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Treatment of continuum in nuclear reactions involving weakly bound systems. A simple model to test different prescriptions describing the coupling to continuum states.

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Abstract. We exploit a model describing the break-up of weakly-bound nuclei that can be used as a laboratory for testing different prescriptions that have been advanced in the literature to take into account the near-by presence of continuum states. In the model we follow the evolution of a single particle wave function in one dimension, initially bound by a Woods-Saxon type potential and then perturbed by a time- and position-dependent external field. Proper choices of this potential can simulate the effect of the interaction between reaction partners in a nuclear collision. These processes generate inelastic excitation probabilities that – distributed over the bound and continuum states of the system – lead to either a partial or a total fragmentation of the final wave function. The comparison with the exact calculations shows that standard coupled channel descriptions based on discretization of the continuum can be accurate only when a proper choice is made of the number of discrete states, of the energy mesh and of the energy cutoff. This may imply, even in simplified cases, the use of a rather large (and unpracticable) number of channels. The use of a more restricted number of channels may lead to misleading results.

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INTRODUCTION

For much longer than a decade we have witnessed a sustained interest in reactions involving weakly-bound nuclear systems. In particular those with projectiles or targets close to the nucleon evaporation lines; under such conditions a sudden ejection of one (or more) of their constituent nucleons may take place. These so-called break-up processes are very important and they have forced us to re-examine closely the role played by the continuum of asymptotically open states which lay close to the particle-emission threshold. From the point of view of reaction theory we are no longer talking about a simple binary process but of a quite complex situation that, if strictly approached, would put to a severe test anyone's expertise in the handling of nuclear reaction formalisms.

It is in the nature of things, however, that people immediately made simplifying assumptions and proceeded to implement detailed calculations for the process right away. These did not just aim to yield simple estimates of the cross sections but have led to quantitative predictions as well. In retrospective – and with benevolence – one can argue that such early analyses fulfill the double purpose of identifying ingredients

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of interest and of testing the possibilities of different formalisms to reproduce the orders of magnitude shown by the measured cross sections.

In this type of studies one should not, however, be guided exclusively by the ability of a given prescription to produce good fits to the experimental data. When unfamiliar approximations are involved (even if they appear obvious and reasonable) it is imperative to check the extent to which they are suitable to function within the new context. To this end one must construct alternative solutions of the problem that are far less objectionable and test thoroughly the consequences of their implementation.

One certainly wishes to avoid in the study of break-up phenomena some of the mistakes incurred in other fields. By the uncontestable fact that the number of continuum states is indeed infinite, *every* single calculation performed so far with a coupled-channel formalism had to resort to some discretization (better or worse) of the space of scattering states. The computing power available at present has normally limited the positive energy states to be accounted for by at most a double-digit number of channels. Is this enough? What can we expect to believe of the results obtained from a calculation performed in a such a restricted space? The shape of the wavefunction representative of the process? The predicted Q-value distribution? Can we develop some feeling about the size of the energy bins that may be appropriate? And what about the effective truncation of the basis to a maximum energy value?

The present contribution is motivated and ellaborated in the spirit of the considerations sketched above. The model we shall soon describe is rather simple. Yet, we trust that it incorporates enough of the correct ingredients to allow for the extrapolation of its findings to other realistic situations. We rush to state that this is not by any means the first time that a time-dependent approach is used in the context of nuclear break-up processes [1]. But we have deliberately restricted ourselves to examine the results extracted from this scheme in close correspondence with those of its coupled-channel counterpart in a *totally equivalent problem*. This has provided us with a solid tool to judge the reliability of the latter technique. After all that is – unavoidably and for the foreseeable future – the only formulation that will be sistematically used for the actual interpretation of experimental data. It is precisely the possibility of investigating *any* aspect of the problem from the two distinct perspectives (and under controlled circumstances) that lends true value to our exercise.

FORMULATION OF THE MODEL AND ITS DIRECT SOLUTION IN THE TIME-DEPENDENT APPROACH

We start illustrating a simple model that can provide for us an adequate representation of a one-nucleon break-up process. Let us briefly review some of the elements that guide our search. The problem posed should admit solutions in terms of a coupled-channels formalism which resorts to a discretization of the continuum. This is, after all, the situation whose soundness we set out to test and have listed as the main motivation of the whole exercise. But, clearly, it should nevertheless be possible to generate the evolution of the wavefunction in an alternative manner, unaffected by a questionable handling of the continuum. To such solutions one could then assign the label of "exact" and they would become the standards of reference to compare with coupled-channels

results. The model should also be simple, so that its solutions turn out to be fast and easy to construct. This is because we intend to use it as the basic source for the numerous checks required to explore different aspects of the two alternative schemes.

