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Coupling to breakup channels using a transformed harmonic oscillator basis

A. M. Moro,[1,3] J. M. Arias,[1] J. Gómez-Camacho,[1] I. Martel,[2] F. Pérez-Bernal,[2,*] R. Crespo,[3] and F. Nunes[4]
[1]*Departamento de FAMN, Universidad de Sevilla, Apartado 1065, E-41080 Sevilla, Spain*
[2]*Departamento de FAIE, Universidad de Huelva, E-21071 Huelva, Spain*
[3]*Departamento de Física, Instituto Superior Técnico, Av. Rovisco Pais, 1049-001 Lisboa, Portugal*
[4]*Universidade Fernando Pessoa, Praça 9 de Abril, 4200 Porto, Portugal*
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The application of a recently proposed procedure for discretizing the continuum to collision processes involving weakly bound nuclei is studied. In particular, the coupling to breakup states in the collision of $d + {}^{208}$Pb at 50 MeV is discussed. For illustrative purposes, only the *s*-wave component of the bound state of the deuteron is considered, and the study is restricted to the case of nuclear *s*-wave breakup. The continuum discretization procedure provides a basis of transformed harmonic oscillator wave functions to accomplish the necessary calculations. Appropriate convergence of the elastic and breakup cross sections with increasing dimension of the basis is reported. In addition, it is shown that the results obtained converge to those of a standard continuum discretized coupled channels calculation, with the advantage that the convergence of the method is determined by only one parameter, namely the dimension of the basis.

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The development of radioactive beam facilities has shed light on a variety of new nuclear structure problems [1] which include neutron and proton rich nuclei close to the drip lines, and in particular halo nuclei. Given that these are weakly bound systems, their modeling should necessarily include in some way the continuum part of the spectrum. This becomes essential when studying nuclear collisions, where the inclusion of the coupling to breakup channels is not only necessary for the description of processes leading to fragmentation, but also when dealing with elastic scattering or transfer reactions.

Reaction calculations where breakup couplings are included have the additional complication that breakup states are not square-normalizable. This problem is generally surmounted replacing the states in the continuum by a finite set of normalized states, and proving that the calculation of scattering observables in the finite basis converges when increasing the number of states considered, or when modifying the parameters which define the normalized states.

Several procedures have been developed to obtain a finite basis of normalized states which describes the continuum. One of the most widely used of these approaches is the method of continuum discretization coupled channels (CDCC) [2]. It consists in discretizing the continuum by means of taking fixed intervals, or bins, of k values. 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. Formally, the CDCC method requires the solution of the Schrödinger equation for all (or, at least, many) energies in the continuum as a previous requirement to calculate the bin wave functions. Thus a practical CDCC calculation requires to fix the maximum k value considered and the interval Δk of the bins, so that the number of bins is given by $M = k_{max}/\Delta k$. To demonstrate convergence in a CDCC calculation one has to show that the scattering magnitudes are not modified with increasing maximum energy (k_{max}) or decreasing the interval Δk. However, when Δk is made smaller, the radius at which the bin wave functions vanish becomes larger, increasing the range of the coupling potential. As a consequence, CDCC calculations are typically very time consuming. In addition, as both Δk and k_{max} parametrize the basis, demonstrating convergence is by no means trivial (see [3] for a recent study of the convergence within CDCC). Despite these difficulties, the method has been successfully applied to a large number of nuclear reactions and is one of the most reliable approaches to reactions involving binary composite systems.

We have recently proposed the use of a transformed harmonic oscillator (THO) basis as an alternative to describe the effect of the continuum [4,5]. In Ref. [4] some applications to simple one-dimensional problems are presented and it is shown that, as the number of states in the THO basis increases, the eigenstates appear densely packed close to the breakup threshold, although some of them lie at higher energies. Besides, it is shown that global structure magnitudes related to the coupling to the continuum, such as sum rules, are very accurately described using relatively small THO basis states. In Ref. [5] this study was extended to the more realistic case of the deuteron, showing similar results to the one-dimensional case. In the present work, we show that the same ideas can be useful in the study of nuclear collisions involving weakly bound nuclei.

