estudio filosófico de los conceptos de espacio y tiempo teniendo en cuenta alguna aportación de la electrodinámica cuántica, es un estudio bastante más vasto de lo que aquí se hace por lo que no se puede presentar en este trabajo ninguna visión filosófica particular respecto a esta materia. Los resultados comentados llevan antes a buscar un enfoque conjunto clásico-cuántico de las cuestiones relacionadas con el espacio-tiempo como un ejemplo particular de la necesidad de usar por lo general este enfoque siempre que tratamos algún aspecto conceptual/filosófico relacionado con las teorías cuánticas.

APPENDIX

BOHR'S QUANTUM POSTULATE AND TIME IN QUANTUM MECHANICS

1 Introduction

Niels Bohr considered that the "discovery of the *elementary quantum of action*, which revealed a feature of *wholeness* inherent in atomic processes" (Bohr, 1958, p. 2) means a departure from the classical physics description, where we assume that the interaction of a physical system with a measuring instrument can ultimately be disregarded. In the case of quantum phenomena we have to be aware that due to the "indivisibility of the quantum of action" (Bohr, 1934, p. 5) we must associate to all "individual atomic processes an element of discontinuity quite foreign to the fundamental principles of classical physics, according to which all actions may vary in a continuous manner" (Bohr, 1934, p. 4). This means that in the case of all atomic processes every energy change results from an indivisible – and because of that discontinuous – transition between different states that cannot be continuously connected. These ideas were summed up by Bohr and presented in what he called the quantum postulate (and its consequences).

In section 2 I will give a historical account of the coming to be of the postulate of the quantum and some of its consequences according to Bohr's views on quantum theory. In section 3, I will consider the temporal description of quantum systems given by the time-dependent Schrödinger equation, taking into account Bohr's views on the interpretation of the formalism of the theory. In particular, considering Bohr's interpretation of the wave function – related to the role he gives to the experimental arrangement in the interpretation of the mathematical formalism of the theory –, it is possible to accommodate the discontinuous changes in individual systems with a temporal description of an ensemble of identical systems in a continuous 'classical' time (that is external to the quantum systems themselves). But as will be shown we must address the question: are Bohr's ideas coherent taking into account his quantum postulate and the use in the description of a quantum system of an external classical time? Following the ideas of Don Howard the answer seems to be no. But from a different perspective (compatible with views put forward, for example, by Paul Teller, Simon Saunders or Henrik Zinkernagel) the answer can be yes.

In a nutshell, according to Bohr it is not possible to define a quantum system independently of the experimental context – (at least in part) classically described – that defines the conditions in which the quantum phenomenon is manifested. In this way it is not possible to take the wave function as describing an isolated quantum system – a concept that has no meaning for Bohr – but a quantum system defined in a particular experimental context, which, at least in part, is classically described. Also, Bohr did not consider the need for the wave function collapse during the observation of a quantum system (Howard, 2004, p. 669). This is possible if the wave function is not associated

with an individual quantum system but to a probabilistic description of identically prepared quantum systems submitted to the same experimental procedure (Teller, 1980, pp. 211-214).

One point of quantum theory that is usually not considered in connection with Bohr's ideas is the concept of time being used in the theory. In reality the use of a classical concept of time is coherent with Bohr's ideas. Even if Bohr did not develop in detail his views regarding space and time in quantum theory, it is possible to give a coherent reading of his ideas by taking into account the need for a classical description of part of the experiment. This makes possible a classical treatment of time, and this even if the quantum postulate implies the impossibility of conceiving the quantum phenomena independently of the measuring apparatus. In particular it is possible to see the temporal parameter of the Schrödinger equation as an external classical time related to the measuring apparatus. This makes it possible to have simultaneously:

A) A quantum system defined in a way that is dependent on the experimental context (due to the quantum postulate).

B) A space-time macroscopic reference frame associated with the measuring apparatus, but defined without taking into account the indissociability of the quantum system to the measuring apparatus.

C) The description of the quantum system using a classical clock with which it has no direct interaction.[50]

Some further remarks are presented in the end of this appendix.

2 The quantum postulate

Around 1912-1913 Bohr developed a model of the atom[51] based on the idea of stationary states – not submitted to the consequences of the classical theory of radiation –, where the electron can jump from one stationary state to another by emission or absorption of radiation with a frequency ν given by the relation $h\nu = E' - E''$, where E' and E'' are the energies of each stationary state. This might seem to be an application of Einstein's ideas on the emission and absorption of light quanta. That is not the case (Mehra & Rechenberg, 2000, pp. 94 & 109).

In his 1913 article Bohr presented a model of the atom in which he incorporated 'quantum' ideas in the classical 'planetary system' model of the atom developed by E. Rutherford. Besides his idea of stationary states – where the classical laws of electrodynamics are put to rest allowing us to consider that there was no emission of radiation, while at the same time the electron was supposed to have a classical orbit described by classical mechanics – the main point in Bohr's approach was the non-classical description of the emission of electromagnetic radiation that could 'explain' the line-spectra of hydrogen. In the beginning of his article, Bohr gave a first treatment of the emission of radiation when an electron passed from one stationary state to

[50] In this way, I will be presenting a reconstruction (in Howard's sense; see Howard, 1994, p. 203) of Bohr's interpretation of the quantum formalism, which in my view makes compatible Bohr's quantum postulate and Bohr's views regarding space and time in quantum theory.

[51] For an account of Bohr's research that lead to his atomic model see e.g. Sánchez Ron (2001, pp. 255-284).

another, based on the so-called Planck's second theory, which was formulated by Planck between 1910 and 1912 (Kuhn 1978). Bohr considered that during the binding of the electron, when the electron passed from a free state of zero energy to a stationary state (or when the electron passed from one stationary state to another stationary state with lower energy), we had an "emission of a different number of Planck's energy-quanta" (Bohr, 1913, p. 139). At the same time Bohr considered that this process corresponded to an "emission of a *homogeneous* radiation" (Bohr, 1913, p. 139). It seems Bohr was not thinking in terms of Einstein's light quanta but in terms of an electromagnetic wave whose energy was, according to one of Bohr's assumptions, given by $h\nu = E' - E''$. This of course is inconsistent with the use of a multi-quantum radiation process in the description of the binding of the electron (Darrigol, 1992, p. 89). In any case Bohr clearly stated that these 'special assumptions' were not essential in the development of his model and that other assumptions might be used. In this article Bohr followed two other different approaches, progressively freeing his model from Planck's considerations on the way (Jammer, 1966, pp. 78-80).

