

Discretizing the Continuum*

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Abstract. Recently we have developed a method to describe approximately the continuum states of a weakly bound system. The method consists on constructing a discrete and normalizable basis by multiplying the ground state of the system by a family of suitable orthogonal polynomials. The Hamiltonian is then diagonalized in the finite basis, giving rise to an accurate description of the excited bound states and to a discretization of the continuum. In this work we present an application of this method to describe the effect of break-up channels in the scattering of deuterons by nuclei. We investigate the case of $d + {}^{208}\text{Pb}$ at 50 MeV, where the Coulomb force, especially the dipole component, is very important. We also present an application of this method to describe thermodynamic properties associated to the vibration and eventual dissociation of ideal diatomic molecules. We investigate the temperature dependence of the heat capacity per molecule.

1 Introduction

Nuclei, molecules and other quantum systems have a discrete number of bound states, which appear at excitation energies below the break-up or dissociation threshold, and an infinite number of continuum states above it.

The main difficulty of treating the continuum arises from the fact that it is described by an infinite continuum of states which are not square-integrable and have an infinite range in co-ordinate space. In some cases, the exact, not normalizable continuum wavefunctions can be explicitly used in the calculation. This is the case for the evaluation of excitation functions for an operator which connect the

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ground state with the continuum states of a system. In this case, the bound character of the ground state allows for an explicit evaluation of the matrix elements. In general, the explicit inclusion of the continuum states in structure or reaction calculations requires a discretization of the continuum. 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.

Different methods are used to generate a discrete basis for the continuum. One simple procedure is to use a box [1]. Then, the wavefunctions are constrained to vanish at a certain distance R . The Sturmian basis consists in finding the bound eigenstates obtained re-scaling the interaction, which have the same binding energy as the original bound state [2]. This basis is complete within the range of the potential. One of the most widely used of these approaches is the method of continuum discretization coupled channels (CDCC) [3]. 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. The Gaussian expansion method [4] consists in taking a non-orthogonal basis consisting on a set of Gaussian functions in geometric progression.

In this work we apply the general orthogonal polynomial method (OP) [5] to discretize the continuum of deuterons and diatomic molecules. In Sect. 2 we briefly outline the orthogonal polynomial method. In Sect. 3 we apply a particular case of the OP method, which is called the transformed harmonic oscillator (THO) method, to describe the break-up effects in the scattering of deuteron by ^{208}Pb . In Sect. 4 we apply another case of the OP method, called the natural orthogonal polynomial (NOP) method to investigate the influence of dissociation in the thermodynamical properties of diatomic molecules.

2 Orthogonal Polynomial Method

The orthogonal polynomial method [5] starts from the knowledge of the bound state wavefunction of the Hamiltonian,

$$h\varphi_0(x) = e_0\varphi_0(x). \quad (1)$$

In this expression, $\varphi_0(x)$ can be the wavefunction of a one-dimensional system, or the radial wavefunction of a three-dimensional system with central forces. However, more complex systems can also be incorporated. For example, in a three-body problem, x can be the hyperradius and $\varphi_0(x)$ the wavefunction corresponding to certain angular and hyperangular momentum components in the ground state. In general, in a problem with n degrees of freedom, x will be a non-compact variable, which can take values up to infinity, while the rest of the variables can be taken as compact (angles or hyperangles) which can be expanded in suitable bases (spherical or hyperspherical harmonics).

We can define an arbitrary local scale transformation $s(x)$, continuous and single-valued. This leads to a positive definite weight function $\omega(s)$, defined as

$$\omega(s) ds = |\varphi_0(x)|^2 dx. \quad (2)$$

This weight function can be used to construct a family of orthogonal polynomials $\{P_n(s); n = 0, 1, 2, \dots\}$ that fulfil

$$\int ds \omega(s) P_n(s) P_m(s) = \delta_{n,m}. \quad (3)$$

From these polynomials, a complete set of orthonormal wave functions can be constructed,

$$\phi_m(x) = \langle x | OP, n \rangle = \varphi_0(x) P_m(s(x)). \quad (4)$$

These wavefunctions are square-normalizable. So, the matrix elements of any operator can be constructed. In particular, the matrix elements of the Hamiltonian are given by

$$\begin{aligned} \langle OP, n | (h - e_0) | OP, m \rangle &= \int dx \phi_n(x) (h - e_0) \phi_m(x) \\ &= \frac{1}{2} \int dx \varphi_0(x) [P_n(s(x)), [h, P_m(s(x))]] \varphi_0(x). \end{aligned} \quad (5)$$

If the potential energy term is local, this is, if it is momentum independent, it will commute with $s(x)$. The double commutator of the kinetic energy term gives

$$\langle OP, n | (h - e_0) | OP, m \rangle = \frac{\hbar^2}{2M} \int ds \omega(s) P'_n(s) P'_m(s) \left(\frac{ds}{dx} \right)^2. \quad (6)$$

The Hamiltonian can be diagonalized in a finite, but arbitrarily large basis, including states from $n = 0$ (the ground state) to $n = N$. The ground state will always appear as an eigenstate of the Hamiltonian. The rest of the eigenstates constitutes a representation of the continuum states, and of other bound states which may exist.