In the case of a three-dimensional problem under central forces, the relevant part of the wave function is the radial one, that can be written as $R(r) = \phi(r)/r$. In the following when referring to the wave function we always mean the radial function $\phi(r)$. The basic idea of the method presented in Ref. [4] is to define a local scale transformation [6] which converts the ground state wave function of a bound nucleus

*Present address: Center for Theoretical Physics, Yale University, New Haven, CT 06520-8120.

$\phi_b(r)$ into a harmonic oscillator wave function $\phi_0^{HO}(s)$. The function $s(r)$, which defines the local scale transformation, is given by

$$\int_0^r |\phi_b(r')|^2 dr' = \mathrm{erf}(s) - \frac{2s\exp(-s^2)}{\sqrt{\pi}}. \quad (1)$$

Next, one generates a set of orthogonal wave functions multiplying the ground state wave function by the appropriate polynomials $P_n(s(r))$,

$$\phi_n^{THO}(r) = P_n(s(r))\phi_b(r), \quad (2)$$

such that the state with $n=0$ coincides with the ground state, and the states with $n>0$ describe the continuum, or other bound states if they exist. From the three-dimensional HO wave functions [7]

$$P_n(s) = \frac{\pi^{1/4}}{2} \sum_{k=0}^{N} \alpha_{nk} s^{2k}, \quad (3)$$

$$\alpha_{nk} = \frac{(-1)^k}{k!} \frac{\sqrt{2(n!)\Gamma(n+3/2)}}{(n-k)!\Gamma(k+3/2)}. \quad (4)$$

Finally, one diagonalizes the Hamiltonian matrix using a finite basis of THO states: the resulting positive energy eigenstates are taken as continuum wave functions. Hereafter N denotes the number of continuum states obtained after diagonalization, thus the THO basis dimension is $N+1$.

The aim of this work is to investigate the adequacy of the THO basis for describing the effect of coupling to breakup states in nuclear reactions. For this purpose, we have considered a test case where the coupling to the continuum is relevant: the elastic scattering and breakup of $d+^{208}$Pb at 50 MeV. In order to study this process two ingredients are needed: the proton-neutron interaction and the interaction of the projectile constituents with the target. At this stage, we do not intend to do a full calculation of the effects of deuteron breakup nor compare with the experimental data but to show that the THO discretization method is an adequate theoretical tool for the modeling of reactions involving weakly-bound nuclei. As an illustration, we consider here a simple theoretical scenario: the deuteron is taken to be a pure s state, the effect of Coulomb breakup is neglected, and the nuclear interaction of the proton and neutron with the target induce the coupling to s-waves breakup states only. Within these restrictions, we perform a convergence study of the THO method and compare with the CDCC method. The realistic case, where the d component is incorporated in the ground state of the deuteron, and both Coulomb and nuclear breakup to $l\neq 0$ states are coupled in, will be presented in a more extensive publication.

Concerning the structure of the projectile, we describe the proton-neutron interaction by means of a Poeschl-Teller potential,