In his second approach Bohr considered that the radiation emitted when the electron passed from one stationary state to another corresponded to a single energy quantum whose energy is equal to $h\nu$. In this case Bohr considered that the relation between the (binding) energy of the electron W and its frequency of (orbital) revolution ω was given by the expression $W = f(\tau)\omega h$, where τ is an integer whole number corresponding to a particular stationary state. By considering the transition between two stationary states and taking into account the Balmer series formula, Bohr found that we must have $f(\tau) = c\tau$, where c is some undetermined number. To determine the value of c, Bohr, following a method used previously by Planck (Jammer, 1966, p. 50; Kuhn, 1978, pp. 278-279; Planck, 1914, pp. 164-166), considered the limit where there should be an agreement with classical electrodynamics. In the case of two successive stationary states $\tau = N$ and $\tau = N - 1$, when "N is great" (Bohr, 1913, 146), we must have $f(\tau)=\tau/2$ to agree with the results from classical electrodynamics.

Finally, Bohr gave up any account of the emission of radiation based explicitly on the concept of energy quanta, and solely by an analogy with classical electrodynamics he tried to make plausible the previous relation between the (emitted) energy W and frequency ω of the electron in the stationary state. In the limit of large N, the frequency of the emitted radiation is given by $\nu = n\omega$, that corresponds to one of the harmonics of ω, which are expected to be emitted according to classical theory (Tomonaga, 1962, p. 93). In this limit of large N, the frequency of the emitted radiation does not depend on the difference of energy of the different stationary states and can be calculated solely from the frequency of one stationary state. Bohr considered that:

> the interpretation of the equation [$W = \tau\omega h/2$] is not that the different stationary states correspond to an emission of different numbers of energy-quanta, but that the frequency of the energy emitted during the passing of the system from a state in which no energy is yet radiated out to one of the different stationary states, is equal to different multiples of $\omega/2$, where ω is the frequency of revolution of the electron in the state considered. (Bohr, 1913, p. 146)

With this approach Bohr develops his model of the atom without having to address directly the problem of the nature of radiation and Einstein's hypothesis of the light quanta.[52]

[52] Bohr associates the expression $E = h\nu$ (that he uses to determine the energy of the electromagnetic radiation) with Planck, and in his article we refers to some of Planck's articles published between 1910 and 1912. In his different formulations of his second theory Planck associated the quanta of energy to the

In 1923 Bohr addressed directly the hypothesis of light quanta (Klein, 1970, p. 21). Bohr considered that the concept of light quanta "excluded in principle the possibility of a rational definition of the conception of a frequency ν" (Bohr, 1924, p. 35), and that "in spite of its heuristic value, however, the hypothesis of light-quanta, which is quite irreconcilable with so-called interference phenomena, is not able to throw light on the nature of radiation" (Bohr, 1923, p. 32). In this article Bohr made an explicit association of the expression $h\nu = E' - E''$ with the emission or absorption of electromagnetic waves by taking more fully into account the correspondence (analogy) with classical electrodynamics that he used already in his 1913 article:

> a process of transition between two stationary states can be accompanied by the emission of electromagnetic radiation, which will have the same properties as that which would be sent out according to the classical theory from an electrified particle executing an harmonic vibration with constant frequency. This frequency ν has, however, no simple relation to the motion of the particles of the atom, but is given by the relation $h\nu = E' - E''$, where h is Planck's constant, and E′and E′′ are the values of the energy of the atom in the two stationary states that form the initial and final state of the radiation process. Conversely, irradiation of the atom with electromagnetic waves of this frequency can lead to an absorption process, whereby the atom is transformed back from the latter stationary state to the former. (Bohr, 1923, p. 33)

Around July of 1925 it was already clear to Bohr that a more classical wave-like picture of the electromagnetic radiation was untenable. This was due to experimental results, related to the so-called Compton scattering, obtained by W. Bothe and H. Geiger. In their experiment, Bothe and Geiger confirmed energy-momentum conservation in individual atomic processes by observing a simultaneous detection (coincidences) of scattered x-rays and recoil electrons in the scattering of x-rays by free electrons (Fick & Kant, 2009, pp. 399-401). Also A. H. Compton and A. W. Simon made an experiment in a cloud chamber that permitted the observation of the track of the recoil electrons and the direction of scattering of the x-rays (due to the occasional production of secondary tracks). They obtained the expected relation, according to the light-quanta hypothesis, between the scattering angles of the x-rays and the electrons (Jammer, 1966, p. 186).

According to Bohr we do not observe directly the scattered x-ray but "photoelectrons released by the scattered radiation" (Bohr, 1925a, p. 204). It is important to take this into account to understand Bohr's reasoning. The experimental result of Bothe and Geiger implies strict energy-momentum conservation in the interaction of the electron and the radiation. This implies that depending on the change of energy and momentum in the recoil electron we will have a change in the energy and momentum of the photoelectron, which is causally dependent on the changes in the first electron due to the strict conservation of energy and momentum in the interaction of the electrons with the radiation. Bohr refers to this situation as a "coupling between the emission of the recoil electrons … and the photoelectrons" (Bohr 1925a, 204). Considering this electromagnetic coupling between two individual transition processes

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resonators (oscillating dipoles) not to the electromagnetic field (Kuhn, 1978, p. 231). Planck did not accept Einstein's idea of the light quanta (Kuhn, 1978, p. 233). Specifically, in is mature formulation of his second theory, Planck proposed to "make the deviation from the laws of classical electrodynamics … as slight as possible" (Planck, 1914, p. 152). In this way, Planck considered that "the absorption of radiation by an oscillator takes place in a perfectly continuous way" (Planck, 1914, p. 161). It is only in the emission of radiation that the behaviour of the oscillators departures from classical theory. According to Planck "the oscillator emits in irregular intervals, subjected to the laws of chance; it emits, however, only at a moment when its energy of vibration is just equal to an integral multiple n of the elementary quantum $\varepsilon = h\nu$, and then it always emits its whole energy of vibration $n\varepsilon$". (Planck, 1914, p. 161)

