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Continuum Discretization by the Transformed Harmonic Oscillator Method: Application to the Scattering of Weakly Bound Nuclei

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Abstract.

The Transformed Harmonic Oscillator (THO) method is used to discretize the continuum of weakly bound nuclei. We focus in the case of the deuteron. For the s states, a finite basis is obtained by multiplying the only present bound state by a family of orthogonal polynomials which depends on the co-ordinate through a local scale transformation. For the p states, that do not have any bound state, a normalizable seed state is defined, and the basis is generated similarly, by multiplying the seed state by the adequate family of orthogonal polynomials. The exact Hamiltonian is diagonalized in this finite basis, and the resulting states, with definite energies and normalizable wavefunctions, are taken as a representation of the continuum. Scattering calculations are then performed using the standard Coupled Channels formalism. We have applied this method to describe the collision of $d+^{208}$Pb at 50 MeV, considering the coupling to s and p breakup states due to nuclear and coulomb forces. Appropriate convergence of the elastic and breakup cross sections with increasing dimension of the basis is found, and the results obtained converge to those of a standard CDCC calculation.

1 Introduction

In nuclear reactions, a standard approach to calculate elastic, inelastic and reaction cross sections is to consider explicitly some of the collective states of the interacting nuclei, and perform a coupled channels calculation including explicitly the coupling to these states. This procedure requires the knowledge of the relevant wavefunctions of the states included in the calculation, which indeed should be normalizable, in order to evaluate the transition potentials. That is the reason why continuum states are normally excluded from a coupled channels approach. Nevertheless, for weakly bound nuclei, the effect of coupling to continuum states plays an important role in the collision, even for the elastic scattering.

The main difficulty of treating the continuum arises from the fact that these states are described by an infinite continuum of states which are not square-integrable and have an infinite range in co-ordinate space. Thus, the continuum is substituted by a discrete set of normalizable states which generate a complete set as the number of states tends to infinity. Then, it is expected that a finite number of these discrete states will play the same role as the true continuum. This is checked by investigating the convergence of the calculation as the number of discrete states included in the basis is increased.

One of the most widely used procedures for this purpose is the method of continuum discretized coupled channels (CDCC) [1]. 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. 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. A practical CDCC calculation requires to fix the maximum break-up energy considered $E_{\max} = \hbar^2 k_{\max}^2/2\mu$ and the number of bins M, so that the width of the bins is given by $\Delta k = k_{\max}/M$. To demonstrate convergence in a CDCC calculation one has to show that the scattering magnitudes are not modified when the maximum energy and the number of bins is increased. 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 $k_{\max}$ parameterize the basis, demonstrating convergence is by no means trivial (see [2] 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.

In this work the Transformed Harmonic Oscillator (THO) method [3] is used to discretize the continuum of weakly bound nuclei. We start with a finite set of harmonic oscillator wavefunctions, which transformed by a local scale transformation, should represent both the bound and break-up states of the nucleus. We define the local scale transformation so that the lowest harmonic oscillator state transforms to the bound state, and so the other HO states transform to a finite set of states which provide a basis for the continuum [4]. The exact Hamiltonian is diagonalized in this finite basis, and the resulting states, with definite energies and normalizable wavefunctions, are taken as a representation of the continuum. This representation will be more accurate as the number of states in the basis is increased. We have shown that the THO method works very well to describe the excitation to the continuum in one-dimensional potentials [4]. We have also shown that scattering problems in one dimension can be described using the THO method [5].

In this paper we apply the THO method to describe the effect of the continuum on the scattering of deuterons on heavy nuclei. In Section 2 we review the THO formalism applied to the description of the continuum of s-wave break-up state [6], and extend it to describe the p-wave continuum. In Section 3 we present the results for the elastic and break-up cross sections of $d+^{208}$Pb at 50 MeV, discussing the consistency of the THO calculations and CDCC calculations. Section 4 contains summary and conclusions.