$$V(r) = -D\frac{1}{\cosh^2(\alpha r)}, \quad (5)$$

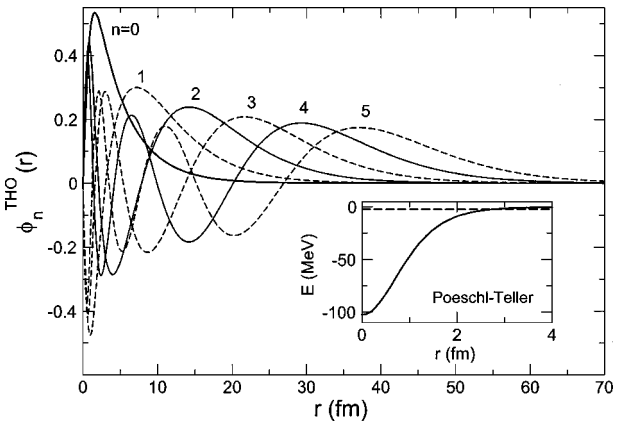

FIG. 1. Radial THO wave functions, $\phi_n^{THO}(r)$, with $n=0$ to $n=5$, obtained by means of the local scale transformation (1). The deuteron ground state wave function ($n=0$) is the solution of the Poeschl-Teller potential sketched in the inset, with parameters that reproduce the deuteron binding energy (marked with dashed line) and its root-mean-square radius.

with depth (D) and range (α) adjusted to reproduce the deuteron binding energy and mean square radius: $D=102.85$ MeV and $\alpha=0.9407$ fm^{-1}. A representation of this potential is shown in the inset of Fig. 1. The use of this potential provides an analytic ground state wave function for the deuteron, which is convenient, although not essential, for the calculations in the THO basis. The interaction of proton and neutron with the target is taken from the Becchetti-Greenless parametrization [8], evaluated at half of the deuteron incident energy. As mentioned above, only the coupling to s-wave breakup states is considered.

Once the ground state radial wave function is obtained by solving the Schrödinger equation with the appropriate potential, Eq. (5) in our case, the function defining the local scale transformation is obtained by direct integration of Eq. (1). With these two ingredients the THO wave functions can be generated by using Eq. (2). In Fig. 1 we present the THO basis functions, from $n=0$ to $n=5$. The wave function with $n=0$ is the *exact* wave function corresponding to the only bound state of the deuteron. It is observed that, as the number of nodes (n) increases, the wave functions extend to larger distances, but they all show a smooth behavior and decay exponentially. In principle the THO basis is infinite but one can truncate it to a finite dimension and study the convergence of different observables as a function of this dimension. In the present case, the internal deuteron Hamiltonian is diagonalized in a truncated basis and provides a finite set of normalized eigenstates which describe approximately the continuum. As in the CDCC, the procedure is useful only if the number of continuum states necessary to provide a good approximation to the converged result is small enough. It is worth to stress that uniquely the $n=0$ basis wave function is an eigenstate of the Hamiltonian, whereas the $n\neq 0$ basis states are not. Consequently the state $n=0$ is decoupled from the other states included in the basis.

In Fig. 2 the eigenstates of the Hamiltonian for the case of a truncated basis of six states ($N=5$) are plotted. It can be

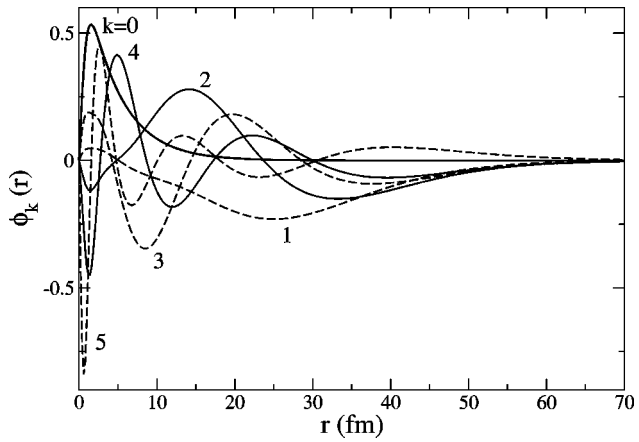

FIG. 2. Radial eigenfunctions of the Pöschl-Teller Hamiltonian, $\phi_k(r)$, with $k=0$ to $k=5$, obtained by diagonalizing the Poeschl-Teller Hamiltonian in a six-dimensional THO basis.

noted that the range of these $\phi_k(r)$ wave functions is determined by the range of the last state included in the THO basis. All eigenfunctions of the Hamiltonian present a smooth behavior and are normalized.