(one occurring with the recoil electron and the other with the photoelectron), Bohr concludes that "no space-time mechanism seemed conceivable that permitted such a coupling and at the same time achieved a sufficient connection with classical electrodynamics" (Bohr, 1925a, 204). That is, it is not possible to maintain a wave-like picture because of the conservation of energy and momentum in individual atomic processes. This does not mean a renunciation of the wave-like perspective and adoption of the light quanta concept. According to Bohr the problem is not simply "distinguishing between two well-defined conceptions of the propagation of light in empty space corresponding to either a corpuscular theory or a wave theory of light" (Bohr, 1925a, p. 204). The real problem being faced is "to what extent the space-time pictures [wave-like or particle-like], by means of which the description of natural phenomena has hitherto been attempted, are applicable to atomic processes" (Bohr, 1925a, p. 204). The paradoxical situation facing Bohr is that there is no simple choice between two incompatible pictures used in the description of natural phenomena. We are in a situation where "the radiative activity of individual atoms is influenced by the presence of other atoms in the sense to be expected in the picture of the wave propagation of light" (Bohr, 1925a, p. 204), but on the other hand we have to recall "the coupling between individual atomic processes [due to energy-momentum conservation], which forces upon us the picture of a corpuscular propagation of light" (Bohr, 1925a, pp. 204). In another article published in December of 1925, Bohr states that one is facing "an essential failure of the [wave-like and particle-like] pictures in space and time on which the description of natural phenomena has hitherto been based" (Bohr 1925b, 848). This situation did not prevent Bohr from grasping the profound conceptual meaning of accepting the "individuality of single [atomic] processes" (quoted in Mehra & Rechenberg, 2000, p. 191) due to the strict conservation of energy and momentum in the interaction of matter and radiation, as had been verified in the experiments of Bothe and Geiger, and Compton and Simon and proposed by Einstein in 1905 within his light-quanta hypothesis.

In a letter to H. A. Lorentz from 24 June 1926, accepting an invitation to attend a meeting, Bohr mentioned the eventual name of the report he would present: "Le Postulat des Quanta et le Nouveau development de l'Atomistique" (Mehra & Rechenberg, 2000, p. 175). What Bohr meant by 'le postulat des quanta' or as it appears in English, the quantum postulate, would appear in print only in 1928. According to the Bothe-Geiger and Compton-Simon experiments, it is necessary to use the idea of an elementary quantum in the description of the interaction between matter and radiation. Because of the indivisibility of the quantum we have to consider that in each single atomic process of interaction between the electron and the electromagnetic radiation we have a "discontinuous change of energy and momentum" (Bohr, 1927, p. 93). From this we may speak of the 'individuality of single processes'. Connected with this idea of individuality is the possibility of a coupling between spatially separated atomic processes, meaning with the term 'coupling' the causal relation between individual processes due to energy-momentum conservation.[53] But the essential point in the quantum theory is the indivisibility of the quantum, as Bohr mentioned:

[53] Scott Tanona gives an account of Bohr's reaction to the Bothe-Geiger experiment that stresses the 'coupling' between different atoms, or more generally the coupling between an atomic system and a measurement instrument (i.e., according to Tanona, a Bothe-Geiger-type coupling with a measurement instrument). In this way Tanona gives to 'individuality' a slightly different meaning than the one adopted here (which relates the term already to the interaction between radiation and matter). Also Tanona stresses Bohr's emphasis on the breakdown of the classical space-time pictures and not on the light-quantum concept (Tanona, 2004, pp. 498-500; see also Murdock, 1987, pp. 29-30).

Its essence may be expressed in the so-called quantum postulate, which attributes to any atomic process an essential discontinuity, or rather individuality, completely foreign to the classical theories and symbolised by Planck's quantum of action. (Bohr, 1928, p. 580)

This has an immediate consequence that Bohr stressed clearly in the same article:

The quantum postulate implies that any observation of atomic phenomena will involve an interaction with the agency of observation not to be neglected … the definition of the state of a physical system, as ordinarily understood, claims the elimination of all external disturbances. But in that case, according to the quantum postulate, any observation will be impossible … if in order to make observation possible we permit certain interactions with suitable agencies of measurement, not belonging to the system, an unambiguous definition of the state of the system is naturally no longer possible. (Bohr, 1928, p. 580)

That is, as a consequence of the 'quantized' interaction, there is no way, as in classical physics, to consider a smaller and smaller interaction that in the limit of an 'infinitesimal' exchange of energy-momentum would enable us to define a quantum system independently of the experimental context where it is being observed.

In his later writings the importance Bohr gave to this consequence of the quantum postulate becomes even clearer. In successive drafts for an article published in 1956, Bohr uses the word 'wholeness', 'indivisibility', and 'unity' (Honner, 1987, p. 69), finally writing "The essential indivisibility of proper quantum phenomena" (Bohr, 1956, p. 87). In several others of his later writings Bohr refers to a 'feature of wholeness' in the atomic processes (Bohr, 1954, p. 71; 1958, p. 2; 1962a, p. 78; 1962b, p. 80). This characterization of atomic processes by their 'wholeness' results from Bohr's insight into the consequences of the "atomistic feature in the energy transmission" (Bohr, 1933, p. 421), that he addressed in published articles since 1928, according to which "all effects of light may be traced down to individual processes, in each of which a so-called quantum is exchanged" (Bohr, 1933, p. 421). We see then that it is Bohr's recognition of the quantized interaction between radiation and matter (embodied in the light-quantum concept) that leads him to the generalization that *all* atomic processes result from indivisible (atomistic) momentum and energy exchanges (i.e. *all* atomic processes are discontinuous).