2 Deuteron Wavefunctions in the THO Method

Let us consider the deuteron. We obtain the $L = 0$ ground state wavefunction $\phi_b(r)$ by solving the Schrödinger equation with the adequate potential. We used a Poschl-Teller potential [7] to obtain an analytic deuteron wavefunction, which is convenient, although not essential for the application of the THO method. Now, the problem consists in generating a suitable set of normalizable wavefunctions that describe the continuum states. For that purpose [4] we define a local scale transformation [8] which converts the ground state wave function of a bound nucleus $\phi_b(r)$ into a harmonic oscillator wave function $\phi_0^{HO}(s)$. The function $s(r)$, which defines the local scale transformation, for the states with $L = 0$ (s-states), is given by [6]

$$N_b \int_0^r |\phi_b(r')|^2 dr' = N_0^{HO} \int_0^s {s'}^2 \exp(-{s'}^2) ds'. \tag{1}$$

N_b and N_0^{HO} are the normalization coefficients required so that the two terms tend to one as r and s tend to infinity. Next, one generates a set of orthogonal wave functions multiplying the ground state wave function by the appropriate polynomials, which in this case are Laguerre polynomials [6]

$$\phi_n^{THO}(r) = N_n L_n^{1/2} \left(s(r)^2\right) \phi_b(r) \,, \tag{2}$$

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.

The deuteron Hamiltonian can be diagonalized in a basis with an arbitrary number of THO states. As shown in [6], the energies of the deuteron obtained from this diagonalization are more densely packed close to the break-up threshold. The eigenstates of the Hamiltonian in the truncated basis present an increasing number of nodes as the energy increases, but all of them have a similar range, determined by the range of the last state included in the THO basis, and all af them decay exponentially for large ditances.

In essence, the procedure sketched above to generate the THO basis starts with the normalizable bound state and multiplies it by a family of orthogonal polynomials on the scaled variable $s(r)$. This allows to construct states with the same L value as the bound state. It is not trivial how to extend this procedure to describe the $L \neq 0$ continuum in the deuteron, for which one does not have any bound state to start with.

We propose here a procedure to generate a normalizable state, for each $L \neq 0$ value, which allows us to build a THO basis multiplying it by the adequate polynomials. We want like to find out, for each L value, which is the state of the continuum of the deuteron which couples most strongly to the bound state. This state will not be, in general, an eigenstate of the deuteron hamiltonian, but it can be expanded in terms of them. In general, it is not possible to know a priori which state will couple more strongly to the ground state. However, when the bound system is in an static external field, or when it is undergoing a scattering process in the adiabatic limit, the effect of the coupling is to perturb the ground state wavefunction. The external field, which in principle is a funcion of the relative coordinate to the target and of the internal coordinate of the deuteron, can be expanded in multipoles. So, we will consider the deuteron in a weak multipole field. The hamiltonian is

$$h^{pert} = h^0 + \epsilon r^L Y_{LM}(\hat{r}). \tag{3}$$

The perturbation that this multipole field creates in the ground state can be written as

$$\phi_b^{pert}(\vec{r}) = \phi_b^{L=0}(r) + \epsilon \psi_L^{seed}(r) Y_{LM}(\hat{r}) \tag{4}$$

where the seed wavefuntion is defined by the expression

$$\psi_L^{seed}(r) Y_{LM}(\hat{r}) = \frac{1}{h^0 - E_B} r^L Y_{LM}(\hat{r}) \phi_b^{L=0}(r) \tag{5}$$

This seed wavefunction is normalizable, and it has the same asymptotic behavior as the ground state. Thus, we argue that the seed state $\psi_L^{seed}(r)$ is, for each L value, the state that couples most strongly to the ground state. It is not an eigenstate of the deuteron hamiltonian, but it can be used to generate the THO basis,

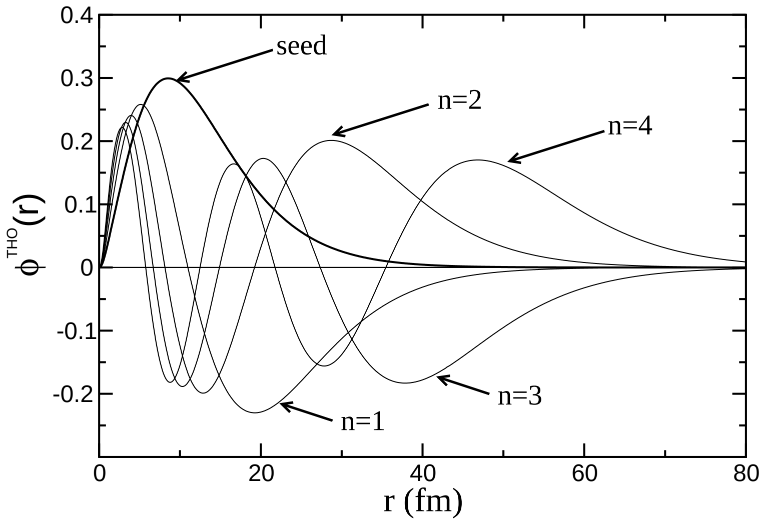

Figure 1. THO wavefunctions for the $L = 1$ continuum states of the deuteron. The seed state is indicated by the thick line.

which, for large number of states, will be an accurate representation of the continuum. This choice of the seed state ensures that, even for a small number of states in the THO basis, those combinations of continuum states which are most likely to couple to the ground state are included in the calculation.