Incorporating all the elements listed above, in what follows we set to describe the evolution of a single-particle wavefunction $\Psi(x,t)$, initially a bound eigenstate of the one-dimentional Woods-Saxon potential

$$V(x) = \frac{V_0}{1+\exp[(|x|-R)/a]} \tag{1}$$

and perturbed by a space- and time-dependent interaction

$$V_{coup}(x,t) = V_C \exp(-t^2/2\sigma_t^2) \exp(-(x-x_0)^2/2\sigma_x^2) \ , \tag{2}$$

As we can see, the coupling is for simplicity assumed to be of gaussian shape. We note, however, that this is not really essential and the expression (2) can be easily changed – within the present implementation of the model – to any other functional dependence as long as it stays separable. The potential $V_{coup}(x,t)$ is meant to simulate the inelastic excitation fields resulting from a collision between two heavy ions. In particular, adjusting the widths σ_t, σ_x, the asymmetry parameter x_0 and the overall strenght V_C one is able to mock up realistic situations that arise from different collision times, bombarding energies, interaction ranges, distances of closest approach, impact parameters, etc.

The evolution of the wavefunction follows, naturally, from the time-dependent Schroedinger equation

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} \ = \ \left[H_0(x) + V_{coup}(x,t)\right] \Psi(x,t) \ , \tag{3}$$

where

$$H_0(x) \ = \ -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial x^2} \ + \ V(x) \tag{4}$$

can be identified as our "unperturbed" hamiltonian. The equation has to be solved (numerically) supplying, as an initial condition at time $t = t_0$, the wavefunction $\Psi(x, t = t_0)$. According to what it was previuously stated we take as the initial state for the time-dependent integration precisely one of those bound eigenstates of the unperturbed hamiltonian $H_0(x)$

An example of solution of the time-dependent equation is shown in Fig. 1, where the N=3 bound state is chosen as the initial configuration and the perturbing external interaction is chosen to be strong enough to generate excitations to the continuum.. It can be immediately seen, in fact, that, evolving in time, a major fraction of the wave function "escapes" the potential well by populating unbound states in the continuum. This can be interpreted as describing final break-up events. As the, now stronger, perturbation was chosen asymmetric ($x_0 \neq 0$), breakup probabilities are different in one direction or the other. We can also see that a fraction of the wave function remains localized in the potential region, corresponding to some finite probability of populating only bound states. The situation can therefore be interpreted as describing a *partial* breakup process. Going

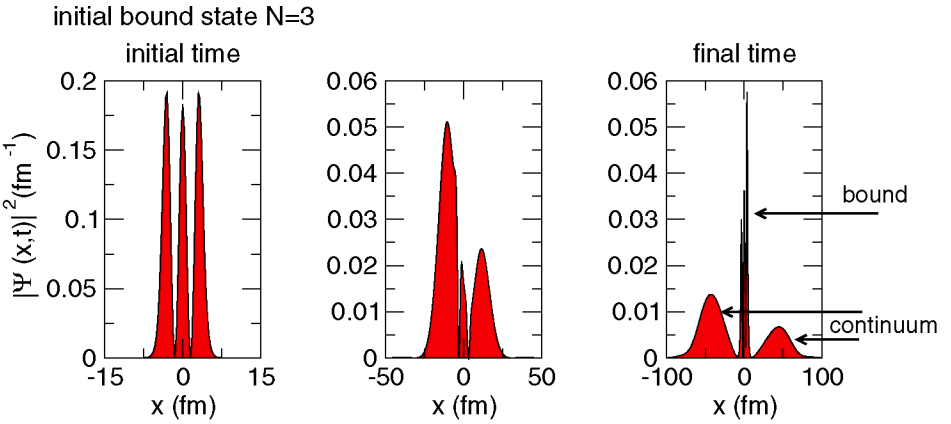

FIGURE 1. Time evolution of the square of the wave function. An asymmetric perturbation has been used, and the initial configuration corresponds to that of the N=3 bound state. Note the increasing range of the abcissas in the different frames; this is necessary to accomodate a distribution of probability that has began to expand outwards, both to left and right.

towards the "left" or towards the "right" is the equivalent, in one dimension, to breaking up emitting the fragment into different orientation angles. The actual situation in the ordinary three-dimensional space is reconstructed – as it was previously mentioned – from the expansion of the incident flux in angular momentum (partial wave) components.

The solution of the problem so far has not involved an expansion of the time dependent wave function into any basis of single-particle states. In particular, it has not yet been necessary to introduce explicitly any scattering states, since continuum effects are automatically incorporated in $|\Psi(x,t)|^2$. In cases involving emerging fragments, however, one might like to predict not only the total break-up probability but also learn about the Q-value distribution of the emitted nucleons. To this end one needs to expand the final wave function into a complete set of energy eigenstates of H_0 including, of course, those lying in the continuum. The resulting continuum Q-value distribution is shown in Fig.2.