One of the most relevant aspects of the "impossibility of separating a behavior of atomic objects from the interaction of these objects with the measuring instruments" (Bohr, 1948, p. 313) is the need of redefining the meaning of the term phenomena. According to Bohr we have to limit the "use of the word *phenomenon* to refer exclusively to observations obtained under specified circumstances, including an account of the whole experiment" (Bohr, 1948, p. 317). In this way we are no "longer in a position to speak of the autonomous behavior of a physical object, due to the unavoidable interaction between the object and the measuring instruments" (Bohr, 1937, p. 293). This implies that for Bohr the wave-function of a 'quantum' system does not have an independent meaning on its own, it can only be defined in the context of an experimental arrangement: we can not speak of the wave-function of an electron by itself, only of its wave function as defined in a particular experimental setup (Teller, 1980, p. 206; Camilleri, 2007, p. 522). This contextualization of the quantum phenomena brings with it, according to Bohr, the need to use classical concepts. Thus, according to Bohr we must consider that:

[An] unambiguous communication of physical evidence demands that the experimental arrangement as well as the recording of the observations be expressed in common language, suitably refined by vocabulary of classical physics. In all actual experimentation this demand is fulfilled by using as

measuring instruments bodies like diaphragms, lenses and photographic plates so large and heavy that, notwithstanding the decisive role of the quantum of action for the stability and properties of such bodies, all quantum effects can be disregarded in the account of their position and motion. (Bohr, 1962b, p. 91)

There is one important aspect of Bohr's interpretation of quantum mechanics not yet mentioned (besides his complementarity, which I will not address). More exactly an aspect that Bohr does not mention himself, i.e. something that is altogether inexistent in Bohr's account of quantum theory, namely the wave packet collapse.

As is well known the wave packet collapse is a central aspect of the so-called Copenhagen interpretation of quantum mechanics. In his "Who invented the 'Copenhagen interpretation'? A study in mythology", Don Howard (2004) calls attention to the fact that Bohr's interpretation, "makes no mention of wave packet collapse or any of the other silliness that follows therefrom, such as a privileged role for the subjective consciousness of the observer" (Howard, 2004, p. 669). This view had already been put forward by Paul Teller in his "The projection postulate and Bohr's interpretation of quantum mechanics":

My position is very simply that Bohr gives the state function a statistical interpretation and a statistical interpretation has no need of the projection postulate [i.e. the collapse of the wave function during measurement]. (Teller, 1980, p. 211)

Teller's view was that to Bohr

The state function must be taken as a purely symbolic device for calculating the statistics of classically or commonly described experimental outcomes in collections of phenomena grouped by shared specifications of experimental conditions. (p. 206)

Accordingly

On Bohr's view the state function describes not one individual case, but a whole ensemble of cases with a common preparation characterized in the language of classical physics or daily discourse. (p. 213)

I agree with Teller's reading or 'interpretation' of Bohr. This means that what we nowdays call the statistical or ensemble interpretation (Isham's minimal interpretation) was basically the interpretation of Bohr or at least we can see it as an interpretation compatible to what we know about Bohr's views on quantum theory, i.e. a Bohrian interpretation. It is this Bohrian interpretation that is being followed in this work.

3 The concept of time in quantum theory and Bohr's quantum postulate

To see the role of the concept of time in quantum theory we have to consider the quantum-theoretic description of time-dependent phenomena by the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = H\,\Psi(t)\,,$$

where H is the Hamiltonian and ψ the wave function of a system. For the present purpose, I will consider the quantum-theoretical description of the spontaneous emission of radiation by an atom. In this case the Hamiltonian is $H = H_{atm} + H_{rad} + H_{int}$, where H_{atm} is the Hamiltonian for an atom, H_{rad} is the Hamiltonian for the

electromagnetic field, and H_{int} is the Hamiltonian describing the interaction between the electromagnetic field and the atom. Considering the case where the electromagnetic field wavelength is much larger than the dimension of the atom, the interaction between the field and the atom can be described using the electric dipole approximation (Loudon, 1973, pp. 42-43). Also, in the case of a weak coupling between the field and the atom, the time-dependent Schrödinger equation can be solved in first-order perturbation theory (Ballentine, 1998, pp. 349-350). To determine the spontaneous emission rate (and from this the lifetime of the excited state), corresponding to the transition of an atom initially in an excited state to the ground state (with the electromagnetic field initially in the vacuum state), a further approximation will be considered: we will consider a time t larger than the inverse of the frequency of the spontaneously emitted photon, but since it is a first-order calculation we must also take t to be smaller than the excited state lifetime (Craig & Thirunamachandran, 1984, pp. 84-86). Solving the time-dependent Schrödinger equation for this case we see that the probability of finding the atom in the excited state follows an exponential decay law, that is, the time dependence is given by $e^{-t/\tau}$, where τ is the excited state lifetime (Allen & Eberly, 1975, p. 167). This means that if we consider an ensemble of equally prepared systems each one consisting of an atom in the same excited state (in a suitable experimental setup), and we measure the time it takes for each atom to decay, for a large ensemble the measured times will fall on an exponential line defined by the lifetime of the atoms. However, as we have seen, according to the quantum theory "the process of transition is indivisible" (Bohm, 1951, p. 426). In this way, when considering just one atom there is only a sole perception of a change in the state of the atom due to the instantaneous emission of radiation at a certain time. Without any external clock there would be no way of timekeeping with just this one atom. There would be no timekeeping before the emission of radiation and after the emission of radiation, only a perception of the change itself due to the emission of a photon. But the time-dependence of the wave function is not related to (what can be called) an internal time related with some dynamical variable, but to a time parameter that is external to the quantum systems. Quantum theory is formulated by considering a background space-time that enters the equations of the theory as parameters not dependent on any physical systems that are described by the theory. In this way the time parameter can be considered as external to the physical systems whose equations of motion are dependent on these space-time parameters. On the other hand, it is possible to define what can be called an internal time by considering some dynamical variable of a quantum system whose behaviour mimics the external time (Hilgevoord, 2005, p. 31). One example is the quantized linear oscillator, described by a quantized angle variable whose eigenvalue runs through the interval [0, 2π], and whose equation of motion describes "the behaviour we expect of the hand of a clock" (Hilgevoord, 2002, p.304): $U(t)|\phi\rangle = |\phi + \omega t\rangle$, where U(t) is the time evolution operator, ϕ is an angle variable, and ω is the constant frequency of the 'quantum clock' (Larmor clock). It is important to notice that the dynamical variable ϕ is described quantum mechanically. For example, if we try to use this 'clock' to measure the time of decay of an atom in an excited state and consider an ensemble of clocks subjected to the same experimental arrangement (each clock being coupled to an atom that is not directly observed), we obtain a time distribution from the ensemble of clocks (for the time of decay) according to the exponential decay law (see Peres, 1995, pp. 406-412).

