

A method of continuum discretization and its application to the scattering of weakly bound nuclei

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In this contribution we present the formalism of a recently proposed procedure of continuum discretization for the description of the scattering of weakly bound nuclei. Convergence checks are presented for some relevant sum rules, using as a representative example the deuteron. Finally, we apply the method to the case of deuteron elastic scattering and breakup, comparing the results with those of the standard method of coupled channels continuum discretization.

Keywords: Continuum discretization; scattering; weakly bound nuclei

En esta contribución presentamos el formalismo de un procedimiento propuesto recientemente de discretización del continuo para la dispersión de núcleos poco ligados. Se presentan asimismo varios tests de convergencia para algunas reglas de suma relevantes, usando como ejemplo representativo el deuterón. Finalmente, aplicamos el método al caso de dispersión elástica y de fragmentación de deuterio, comparando los resultados con los obtenidos a partir del método standard de discretización del continuo (CDCC).

Descriptores: Discretización del continuo; dispersión; núcleos débilmente ligados

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1. Introduction

In recent years, many of the efforts in Nuclear Physics have been devoted to the experimental and theoretical study of nuclei close to the drip lines. For these nuclei new structures are being observed challenging the established nuclear structure models. Nowadays, our main source of information of these exotic nuclei is through scattering experiments in which accelerated beams of radioactive nuclei are collided with stable targets. An important consideration of these experiments is that exotic nuclei are often very weakly bound systems and, consequently, they present a high probability of breakup in the Coulomb and nuclear fields of the target nucleus. Thus, in order to extract reliable information on nuclear structure from reaction experiments it is essential to include in the formalisms the coupling to continuum states.

Of special interest are the so called halo nuclei, which are very weakly bound systems with one or two outer particles with a high probability of exploring the classically forbidden region.

Reaction calculations where breakup couplings are included have the additional complication that breakup states are not square-normalizable. This problem is frequently overcome by replacing the states in the continuum by a finite set

of normalized states. Convergence checks with respect to the number of states considered or the parameters characterizing these states are required in order to make the method reliable.

Several methods have been developed to obtain a finite basis of normalized states to describe the continuum. Probably, the most widely used of these approaches is the method of continuum discretization coupled channels (CDCC) [1]. The method is based on the partition of the continuum into a set of energy intervals (bins). Each bin is characterized by a single radial wave function, which is obtained as an average of the continuum wave functions over the bin. In this averaged radial wave function, the oscillations of the different components tend to cancel beyond a certain distance, and so the bin radial wave function becomes normalizable. Then, for each bin, a representative normalized square integrable relative motion wave function of the form

$$\psi_{i,\ell m}(\mathbf{r}) = \frac{\phi_{\ell}^i(r)}{r} Y_{\ell m}(\hat{r}), \quad (1)$$

is defined. Its radial wave function is a superposition of the scattering states $\tilde{\phi}_{\ell}(k)$ within the bin defined by the interval $\Delta k_i = k_i - k_{i-1}$, with a certain weight function $f_i(k)$, i.e.,

$$\phi_{\ell}^i(r) = \sqrt{\frac{2}{\pi N_i}} \int_{k_{i-1}}^{k_i} f_i(k) \tilde{\phi}_{\ell}(k, r) dk, \quad (2)$$

with $N_i = \int_{k_{i-1}}^{k_i} |f_i(k)|^2 dk$. For a non-resonant continuum, typically $f_i(k) = 1$, in which case $N_i = \Delta k_i$. In general, the integral (2) has to be solved numerically. This means that, for each bin function, $\phi_i^2(r)$, the CDCC method requires the solution of the Schrödinger equation for many values of k .

For the calculation of scattering observables it is also necessary to consider the coupling between the ground state and the continuum bins, and between the bins themselves, due to the nuclear and Coulomb potential. In practice, this commonly leads to a set of coupled equations for all the values of i and ℓ . In order to make the number of equations finite, it is necessary to perform a double truncation in both angular and linear momentum. Thus, the continuum is restricted to the subspace $0 \leq \ell \leq \ell_{\max}$ and $0 \leq k \leq k_{\max}$. To demonstrate convergence in a CDCC calculation it is necessary to check that the calculated scattering magnitudes are not modified when increasing maximum energy (k_{\max}) and angular momentum (ℓ_{\max}) or when decreasing the bin widths, Δk_i .