In Fig. 3 we present the energies of the deuteron Hamiltonian diagonalized in a THO basis as a function of the basis dimension. One can verify that the energy density of these states is higher close to the breakup threshold.

An attractive feature of this method is that the only requirement to construct the THO basis is solving the Schrödinger equation for the ground state, either analytically or numerically. The THO basis is then obtained by means of Eqs. (1) and (2). As the continuum wave functions are obtained through the Hamiltonian diagonalization, their calculation does not require the integration of the Schrödinger equation. Furthermore, the scattering calculation is equivalent to a standard coupled channels calculation with bound states, whose internal energies and wave functions are given by the diagonalization of the deuteron Hamiltonian in this THO basis. The only discrete parameter to be changed in order to investigate convergence is the number of states to be

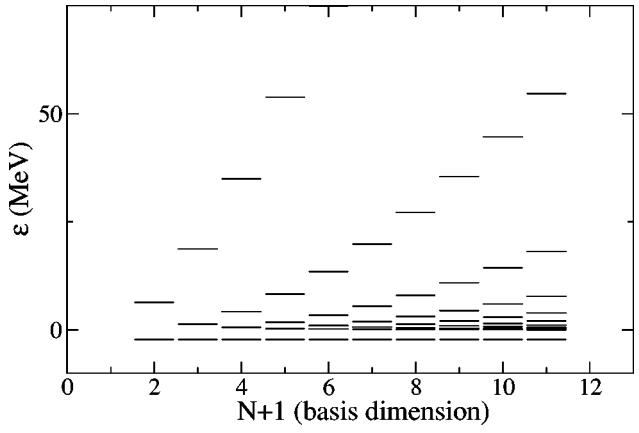

FIG. 3. Ground state and continuum energies obtained upon diagonalizing the deuteron Hamiltonian as a function of the dimension of the THO basis $(N+1)$. Note that for $N>5$ the last state is out of scale.

TABLE I. Convergence of the breakup cross section (σ_{bu}), average excitation energy ($\langle\epsilon-\epsilon_0\rangle$), and average inverse excitation energy $[\langle(\epsilon-\epsilon_0)^{-1}\rangle]$ in the CDCC calculation, with respect to the number of continuum bins (M). All calculations were performed keeping $k_{max}=0.85$ fm^{-1} (corresponding to a maximum excitation energy of $\epsilon_{max}=30$ MeV) and using a different number of continuum bins.

M	σ_{bu} (mb)	$\langle\epsilon-\epsilon_0\rangle$ (MeV)	$\langle(\epsilon-\epsilon_0)^{-1}\rangle$ (MeV^{-1})
2	86.8	6.20	0.166
4	86.1	5.81	0.219
6	87.0	5.85	0.222
8	84.8	5.94	0.224
10	82.5	6.04	0.223
12	81.8	6.07	0.224

included in the basis. Using this input, we solve the coupled channels calculations using the computer code FRESCO [9].

In Table I we present the results of a standard CDCC calculation for the total breakup cross section, as well as the average final excitation energy and the average inverse excitation energy, using in both cases the breakup cross sections as weights. We have kept fixed the maximum excitation energy at 30 MeV and have done calculations varying the number of continuum bins and, accordingly, the bin size Δk.

In Table II we present the same observables as in Table I, but now using the THO method. It is found that the convergence with respect to the number of states is very satisfactory. Taking the results for $N=10$ as reference, we find that the THO calculations with four, six, and eight continuum states give similar results. Even the THO calculation with just two continuum states gives as reasonable an estimate as the corresponding CDCC.

An unusual feature of the THO method is that the diagonalization of the internal Hamiltonian in the THO basis may give rise to closed channels, i.e., states with excitation energies larger than the scattering energy. Although these states do not contribute directly to the outgoing flux, they might be significantly excited in the proximity of the target, thus af-

TABLE II. Calculated total breakup cross section (σ_{bu}), average excitation energy ($\langle\epsilon-\epsilon_0\rangle$), and average inverse excitation energy $[\langle(\epsilon-\epsilon_0)^{-1}\rangle]$, using the THO basis, for different choices of the number of continuum states (N). The column N_{coup} indicates the number of continuum states which are coupled together in the coupled channels calculation.