We see then that in the case under consideration of an atom in an excited state, its description, as just mentioned, presupposes an external time flowing independently of the atom. This means that in the quantum theory we cannot really think in terms of one

isolated system: the temporal behavior as described in the quantum theory is not perceptible from the behavior of one isolated system but only by taking into account an ensemble of equally prepared systems.

The exponential decay law considered in the case of the spontaneous emission of electromagnetic radiation is common in the temporal behavior of different physical systems. The first known example is the disintegration of radioactive substances that follows an exponential law of decay (Rutherford & Chadwick & Ellis, 1930, pp. 4-8). Considering this, we could imagine a situation where "all 'regular' clocks were abolished from our laboratories, and we were forced to use radium clocks, in which the defining events are the disintegration of individual atoms" (Campbell, 1927, p. 779). In this situation, if we had only a few radium atoms (or equivalently in case of the spontaneous emission, a few atoms in an excited state), from the sequence of more or less simultaneous groups of decays, it would not be possible to construct an exponential curve and with it have a rough timekeeping procedure. But for a very large ensemble, we have, as time goes by, a clearer notion of the temporal behavior of the ensemble as a whole, even without an explicit reference to an external clock. On similar lines, in the case being considered of the temporal description of the spontaneous emission, each individual atom, according to the quantum postulate, will have a discontinuous change of state at a particular (external) time, and it is only possible to determine the probability for this change. But considering a large ensemble of identical systems, by measuring the time of decay of each one we obtain a distribution that fits an exponential curve. In this way the regularity of the temporal behavior of a quantum system is only made 'visible' by considering a large ensemble of equally prepared systems (Peres, 1995, p. 403). But we must recall that the time dependence of each equally prepared quantum system is determined in terms of an external classical time measured by a 'classical' clock.

I will now address the problem of seeing how this use of a classical external time fits into Bohr's account of quantum theory. For Bohr, the space and time description of a quantum phenomenon is dependent on the definition of a space-time reference frame through "fixed scales and clocks" (Bohr, 1949, p. 40). This coordinate system is "fixed in the ordinary way by means of solid bodies and unperturbable clocks" (Bohr, 1928, p. 584).[54] That is, for Bohr the reference frame is defined by the macroscopic experimental arrangement.

Not only is the existence of a coordinate system linked to an experimental arrangement, but also for its definition we have to disregard the quantum postulate – in what regards the stipulation of a reference frame 'connected' with the experimental setup – and consider it defined entirely on classical terms. This is because, according to Bohr, "if we want to use the idea of space-time we must have watches and rods which are outside and independent of the object under consideration" (Bohr, 1985, p. 369). This classical operationally defined space-time coordinate system (i.e. a coordinate system presupposed by an inertial material frame of reference so large and heavy that all quantum effects can be disregarded so that it has a well-defined position and momentum in relation to the background space-time) not in directly interaction with the quantum

[54] In this work I will make the simplifying assumption that we can identify directly the space-time reference frame with the background space-time, i.e. that the reference frame is inertial. This means that I am taking the effective laboratory frame to be an inertial frame or at least to be, for all practical purpose, nearly inertial. It is important to notice that by definition an inertial reference frame is one in which Newton's laws of motion are valid. This implies that the operationally defined inertial reference frame (the material frame of reference) must itself be describable by classical dynamics (for details on this subject see Dickson, 2004).

system, can be seen as implemented in the formalism of the quantum theory as external space and time parameters that appear in the Schrödinger equation and wave function.

That we must consider, according to Bohr's view, the space and time parameters as related to the experimental arrangement, can be expected by taking into account Bohr's interpretation of the quantum formalism. Due to the quantum postulate the wave function (and the Schrödinger equation) cannot be seen as something intrinsic to a quantum system and independent of the experimental arrangement that enables the observation of the phenomena we associate with the quantum system. This means also that part of the conceptual content and mathematical description of the wave function is dependent on the existence of an experimental arrangement. In particular the time parameter that appears in the Schrödinger equation and wave function depends on a background space-time, that we can see as justified, according to Bohr's interpretation of the quantum formalism, by taking into account – due to the quantum postulate – the unavoidable interaction of the quantum system with the experimental arrangement *with its entirely classically described* "fixed measuring rods and synchronized clocks" (Bohr, 1955, p. 90).

To sum up: on one hand we must take the quantum system – due to the quantum postulate – not to be definable without taking into account the experimental setup; and on the other hand we must take the reference frame to be independent of the quantum system so that it can be described entirely in classical terms. This situation is not inconsistent. In reality it is possible to present a coherent view on the consequences of the quantum postulate in what regards the classical description of space and time, by noticing that, according to Bohr, not all of the experimental arrangement has to be considered in direct interaction with the quantum system, only the "significant parts of the experimental arrangement" (Bohr, 1962b, p. 92). This is what makes it possible to consider that the watches and measuring rods "are outside and independent of the object under consideration" (Bohr, 1985, p. 369). That is, at the same time the quantum system and its mathematical description cannot be defined without taking into account, due to the quantum postulate, the interaction with the measuring instruments, but in what regards the rods and clocks belonging to the experimental arrangement (necessary for the definition of the space-time reference frame), they are independent of the quantum system (i.e. not in direct interaction), and so not submitted to the consequences of the quantum postulate being treated as totally classical entities.