It should be noticed that the OP method has a large degree of flexibility. If the local scale transformation is chosen according to some physical consideration, then the weight functions and the family of polynomials will be determined. However, the weight function can be chosen, and then the local scale transformation and the family of polynomials follow. Alternatively, the family of polynomials is chosen, and then the weight function and the local scale transformation are derived.

3 Break-Up Effects in Deuteron Scattering

The transformed harmonic oscillator (THO) method, which was originally proposed in ref. [6], can be described as a particular case of the general orthogonal polynomial method, taking as weight function $\omega(s) = s^2 \exp(-s^2)$. We have applied this method to discretize the continuum of $l = 0$ states of the deuteron [7]. The THO basis for s states is

$$\varphi_{m0}^{\text{THO}}(r) = L_m^{1/2}(s(r)^2) u_D(r), \quad (7)$$

where $u_D(r)$ is the bound deuteron wavefunction, which we take as a pure s -state. In this work we have extended the procedure to the continuum of deuteron states with $l \neq 0$. This leads to a THO basis for $l \neq 0$ states given by

$$\varphi_{nl}^{\text{THO}}(r) = (s(r))^l L_n^{l+1/2}(s(r)^2) u_D(r), \quad (8)$$

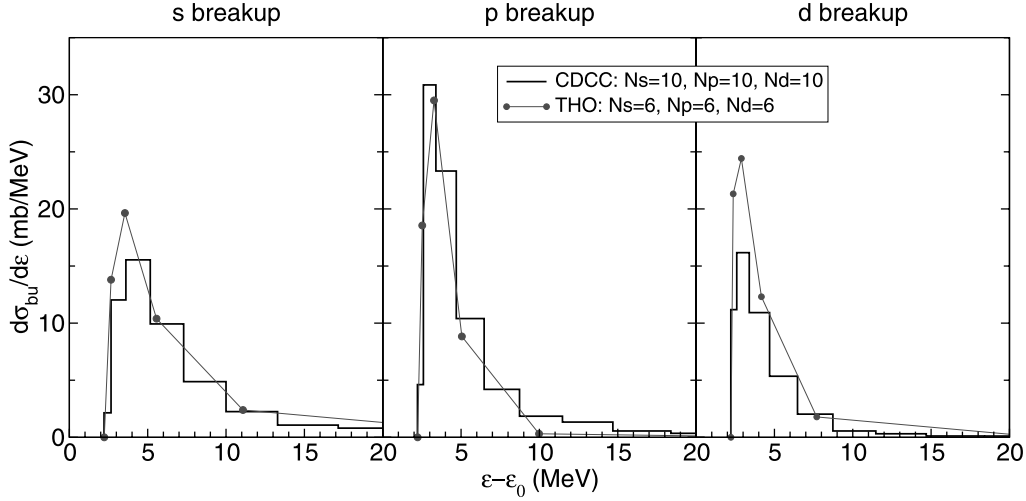


Fig. 1. Break-up distributions of the reaction $d + {}^{208}\text{Pb}$ at 50 MeV, including s , p , and d break-up channels. THO and CDCC calculations are compared

where $L_n^\alpha(s)$ are Laguerre polynomials. The properties of this family of polynomials ensure that the basis functions are orthogonal and complete for each l value. Note that the basis functions have the r^l behaviour close to the origin which is required by continuity of the function and its derivatives. Note that this basis is different from the one used in ref. [8], where a specific seed state was taken to generate the states with $l \neq 0$.

We have diagonalized the deuteron Hamiltonian in the s , p , and d channels in a finite basis. The corresponding eigenfunctions and energies have been used in a coupled-channels calculation for the reaction $d + {}^{208}\text{Pb}$ at 50 MeV. Details of this calculation can be found in refs. [7, 8]. The calculation includes explicitly Coulomb and nuclear couplings, between the bound states and the continuum, as well as continuum-to-continuum couplings. The results for the break-up cross section, shown in Fig. 1, are in broad agreement with the CDCC calculations. A detailed study of the convergence of the THO method, as compared to the CDCC method, is in progress.

4 Thermodynamical Properties of Diatomic Molecules

Let us consider a dilute gas of diatomic molecules. We take the Boltzmann constant as $k = 1$, so that temperatures and energies have the same units. When the temperature is large compared to the typical rotational energies, but small compared to the vibrational energy, the molecule has 5 effective degrees of freedom (3 translations and 2 rotations). Hence, the heat capacity per molecule is $C_v = \frac{5}{2}$. However, as the temperature is larger, the vibrations start playing a role. When the temperature is higher than the dissociation energy, the molecule dissociates, and then there are 6 effective degrees of freedom (3 translations per atom); so, the heat capacity per molecule becomes $C_v = \frac{6}{2}$.