N	N_{coup}	σ_{bu} (mb)	$\langle\epsilon-\epsilon_0\rangle$ (MeV)	$\langle(\epsilon-\epsilon_0)^{-1}\rangle$ (MeV^{-1})
2	2	89.2	3.98	0.273
4	3	83.8	5.48	0.231
6	5	84.0	5.46	0.226
8	7	83.5	5.66	0.224
10	8	83.5	5.85	0.220
10	10	82.8	5.87	0.221

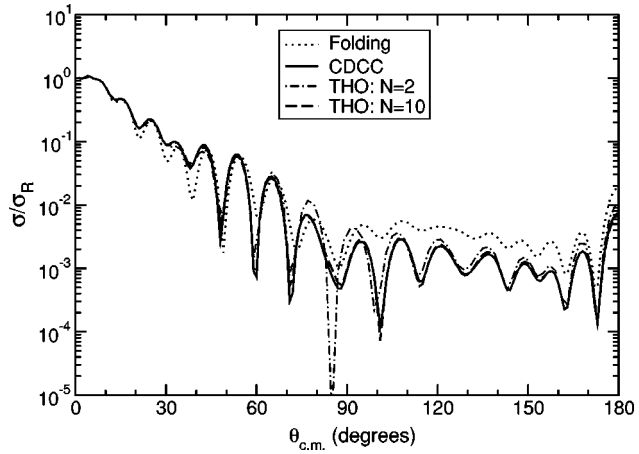

FIG. 4. Elastic differential cross section angular distribution as a ratio to Rutherford cross section for the reaction $d+\mathrm{Pb}$ at 50 MeV. All calculations were performed with the Becchetti-Greenless prescription for the proton-target and neutron-target optical potentials.

fecting the elastic and breakup cross sections. The direct method of solving differential equations used in FRESCO is numerically unstable for these states with high excitation energies. Therefore, in order to investigate the importance of these states, *R*-matrix coupled channel calculations were performed. We found that states with excitation energies above 30 MeV play a minor role and, consequently, closed channels do not affect the scattering observables for this reaction. With the exception of the last row, the calculations presented in Table II are performed excluding the coupling to closed channels. The number of states which are coupled in each case is indicated by the row labeled N_{coup}.

In Fig. 4 we compare the elastic differential cross sections obtained within the CDCC approach ($\epsilon_{max}=30$ MeV and $M=10$ bins of uniform width in k) and the corresponding THO results for $N=10$ (dashed line). It is observed that the agreement between both calculations is excellent. We also present the result of a minimal THO calculation, including only two states (dotted-dashed line). We see that this very schematic calculation does indeed describe the effect of coupling to the continuum reasonably well. As an illustration of the relevance of breakup states in the elastic scattering, we have also included the calculation with the folded potential, i.e., ignoring the coupling to the breakup channels.

In Fig. 5 the breakup cross section as a function of the excitation energy of the deuteron is depicted for the CDCC and THO approaches. In the THO method, we present results with two different numbers of basis states, $N=8$ (open circles) and $N=10$ (filled circles), in order to show the convergence of the results. In the CDCC case, it 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 consistency between the THO calculations with different numbers of states and the CDCC calculation indicates the validity of the THO method to calculate breakup excitation functions.