COUPLED-CHANNEL APPROACH

As an alternative to the direct numerical solution of the time-dependent Schroedinger equation one can resort to the familiar coupled-channel formalism, where the Schroedinger equation is solved by expanding the total wave function in a basis of eigenstates $\Phi_n(x,t)$ of the hamiltonian H_0. This is the preferred approach in most situations, where the direct numerical solution of the full time-dependent many-body wave function is very complicated. For these reasons it is also the conventional approach that is used in most of the current computer codes available in the market. We will use here a simplified version of the coupled-channel scheme, adapted to our one-dimentional problem.

If the basis states are identified with the eigenstates of a finite potential, the complete

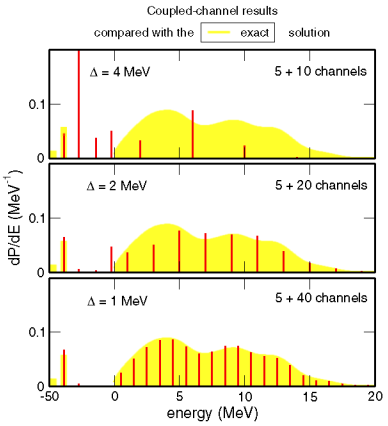

FIGURE 2. Case of partial break-up starting from a well-bound orbital (N=3). Comparison of final Q-value distribution obtained in the exact calculation and with the discretized continuum. In the later case, different energy meshes are used in the different frames. The energy cut-off was fixed at 20 MeV.

set of states necessarily includes the discrete bound states but also the continuum states at positive energies. This is indeed the case of the potential considered in this work. In our context – and using the positive energies E as a label for the continuum states, $\Phi(E,x)$ – the expansion of the full wave function does in fact incorporate continuum amplitudes $a(E,t)$ in the form

$$\Psi(x,t) \;=\; \sum_{N=1}^{\infty} a_n(t)\Phi_n(x) + \int dE \Big(a_-(E,t)\;\Phi_-(E,x) + a_+(E,t)\;\Phi_+(E,x) \Big) \qquad (5)$$

having taken into account that for each positive energy E there are two independent solutions. We have chosen these, quite naturally, as the solutions of the scattering problem at energy E with boundary conditions of incoming plane wave from the left (Φ_-) and from the right (Φ_+).

With the full (bound plus continuum) basis the standard coupled equations for the discrete part of the amplitudes, $a_n(t)$

$$i\hbar\dot{a}_n = \sum_{m=1}^{\infty} \mathrm{e}^{-i(E_n - E_m)t} < \Phi_n | V_{coup}(t) | \Phi_m > a_m(t) \qquad (6)$$

has to be generalized to now include terms that not only couple to the other discrete amplitudes but also to the continuum ones. In addition, we have other analogous coupled equations for the continuum ampliudes $a_\pm(E,t)$.

So far we have not performed any sort of energy discretization. But in order to solve the continuum differential set of equation it is imperative to reduce the channels to a finite (preferably small) number. Different prescriptions have been proposed to provide a discrete basis. A first, simple, procedure consists in slicing the energy continuum in equally-spaced bands. Each slice, assumed to be associated to a single state, is then

chosen to be represented by the true continuum wave function corresponding to the central energy of the band. The norm of each of those effective, discrete "states" must be weigthed by a factor $\sqrt{\Delta E}$ to restore correct units for the distribution of continuum probabilities over the chosen energy mesh of size ΔE. In a second popular procedure [2], normally used in CCDC codes, again each slice is made to corresponds to a single state. But this time the effective configuration is obtained by *averaging* over the continuum states in the interval ΔE with some weighting function $w(E)$.

An example of the comparison between the "exact" results and those obtained within the coupled-channel approximation is given in Fig. 2, for different choices of the energy mesh (and consequently different number of basis states). The comparison focuses on the Q-value distribution of the final break-up wave function. In the former case this is obtained by projecting the final wave function on the set of basis states (bound plus continuum). For the positive energy part this gives rise to a continuum Q-value distribution (reported as the solid yellow curves), without the need of actually implementing a continuum discretization. In the coupled-channel approach, on the other hand, the projection is done over the discretized states we consider and are directly given by the final amplitudes a_n. The corresponding Q-value distribution will therefore consist of discrete lines, whose number and position will depend on the parameters of the discretization model. We can see from the figure that even in this unidimensional case a number of dozens of channels is needed to give a proper account of the process. No significant difference was found by using either procedure for the discretization.

Further examples can be found in Ref. [3, 4, 5], where different situations have been considered. We can summarize these results by stating that the comparison with the exact calculations shows that standard coupled channel descriptions based on discretization of the continuum can be accurate only when a proper choice is made of the number of discrete states, of the energy mesh and of the energy cutoff. This may imply, even in simplified cases, the use of a rather large (and unpracticable) number of channels. The use of a more restricted number of channels may lead to misleading results.

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