The question that we want to address is, how does C_v change with temperature in the range which goes from the vibrational temperature to the dissociation temperature. The partition function [9] is given by

$$Z(\beta) = \sum_n \exp(-\beta E_n), \quad \beta = 1/T, \quad (9)$$

from which the average energy can be obtained as $E(\beta) = -d \log(Z(\beta))/d\beta$ and so the heat capacity per molecule becomes

$$C_v(T) = dE(\beta)/dT = \beta^2 \frac{d^2 \log Z(\beta)}{d\beta^2}. \quad (10)$$

If the vibrations are harmonic, $E_n = n\hbar\omega$, and the specific heat is given by the expression

$$C_v(T) = (\beta\hbar\omega)^2 \frac{\exp(\beta\hbar\omega)}{(\exp(\beta\hbar\omega) - 1)^2}. \quad (11)$$

Obviously, a harmonic molecule cannot reach the dissociation. Instead, we consider a Morse Hamiltonian. The interaction is, in the adequate units,

$$V(x) = \left(j + \frac{1}{2}\right)^2 (e^{-2x} - 2e^{-x})/2. \quad (12)$$

This potential has a number of bound states given by the integer part of j . The potential and energy levels are shown in Fig. 2 for $j = 6$.

To obtain the wavefunctions and energies of the bound states and the discretized continuum, we make use of the natural orthogonal polynomial (NOP) method [5, 10]. The local scale transformation is chosen so that $s = (2j + 1)e^{-x}$. The NOP basis for vibrational and dissociation states [5] is

$$\varphi_m^{\text{NOP}}(x) = L_m^{2j-1}(s(x))\varphi_0(x). \quad (13)$$

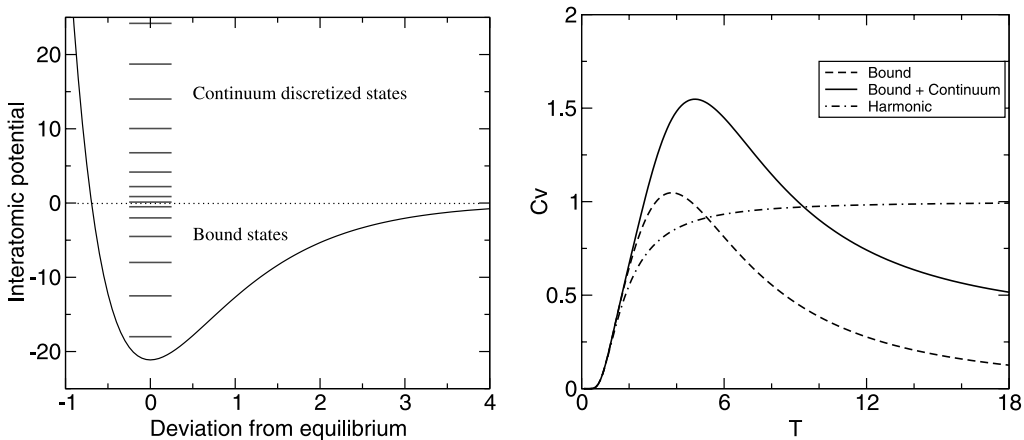


Fig. 2. Bound states and low-energy discretized continuum states of a Morse potential, and its contribution to C_v . The vibrational energy is 5.5, and the dissociation energy is 18

This expression can be generalized [10] to give

$$\varphi_m^\sigma(x) = L_m^{2\sigma-1}(s(x))s(x)^{\sigma-j}\varphi_0(x). \quad (14)$$

The Morse Hamiltonian is tri-diagonal in the NOP basis. Besides, an adequate choice of σ allows to decouple the bound states from the continuum. This means that the energies and wavefunctions of the bound states are exactly described [10]. As far as the continuum is concerned, we obtain that the density of states depends on the size of the basis, although in all cases this density is larger for the energies close to the dissociation energy. We have performed a calculation including 100 states, from which the 6 bound states and 94 continuum discretized states are obtained. In Fig. 2 we present the vibrational and dissociative contribution to C_v . It can be seen that the harmonic approximation is only valid at temperatures which are small compared to the vibrational temperature. The calculation which includes only the contribution of bound states underestimates C_v at high temperatures, for which we expect that the vibrational and dissociative contribution to C_v should go to $\frac{1}{2}$. The calculation including the continuum shows a clear maximum at temperatures about 5. We find that, as the number of states in the basis increases, so does the value of C_v at the maximum. So, we suspect that the temperature at which this maximum occurs may correspond to a phase transition associated to the dissociation of the molecule.

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