Despite the limitations cited above, the CDCC has been successfully applied to a large number of nuclear reactions and it is one of the most reliable approaches to the study of reactions involving binary composite systems. The aim of the Transformed Harmonic Oscillator (THO) method is to construct a finite set of normalized and orthogonal states which can be used as an alternative representation of the continuum spectrum of a weakly bound nucleus and that overcomes or, at least, reduce some of the limitations of other discretization procedures, such as the CDCC.

The present paper is structured as follows. In Sec. 2 the basic ideas of the THO method are presented. Section 3 is devoted to show results for some structure sum rules for transitions involving the bound state and the continuum for the deuteron. In Sec. 4 we apply the method to describe some scattering observables of the reaction $d + {}^{208}\text{Pb}$ at 50 MeV, comparing the results with the standard CDCC method. Finally, Sec. 5 is left for conclusions.

2. The THO method

The THO presented here was first formulated and applied to simple one dimensional problems [2]. Subsequently, it was extended to the three dimensional case and successfully applied to describe global structure magnitudes related to the coupling of the continuum [3] and scattering observables [4]. In the present work, we will concentrate on the formulation of the method in the three dimensional case and its application to deuteron structure and scattering.

In both the one- and three-dimensional cases, the standpoint of the method is to define a local scale transformation (LST) [5] which is such that converts the bound state wave function of the weakly bound system, represented by $\phi_b(r)$, into a harmonic oscillator (HO) wave function. The function, $s(r)$ defining the LST is given by

$$\phi_b(r) = \sqrt{\frac{ds}{dr}} \phi_0^{\text{HO}}[s(r)]. \quad (3)$$

Once the $s(r)$ is known, a set of orthogonal wave functions, the THO basis, is generated by applying the same LST used for the ground state to the rest of HO wave functions, *i.e.*,

$$\phi_n^{\text{THO}}(r) = \sqrt{\frac{ds}{dr}} \phi_n^{\text{HO}}[s(r)]. \quad (4)$$

Due to the simple analytical structure of the harmonic oscillator wave functions, this is equivalent to multiply the ground state function by the appropriate orthogonal polynomials $P_n(s)$ [4]

$$\phi_n^{\text{THO}}(r) = P_n[s(r)]\phi_b(r). \quad (5)$$

Notice that the new functions $\phi_n^{\text{THO}}(r)$ are orthogonal by construction and constitute a complete set. Also, they decay exponentially at large distance, thus reproducing the correct asymptotic behavior of the bound wave functions. However, in general, they are not eigenstates of the internal Hamiltonian. Then, one has to diagonalize the Hamiltonian using a truncated THO basis. As a result of the diagonalization a new set of functions, $\{\phi_k^N(r); k = 0, \dots, N\}$, with eigenvalues $\epsilon_0, \dots, \epsilon_N$ are generated. Here, $N + 1$ is the number of functions retained in the THO basis, $k = 0$ standing for the ground state. Thus $\phi_0^N(r) = \phi_0^{\text{THO}}(r) = \phi_b(r)$ and so $\epsilon_0 = \epsilon_b$, while the rest of eigenstates lie at positive energies and they constitute our representation of the continuum.

3. Convergence of the method

In order to check the adequacy of the THO method, we evaluate in this section several sum rules which involve the coupling of the ground state with the continuum wave functions. In particular, we will focus in the case of the deuteron. For the sake of simplicity, we consider a simple scenario in which the deuteron ground state is assumed to be in a pure $\ell = 0$ state and only the s -wave continuum is considered.

The proton-neutron interaction is described by means of the Poeschl-Teller potential,

$$V(r) = -D \frac{1}{\cosh^2(\alpha r)}, \quad (6)$$

with the depth (D) and range (α) adjusted to reproduce the experimental binding energy and rms of the deuteron: $D = 102.73$ MeV and $\alpha = 0.9407$ fm⁻¹.