So, it can be used to define the local scale transformation $s(r)$, which will be different for each L-value, through the expression

$$N_L^{seed} \int_0^r |\psi_L^{seed}(r')|^2 dr' = N_L \int_0^s (s')^{2L+2} \exp(-{s'}^2) ds' \tag{6}$$

Once this transformation is defined, we can build the THO basis for the states with a given L through the expression

$$\phi_{nL}^{THO}(r) = N_{nL} L_n^{L+1/2} \left(s(r)^2\right) \psi_L^{seed}(r) \tag{7}$$

The wavefunctions so obtained are presented in Figure 1, for the case of $L = 1$. The long range of these wavefunctions should be noticed. When these basis functions are used to diagonalize the deuteron hamiltonian for $L = 1$, we find that many states appear at energies close to the break-up threshold. So, we can expect that the low energy continuum is well described in this method.

3 Scattering Calculations

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,

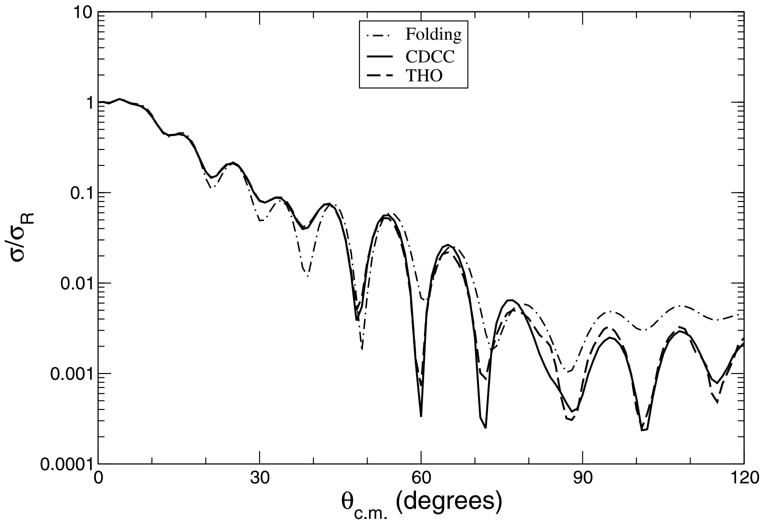

Figure 2. Elastic differential cross section for the reaction $d\,+\,^{208}\mathrm{Pb}$ at 50 MeV. The coupling to s and p break-up states is included.

we have considered a test case where the coupling to the continuum is relevant: the elastic scattering and breakup of $d+^{208}\mathrm{Pb}$ at 50 MeV. The deuteron is taken to be a pure s-state, in the gound state, and spin-orbit interactions are not considered. For the break-up states, we consider s and p break-up, and include explicitly the effect of nuclear and coulomb break-up. The interaction of proton and neutron with the target is taken from the Becchetti-Greenless parameterization [9], evaluated at half of the deuteron incident energy. Within these restrictions, we perform a convergence study of the THO method and compare with the CDCC method.

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. (2,7). 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 included in the basis.

We performed the THO coupled channels calculations and the CDCC calculations using the computer code FRESCO [10]. In the case of the CDCC calculations, several tests calculations were made to determine the adequate values of