This reading of Bohr's ideas implies considering the part of the experimental arrangement not directly in interaction with the quantum system as describable by classical physics. What about the parts that are in interaction? According to Paul Teller's account of Bohr's interpretation of quantum mechanics:

> Bohr acknowledges that one may include the immediate macroscopic measuring device as part of the object described with the formalism of quantum mechanics, as long as there remains some further part of the total experimental context which receives a classical description. (Teller, 1980, p. 215)

I agree with Teller's reading of Bohr. Let us consider the two-slit electron diffraction experiment. According to Bohr, depending on what we want to measure, the position or momentum of the electron, we must use a first diaphragm rigidly fixed to the apparatus (in the case of a position measurement) or not rigidly connected to the apparatus (in the case of a momentum measurement). In the second case the position and momentum of the diaphragm are treated quantum mechanically:

> In the arrangement suited for the control of the momentum of the first diaphragm, this body can no longer be used as a measuring instrument for the same purpose as in the previous case [(the position

measurement)], but must, as regards its position relative to the rest of the apparatus, be treated, like the particle traversing the slit, as an object of investigation, in the sense that the quantum-mechanical uncertainty relations regarding its position and momentum must be taken explicitly into account. (Bohr, 1935, p. 698)

How is it possible to treat classically the diaphragm in one case and in the other to treat it quantum mechanically? According to Bohr, this is made acceptable by taking into account his correspondence principle. Bohr mentions the "necessity of discriminating in each experimental arrangement between those parts of the physical system considered which are to be treated as measuring instruments and those which constitute the objects under investigation" (Bohr, 1935, p. 701). Bohr considers that "the place within each measuring procedure where this discrimination is made is … largely a matter of convenience" (p. 701). Accordingly, there is no

inconsistency in the quantum-mechanical description, connected with a change of the place where the discrimination is made between object and measuring agencies … we only have a free choice of this place within a region where the quantum-mechanical description of the process concerned is effectively equivalent with the classical description. (p. 701)

To provide a more elaborated characterization of the reconstruction being proposed in this paper I will make a contrast with Don Howard's reconstruction of Bohr's interpretation of quantum mechanics, which in my view makes it very difficult to give a coherent reading of Bohr's ideas when taking into account his views on space and time in quantum mechanics. According to Howard:

Bohr demanded a classical description only of those properties of the measuring instrument that are correlated, in the measurement interaction, with the properties of the observed object that we seek to measure … this implies, as well, a classical description of the associated measured properties of the observed object itself. A quantum description would be possible for the remaining properties of instrument and object, the properties not crucially involved in the measurement. (Howard, 1994, p. 203)

In the articulation of his argument, Howard first makes it plausible, by quoting Bohr, the idea that not all of the measuring instrument has to be described in classical terms. Howard focuses on the description of the diaphragm in the previously mentioned experiment (which he refers to as diaphragm A), which as mentioned in a particular experimental setup had to be rigidly connected with the rest of the measuring apparatus while in another experimental setup had to be detached from the support that defines the frame of reference. Howard considers that in both cases – of a movable or fixed diaphragm – we can consider the diaphragm as part of the measuring instrument. I think the quotation of Bohr cited by Howard (the passage in page 698 of Bohr's 1935 article quoted above) is ambiguous enough to accommodate also Howard's reading. Also, in a different article, regarding the particular experimental arrangement for measuring the momentum, Bohr mentions that "certain parts of the whole device must naturally be given the freedom to move independently of others" (Bohr, 1949, p. 48), and this goes along the lines of Howard's proposal. But I think that, according to the reconstruction of Bohr's ideas proposed here, this possibility of giving a classical or quantum-mechanical description of the diaphragm is taken care of by taking into account Bohr's line of argumentation related to his correspondence principle: there is a freedom of choosing to treat part of the experimental setup quantum mechanically (usually as part of the object under investigation) or classically (usually as part of the measuring

apparatus). That is, we can choose where to make the 'Heisenberg cut' according to our convenience without entailing any inconsistency.[55]

More complicated in my view is another point of Howard's argumentation. Howard considers also that

> In neither arrangement will the whole of diaphragm *A* be given a classical description. In the second arrangement, the position is described quantum mechanically; in the first, we may infer, the momentum will be so described. What will be described classically are, by implication, only those properties of diaphragm *A* that are correlated with the observed system in the measurement. (Howard, 1994, p. 214)

According to Howard, further evidence for this interpretation can be found in two passages from Bohr (1939a). The first one is:

> We must recognize that a measurement can mean nothing else than the unambiguous comparison of some property of the object under investigation with a corresponding property of another system, serving as a measuring instrument, and for which this property is directly determinable according to its definition in everyday language or in the terminology of classical physics. (p. 311)

While this passage cannot be said to contradict or give direct evidence to Howard's claim, the second passage seems to me to be a typical Bohrian reference to a consequence of the correspondence principle:

> In the system to which the quantum mechanical formalism is applied, it is of course possible to include any intermediate auxiliary agency employed in the measuring process. Since, however, all those properties of such agencies which, according to the aim of the measurements have to be compared with the corresponding properties of the object, must be described on classical lines, their quantum mechanical treatment will for this purpose be essentially equivalent with a classical description. (pp. 315-316)

But again (as in the case mentioned above), no clear conclusion can be given in relation to Howard's interpretation of these quotations without taking fully into account Bohr's views regarding quantum mechanics, or more exactly a 'self-consistent' reconstruction of Bohr's writings making compatible Bohr's quantum postulate and Bohr's doctrine of a classical space and time.[56]

To set my case I will need to consider Howard's full-blown development of his views. In another passage Howard spells out his main point again:

> This means that the only *essential* use of classical methods of description will be in connection with that property of the instrument that is correlated with the property of the object that the instrument is designed to measure. (Howard, 1994, p. 216)

From this several things will follow:

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[55] In the view presented here, the 'Heisenberg cut' is an unavoidable aspect of considering a (classically described) reference frame taken to be, according to Bohr's views, outside and independent of the quantum system under consideration. Accordingly the meaning I give to 'wholeness' or 'unity' is not like in Howard's case of an entanglement between the quantum system and the experimental arrangement in its totality, but results from the indivisibility of the quantum interaction, which entails – according to the quantum postulate – the impossibility of defining the quantum system independently of the experimental arrangement (see also footnote 53).

[56] However, in this particular case we do not have to look far to notice that this quotation taken out of context can have a broad array of (re)interpretations. Just a few lines below Bohr writes: "the only significant point is that in each case some ultimate measuring instruments, like the scales and clocks which determine the frame of space-time coordination – on which, in the last resort, even the definitions of momentum and energy quantities rest – must always be described entirely on classical lines, and consequently kept outside the system subject to quantum mechanical treatment". (Bohr, 1938a, p. 316)

A) We must interpret Bohr's reference to classical concepts as not related to the correspondence principle, since, according to Howard, only certain properties of both the measurement apparatus and the object must be considered from a classical perspective. In this way, we must look for some other type of 'essential equivalence' between the quantum and classical description.[57] In Howard's view the kind of convergence between quantum and classical descriptions demanded by the correspondence principle is a wholesale convergence, not an 'essential equivalence' between selected sets of properties (Howard, 1994, p. 217; see also Howard, 2005, pp. 28-29).