Once the ground state wave function is obtained, the set of THO functions are calculated using Eq. (5). Finally, the deuteron Hamiltonian is diagonalized in a truncated THO basis. The resulting eigenfunctions are represented in Fig. 1. It is interesting to study the systematic of the eigenvalues with respect to the basis dimension. This is illustrated in Fig. 2, where the energy levels resulting from the diagonalization are schematically represented versus the basis dimension $M = N + 1$. In the case of the deuteron (which is also

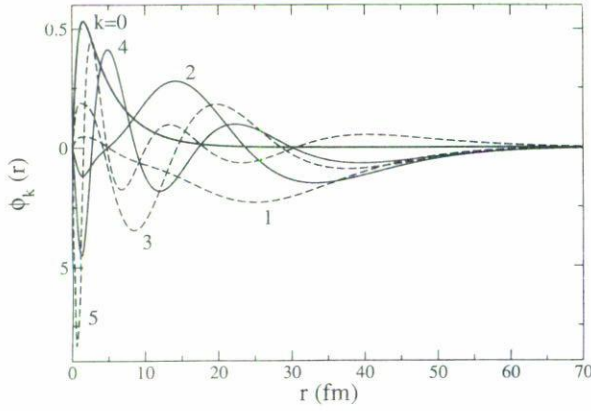


FIGURE 1. Radial part of the functions: $\phi_k^N(r)$, $k = 0, \dots, 5$ that result from the diagonalization of the deuteron Hamiltonian (using a Poeschl-Teller potential) in the THO basis. The parameters of the potential are adjusted to give to binding energy and rms of the deuteron.

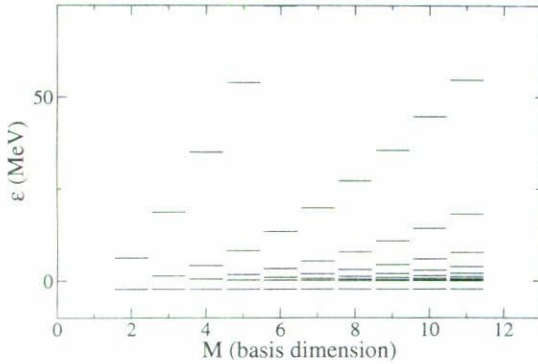


FIGURE 2. Energy levels resulting from the diagonalization of the deuteron Hamiltonian in the a truncated THO basis versus the basis dimension.

the case of other interesting systems, such as many halo nuclei) there is only one bound state. Accordingly, the diagonalization of the Hamiltonian in the THO basis gives rise to a eigenstate with eigenvalue $\epsilon_0 = \epsilon_b = -2.22$ MeV (actually, the deuteron ground state) and a set of positive eigenvalues, which are taken as a representation of the continuum. Another interesting property is that the positive eigenvalues do not appear uniformly distributed along the continuum, but concentrated above the threshold. As we shall see in the next section, this property has notable consequences when the method is applied to scattering problems.

As a first check to evaluate the reliability of the THO basis to represent the continuum, we have calculated the following sum rules which depend on the coupling between the ground state and the continuum states for a given operator O :

- Total Strength (TS): $TS(O; N) = \sum_i |\langle N i | O | N 0 \rangle|^2$
- Energy Weighted Sum Rule (EW): $EW(O; N) = \sum_i (\epsilon_i^N - \epsilon_b) |\langle N i | O | N 0 \rangle|^2$
- Polarizability (PO): $PO(O; N) = \sum_{i \neq 0} (\epsilon_i^N - \epsilon_b)^{-1} |\langle N i | O | N 0 \rangle|^2$

TABLE I. Convergence of the total strength (TS), energy weighted sum rule (EW) and polarizability (PO) for the local operator $O(r) = r$ as a function of the size of the THO basis, $M = N + 1$. Lengths are given in units of α^{-1} and energies in units of $(\hbar^2 \alpha^2 / 2\mu)$.

M	TS($O; N$)	EW($O; N$)	PO($O; N$)
4	12.9070	0.9586	35.6318
6	12.9075	0.9713	35.7034
8	12.9078	0.9819	35.7081
10	12.9080	0.9880	35.7083
Exact	12.9082	1.0000	35.7083

TABLE II. The same as in Table I, but for the short range operator $O(r) = V(r)$.