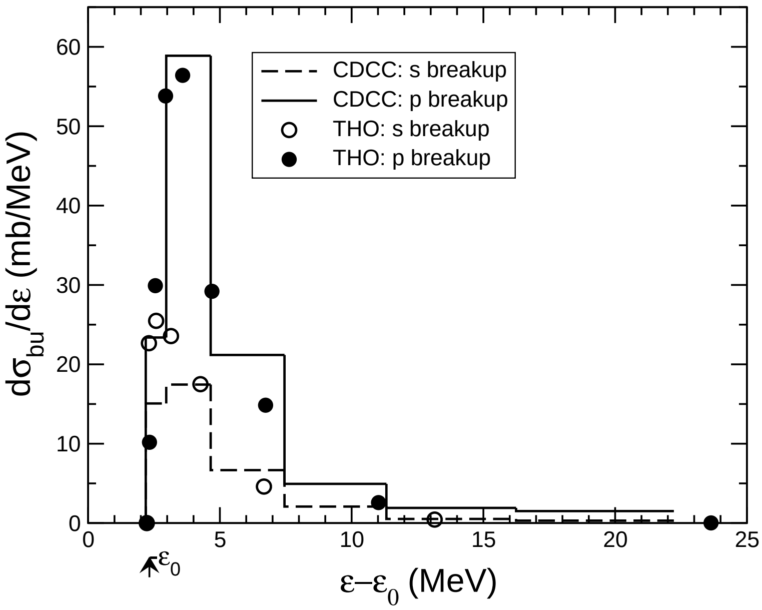

Figure 3. Differential breakup cross sections to s and p states as a function of the proton-neutron relative energy in the outgoing channel, for the reaction $d\,+\,^{208}\mathrm{Pb}$ at 50 MeV.

the maximum energy and number of bins. It was found that maximum energy of 20 MeV and 6 bins for the s and p channels gave a reasonably converged result. For the THO calculations, 8 states for the s and p channels gave a converged result.

In Figure 2 we compare the elastic differential cross sections obtained in the THO and CDCC approaches. It is observed that the agreement between both calculations is very good. 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 Figure 3 the differential 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, 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 calculation and the CDCC calculation indicates the validity of the THO method to calculate break-up excitation functions.

A feature of the THO method is that it provides a detailed description of the continuum in the low energy region where break-up is more relevant. We have

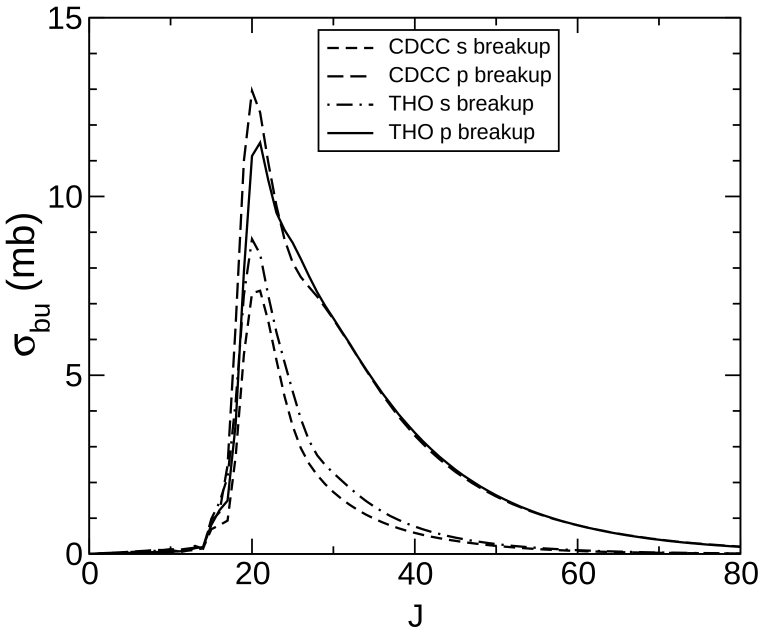

Figure 4. Partial breakup cross sections to s and p states as a function of the total angular momentum J, for the reaction $d + {}^{208}\mathrm{Pb}$ at 50 MeV.

checked that, changing the deuteron Hamiltonian to decrease (increase) the binding energy, then the break-up 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 Figure 4 the partial cross sections for the different J values is presented. As in the other observables, the agreement between the CDCC and the THO methods is very good. It is interesting to notice that the p break-up cross sections extend to large J values. This is due to the effect of the long range dipole coulomb potential. Moreover, there is also a significant contribution of s break-up at large J values. This is due to the effect of continuum to continuum dipole coulomb coupling between the p and the s break up states.

4 Summary and Conclusions

We have shown in this paper 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 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. (1,2) provide the THO basis which can be used to diagonalize the nuclear Hamiltonian. If the system does not have any bound state for some L value, a normalizable seed state can be generated from eq. (5), and then the THO basis can be obtained from eqs. (6,7).

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 in a case in which long range coulomb potentials are considered. 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.

Acknowledgments

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