B) According to Howard we will find this 'essential equivalence' by looking at the case of an ensemble of identically prepared composite systems (consisting on the measurement setup and the 'quantum object') described by a density matrix built with non-factorizable state functions (due to the entanglement between the measurement setup and the 'quantum object') – the pure case. With a proper selection of sub-ensembles describing factorizable state functions (according to Howard corresponding to the classical idea of separability) the ensemble can be seen as a mixture of elements of the sub-ensembles. According to Howard in each experimental context it is possible to find the proper mixture that gives exactly the same predictions as the original density matrix for the entangled pair (Howard, 1994, pp. 220-222; see also Shlosshauer & Camilleri, 2008, pp. 17-18). Howard considers this approach as the key to a reconstruction of Bohr's views on the need of classical concepts:

> It is upon this disarmingly simple mathematical fact—the equivalence, context by context, of pure cases and mixtures—that I build my interpretation of Bohr's doctrine of classical concepts. I claim that we make the clearest sense out of Bohr's stress on the importance of a classical account of experimental arrangements and of the results of observation, if we understand a classical description to be one in terms of appropriate mixtures. More specifically, I would reconstruct the doctrine of classical concepts as follows. Given any measurement interaction, a description in terms of a pure case is correct, in the sense that it yields all of the right predictions. This is the proper quantum mechanical account of the interaction, and such an account can always be given for all aspects of the interaction, including all parts of both instrument and object. Such a description reflects the essential nonseparability of the quantum mechanical interaction formalism, the nonseparability that Bohr stresses as a fundamental lesson of the quantum mechanical account of the instrument/object interaction; it reflects, too, the non-classical character of quantum statistics. On the other hand, precisely because of its nonseparability, a description in terms of a pure case does not permit us to distinguish instrument and object in the way that Planck and Einstein thought necessary to ensure objectivity. But here is where the concept of an appropriate mixture finds its place. Once we specify the kind of measurement being performed, an appropriate mixture can be constructed that gives all of the right predictions for the parameters involved in such a measurement; and, at least with respect to those parameters, we can separate the states of the instrument and the object and give a purely classical, ignorance interpretation of their statistics. The proper "classical" description, then, is a description in terms of an appropriate mixture. (Howard, 1994, pp. 222-223)

C) One of the implications of all this is clearly spelled out in the following sentence:

[57] In Howard's reading of Bohr's Como lecture (Bohr, 1928), Bohr takes the object and instrument to form an entangled pair that is described quantum mechanically. In order to assign a measured value to the quantum system we must consider the object and instrument not to be entangled (in what regards the property of the measuring instrument that is correlated, in the measurement, with the property of the observed object that we seek to measure). According to Howard, "doing that is what Bohr means by a description in terms of 'classical concepts'" (Howard, 2005, p. 28). In this way according to Howard reading of Bohr, "the descriptions are 'classical' simply in the sense that entanglement is denied and separability is affirmed" (p. 28). For more details on Howard's use of the term 'classical' see point B and the quotation within.

> The fourth question asked why, in the description of a measuring instrument, the only *essential* use of classical methods of description is in the account of that parameter of the instrument that is correlated with the measured property of the object. The answer is that only in connection with these properties need we assume the separability of instrument and object. And the appropriate mixture reconstruction reflects this fact by its context dependence: A different mixture is appropriate to every different context, in the sense that an appropriate mixture yields the correct predictions only for those parameters measurable in that context. All other parameters—of both object and instrument—are correctly described only quantum mechanically, in terms of the pure case density matrix. (Howard, 1994, p. 224)

In this way, we would not need a description of the apparatus in classical terms. The classical description (in Howard's sense) is only necessary for the part that we can consider to be in direct interaction with the object and even in this case only for the parameter involved in the measurement. In the case being considered, for a fixed diaphragm we would have to give a classical description of the position of the diaphragm and the object, and in the case of a moving diaphragm it would be necessary to give a classical description of the momentum. All the rest would be described quantum mechanically.

This interpretation faces problems when we consider Bohr's views on the concepts of space and time in quantum mechanics. As Jan Hilgevoord mentions, there seems to be a problem related to the use of the time concept in quantum mechanics that has posed a challenge to several physicists but to which Bohr makes no reference (Hilgevoord, 2005): the inexistence of a time operator in quantum mechanics. Bohr does not mention this because in his interpretation of quantum mechanics there is simply no motive not to consider space and time from a classical perspective (Hilgevoord, 2005, pp. 47-48). This should be clear from the presentation made above of Bohr's reliance on classical concepts of space and time in his interpretation of quantum mechanics. However, and I must stress this point, it is important to notice that for Bohr the classically described space-time reference frame (which is part of the experimental arrangement) is taken to be outside and independent of the observed quantum system.

This is in direct contradiction with Howard's reconstruction. As we have just seen Howard considers that:

1) The only essential use of classical methods of description (in Howard's sense) will be in connection with that property of the instrument that is correlated with the property of the object that the instrument is designed to measure.

2) A quantum description would be possible for the remaining properties of instrument and object, the properties not crucially involved in the measurement.

As it stands I consider this view incompatible with Bohr's account of reference frames in the experimental arrangements. Bohr wrote *explicitly* that "if we want to use the idea of space-time we must have watches and rods which are outside and independent of the object under consideration" (Bohr, 1985, p. 369), and in similar lines that "some ultimate measuring instruments, like the scales and clocks which determine the frame of space-time coordination … must always be described entirely on classical lines, and consequently kept outside the system subject to quantum mechanical treatment" (Bohr, 1939a, p. 316). As I have shown this view is compatible with Bohr's quantum postulate. As it stands Howard's reconstruction seems to be at odds with Bohr's views on space and time in quantum mechanics. In particular, according to Howard's views, we would have to consider that the entire quantum mechanically described apparatus is entangled with the quantum object (since Howard considers that only for the relevant parameter of

the measurement we need a 'classical' separability of apparatus and object). It is not clear how, in these circumstances, an external classical time might fit into Howard's reconstruction.