M	TS($O; N$)	EW($O; N$)	PO($O; N$)
3	0.4252	0.1126	0.551771
6	0.4883	0.4676	0.551867
9	0.4978	0.6906	0.551868
12	0.5012	0.7737	0.551869
14	0.50142	0.7925	0.551869
Exact	0.501464	0.803147	0.551869

The summations run from 0 to N . We have used the abbreviated notation: $|N i\rangle \equiv |\phi_i^N\rangle$. Two different operators have been considered: a long range operator, $O(r) = r$, to describe effects of long-range external fields, such as the Coulomb potential, and a short-range potential, $O(r) = V(r)$, to describe couplings associated with the nuclear interaction.

In Tables I and II we present the calculated sum rules for different values of N , along with the exact results for $N \rightarrow \infty$. The latter were obtained from the expressions:

- $TS(O) = TS(O; N \rightarrow \infty) = \int dr |O(r)\phi_b(r)|^2$
- $EW(O) = EW(O; N \rightarrow \infty) = \int dr \left| \frac{dO(r)}{dr} \phi_b(r) \right|^2$
- $PO(O) = PO(O; N \rightarrow \infty) = \frac{1}{2} \frac{d^2}{dt^2} \langle \phi_0(t) | H - \epsilon_b | \phi_0(t) \rangle$,

where $|\phi_0(t)\rangle$ represents the ground state for a perturbed Hamiltonian $H(t) = H + tO(r)$.

Comparing the exact values with those for finite N we find that the convergence of the method is very satisfactory. It remains to assess the adequacy of the THO basis to represent properly the continuum in the description of scattering processes. It is important to note that these processes involve not only ground state to continuum transitions but also continuum-continuum couplings.

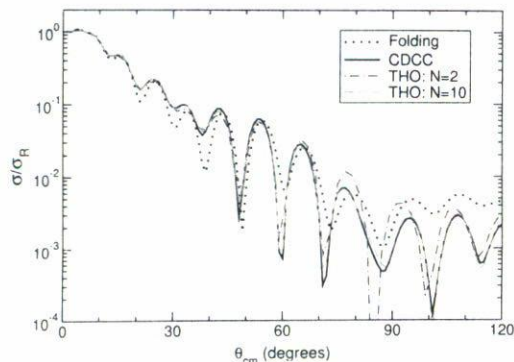


FIGURE 3. Elastic scattering differential cross sections (as ratio to Rutherford cross section) for the reaction $d + {}^{208}\text{Pb}$ at 50 MeV. The dotted line is the Watanabe folding potential. The solid line is the CDCC calculation. The dotted-dashed and dashed lines represent the THO calculation with $N = 2$ and $N = 10$ states, respectively.

4. Application to deuteron scattering

In this section we apply the THO formalism to the reaction $d + {}^{208}\text{Pb}$ at 50 MeV for which standard CDCC calculations revealed that the deuteron continuum is relevant.

We used the same binding potential as in the previous section. The proton-target and neutron-target interactions were described in terms of optical potentials, using the Becchetti-Greenless parameterization [6], evaluated at half of the deuteron incident energy. Only the coupling to s -wave breakup states was considered. Moreover, we neglect Coulomb breakup and thus we assume that the Coulomb interaction between the projectile and target has only a monopole part. Due to these restrictions, we will compare our results with those of the CDCC calculations, instead of experimental data.

Using the set of wave functions $\{\phi_k^N(r); k = 1, \dots, N\}$ as a representation of the continuum, the scattering calculation is equivalent to a standard coupled channels calculation for bound states. In both cases, namely the THO and CDCC methods, we have solved the coupled channels equations using the computer code FRESKO [7]. In order to achieve convergence of the CDCC, a maximum excitation energy of $\epsilon_{\text{max}} = 30$ MeV was considered. This energy interval was divided in 10 bins of uniform width in k .