A feature of the THO method is that it provides a detailed description of the continuum in the low energy region where

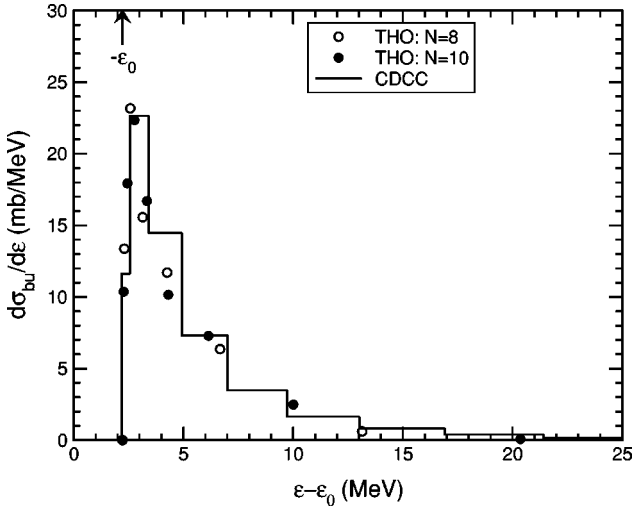

FIG. 5. Breakup cross section as a function of the proton-neutron relative energy in the outgoing channel, for the reaction $d+\mathrm{Pb}$ at 50 MeV. The CDCC calculation with ten continuum bins of uniform size in k, up to a maximum excitation energy of $\epsilon_{max}=30$ MeV is compared with two calculations using the THO basis with $N=8$ and $N=10$ states.

breakup is more relevant. We have checked that, changing the deuteron Hamiltonian to decrease (increase) the binding energy, then the breakup strength moves to lower (higher) energies, and so do the eigenvalues of the Hamiltonian in the THO basis. To achieve this in a CDCC calculation, one needs to adjust the bin size by hand.

In Fig. 6 we show the angular distribution of the breakup cross section. The THO calculation with $N=10$ states is in good agreement with the CDCC calculation, especially at forward angles for which the cross sections are most important. The THO calculation with $N=2$ states provides a reasonable approximation to the converged result.

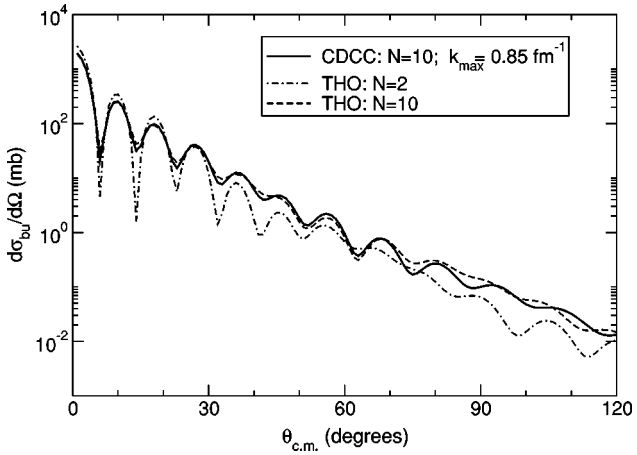

FIG. 6. Breakup cross section as a function of the deuteron center-of-mass scattering angle, for the reaction $d+\mathrm{Pb}$ at 50 MeV. The CDCC calculation with ten continuum bins of uniform size in k, up to a maximum excitation energy of $\epsilon_{max}=30$ MeV is compared with two calculations using the THO basis with $N=2$ and $N=10$ states.

In conclusion, we have shown in this Rapid Communication that the continuum discretization method proposed in Ref. [4] can be applied to problems of current interest in nuclear physics, in particular to the case of collisions involving weakly bound nuclei. The only previous requirement for the application of the method is the knowledge of the ground state wave function of the nucleus, either in an analytical or numerical form. Then, Eqs. (1) and (2) provide the THO basis which can be used to diagonalize the nuclear Hamiltonian. We have performed a series of schematic calculations for the case of the $d+^{208}$ Pb elastic scattering and breakup at 50 MeV. The comparison of THO and CDCC results has demonstrated the validity of the first method and has shown that the THO discretization method works properly even though the basis is truncated to very few states. One of the greatest advantages of the THO method is that it automatically distributes the basis states in the relevant energy regions of the continuum, offering an easy, computationally efficient, alternative to the standard CDCC method.

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