Parts of the views being developed here have been noticed before. For example by Simon Saunders who made the following remark:

> The conditions of an experiment must ultimately involve rigid connections to bodies of arbitrarily large mass. In that case the uncertainty relations, for the latter bodies, become irrelevant (so long as there is non-zero latitude in *both* position and momentum). Bohr admitted as much when he remarked that the freedom of choice in the divide between quantum and classical was restricted to "a region where the quantum mechanical description of the process concerned is effectively equivalent with the classical description" [5, p.701], and later, when he said that the requirements of unambiguous description of the apparatus "is secured by the use, as measuring instruments, of rigid bodies sufficiently heavy to allow a completely classical account of their relative positions and velocities" [9, p.3]. (Saunders, 2005, p. 24)

In similar lines Henrik Zinkernagel remarked that:

> Bohr actually agreed that the measurement apparatus can also be described by quantum theory. However, he writes (1939, p. 104):
>
> ...in each case some ultimate measuring instruments, like the scales and clocks which determine the frame of space-time coordination – on which, in the last resort, even the definitions of momentum and energy quantities rest – must always be described entirely on classical lines, and consequently kept outside the system subject to quantum mechanical treatment.
>
> The point is that we can treat a measuring apparatus (or part of this) as a quantum system, but only when some other system is then treated classically. (Zinkernagel, 2006, p. 5)

Zinkernagel's and Saunders's reading of Bohr seems to go along similar lines as the one being presented here, as is the case with the previous quotation from Teller (see page 8). Teller mentions that, according to Bohr, even if we have the possibility of describing quantum mechanically the immediate macroscopic measuring device (i.e. the part of the instrument in interaction with the object under investigation), we have to describe classically some further part of the experimental arrangement. Saunders stresses the need of a material frame of reference (bodies of arbitrarily large mass) to describe any experiment, and, quoting Bohr, that this material frame of reference must be described by classical dynamics. Zinkernagel quotes Bohr saying that the material frame of reference must be described entirely by classical dynamics and taken to be outside the system subjected to a quantum mechanical description (in an hypothetical revision of Howard's approach this might imply taking from the start the material frame of reference to be disentangled from the quantum system).

I think it is fair to say that we are all reading Bohr as implying the need for a classical physics account of (at least) part of the experimental arrangement (the one not directly in interaction with the quantum system), stressing in particular the need for a classical account of the reference frame. This view is clearly at odds with Howard's. Howard's reconstruction implies an all-quantum description of the entangled pair instrument & object, giving just a classical description (in Howard's sense), for both the instrument and object, of the property being measured. On the reconstruction being presented here (which I must stress is compatible with the interpretation being given to the quantum postulate), according to Bohr, we must describe classically[58] the material frame of reference, taken to be independent[59] from the object of observation. In this way

[58] In the sense of using classical theories, not in Howard's sense.

[59] In my sense this means not in direct interaction; in Howard's sense it might mean disentangled.

I consider Howard's, nevertheless very interesting, reconstruction of Bohr's interpretation of quantum mechanics to be incompatible (at least as it stands at the moment) with Bohr's conception of space and time in quantum mechanics (related to an operationally defined and classically described reference system). In exact opposition to Howard's views, Bohr's doctrine of a classical space and time implies treating classically (in the usual sense) the parts of the measuring apparatus that are not in interaction with the quantum system.

4 Conclusions

In the quantum theory we can only recover a temporal description of the behavior of physical systems when considering an ensemble of identically prepared systems that are subjected to similar experimental arrangements. In fact, we cannot from one single system have a well-defined sense of temporal flow. This might lead one to consider that there is a tension between the idea of a continuous time and the discontinuous jumps between the possible states of a quantum system. In part the tension is avoided by constructing the theory considering a background space-time on which it is not the temporal behavior of an individual system – due to the discontinuity – that is described but the temporal behavior of an ensemble. Another related point is that the discontinuity is implemented in the theory already with the previous 'input' of a background time, that is, we talk about discontinuous changes as implied in the quantum postulate from the perspective of a macroscopic continuous space-time related to the experimental arrangement from which it looks as if the quantum system has discontinuous changes. As Bohr stressed, the point is that, as a consequence of the quantum postulate we cannot regard the physical properties of the quantum system as intrinsic and independent of the experimental arrangement being used (with its related classical reference frame). According to Bohr:

> No result of an experiment concerning a phenomenon which, in principle, lies outside the range of classical physics, can be interpreted as giving information about independent properties of the object; but is inherently connected with a definite situation in the description of which the measuring instruments interacting with the objects also enter essentially. (Bohr, 1939b, p. 269)

> While within the scope of classical physics we are dealing with an idealization, according to which all phenomena can be arbitrarily subdivided, and the interaction between the measuring instruments and the object under consideration neglected, or at any rate compensated for, it was stressed that such interaction represents in quantum physics an integral part of the phenomena, for which no separate account can be given if the instruments shall serve the purpose of defining the conditions under which the observations are obtained … The characteristic new feature in quantum physics is merely the restricted divisibility of the phenomena, which for unambiguous description demands a specification of all significant parts of the experimental arrangement … the whole purpose of the formalism of quantum theory is to derive expectations for observations obtained under given experimental conditions. (Bohr, 1962b, pag. 91-92)

In this way the characterization of the discontinuous behavior of the quantum system, that is, of the phenomena being observed, rests on the previous notion of a time coordinate (associated with clocks that are part of the measurement apparatus). We have no intrinsic notion of discontinuity by itself; this notion arises in the context of a theory that, following Bohr's view on the interpretation of the formalism, does not treat the phenomena we observe and relate to a 'quantum object' (like for example an electron) with something that has a meaning independent of the experimental arrangement that permits its observation. We have a discontinuity in the context of an operational notion of a continuous time that is simultaneously inscribed in the formalism of the theory as

an external parameter in the Schrödinger equation. It is from the perspective of this external time, which we use in the description of the functioning of any measurement apparatus, that the discontinuity we associate with the phenomena appears, simultaneously with a statistical description of the (continuous) temporal behavior of an ensemble of equally prepared systems.

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