In Fig. 3 we present the differential elastic cross section angular distribution. The dotted line corresponds to the calculation with the Watanabe folding potential. This is obtained by folding the proton-target and neutron-target potentials in the ground state of the deuteron and, therefore, ignores completely the deuteron continuum. The solid line is the converged CDCC calculation. The differences with the folding calculations give an insight of the importance of the continuum at the different angles. The dashed line corresponds to the THO calculation with $N = 10$ continuum states, for which convergence was achieved. It is noticeable the excellent agreement between the THO and the CDCC. We present also a THO calculation with $N = 2$ continuum states, which gives already a very reasonable description of this observable.

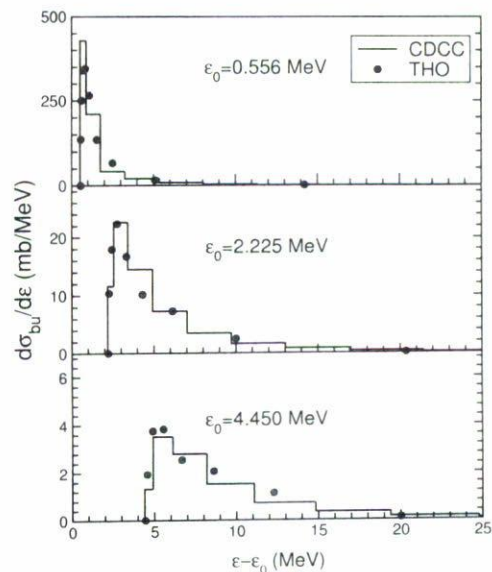


FIGURE 4. Breakup cross section as a function of the excitation energy of the deuteron, ϵ , for the reaction $d + {}^{208}\text{Pb}$ at 50 MeV, and three different values of the deuteron binding energy: $\epsilon_b = 0.556$ MeV (upper panel), $\epsilon_b = 2.226$ MeV (middle panel) and $\epsilon_b = 4.45$ MeV (bottom panel), the second one corresponding to the physical value. The histograms corresponds to the CDCC calculations and the dots to the THO with $N = 10$.

In Fig. 4 the breakup cross section as a function of the excitation energy of the deuteron is depicted for the CDCC and THO approaches. In the CDCC case, this distribution is obtained dividing the cross section for each bin by the width of the bin. In the THO case, it is obtained dividing the cross section of each continuum state, corresponding to an energy ϵ_i , by an energy width which is given by $(\epsilon_{i+1} - \epsilon_{i-1})/2$. The THO calculations were performed with $N = 10$ states. The calculations of the central panel were carried out with the experimental value, $\epsilon_b = -2.22$ MeV. It is noticeable that the eigenvalues associated with the THO states tend to concentrate within the continuum region where the breakup results are more important and vary more abruptly. This distinctive feature permits an adequate description of the breakup distribution with a relatively small number of continuum states, without the need of adjusting by hand the bins widths, as in a typical CDCC calculation.

In order to check the generality of this result, we have performed test calculations in which the binding energy of the deuteron is artificially reduced or increased with respect to its experimental value. In the first case (upper panel), there is an increment in the breakup probability, and the maximum of the distribution approximates to the breakup threshold. This behavior is perfectly accounted for by the distribution of THO states. On the other side, when the binding energy is incremented (lower panel), the breakup probability decreases and the distribution becomes smoother. Again, the THO states distribute according to this behavior, giving a very reasonable description of the breakup distribution.

5. Conclusions

In conclusion, we have shown in this contribution that the continuum discretization developed in Refs. 2–4 and discussed here is a reliable alternative to other methods of continuum discretization.

An attractive feature of this method is its simplicity. The construction of the continuum basis only requires the knowledge of the ground state, either analytically or numerically. Then, the THO basis is obtained just by multiplying this ground state by the appropriate set of orthogonal polynomials. Finally, the wave functions that represent the continuum are obtained by diagonalization of the Hamiltonian in the THO basis. Thus, the calculation does not require the integration of the Schrödinger equation to obtain the continuum states. Moreover, the convergence of the method is controlled by only one integer parameter, the basis dimension. This

is in contrast with the CDCC method, for which convergence with respect to several parameters has to be checked. The tests performed in the case of the deuteron structure and scattering suggest that the present method can be considered as a reliable tool to model the scattering involving loosely bound nuclei.

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