Continuum coupling in one-dimensional scattering using a transformed harmonic oscillator basis

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The coupling to the continuum is studied in a one-dimensional problem that describes the interaction of a weakly bound composite object with a wall in a semiclassical approach. A transformed harmonic oscillator basis is introduced to provide an appropriate discrete and finite basis for treating the continuum part of the spectrum. The convergence of the scattering magnitudes is investigated as the number of states in the basis is increased. The role of bound-to-continuum and continuum-to-continuum coupling is investigated.

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I. INTRODUCTION

A composite quantum-mechanical object is described by an internal Hamiltonian that includes the kinetic energy of the constituents, as well as the interactions between these. The eigenstates of the internal Hamiltonian will be given, in general, by a finite (or, at least, discrete) number of bound states, and a continuum of breakup states, which can be characterized by the relative momentum of the fragments. When such an object, initially in its ground state, which is bound, undergoes a scattering process from a structureless target the dynamics of the system is governed by the total Hamiltonian that includes the internal Hamiltonian of the object plus the interaction with the target. As a result, the object may be excited to other bound states, or to the continuum of breakup states. Even if the object ends up in the ground state, the scattering magnitudes will be affected by the coupling to bound and breakup states.

The effect of coupling to bound states can be described by means of a coupled-channels calculation. In a time-independent formalism, it involves the solution of a finite number of second-order coupled differential equations on the relative coordinate, which appear as a result of projecting the Schrödinger equation on the bound wave functions. In a semiclassical time-dependent formalism, one has to solve a finite number of first-order coupled differential equations on the time variable. In both cases, the procedure is rather straightforward, although it may be computationally difficult, if many bound states are considered.

The effect of coupling to breakup states is more difficult to describe. The continuum wave functions have an infinite range and are not normalizable. Thus, the coupling potentials from bound states to the continuum states have a very long range, and the coupling potentials from continuum-to-continuum states have an infinite range. That makes it necessary to use some discretization procedure to substitute the continuum of breakup states by a finite number of normalizable states, which, in the adequate limit, should represent the effect of coupling to the true continuum. Several methods have been proposed for this purpose. The *R*-matrix method [1] solves the many-body problem in a box and then make the matching with the adequate boundary conditions. The Sturmian basis [2–4] uses bound states of scaled potentials, which are orthogonal when weighted with the potentials. The Siegert pseudostate formulation [5] provides a finite basis representation of the outgoing wave solutions to the radial Schrödinger equation for cutoff potentials. The Gamow states [6] are non-normalizable solutions of the Schrödinger equation corresponding to outgoing boundary conditions characterized by complex energies. The method of continuum discretization coupled channels [7] discretizes the continuum by means of taking fixed intervals, or bins, of k values in the continuum states. Finally, a complete basis of single particle wave functions, such as the harmonic oscillator, can be used to expand both bound and scattering states [8].

We have recently proposed the use of a transformed harmonic oscillator (THO) basis to describe the effect of the continuum [9,10]. The basic idea is to define a local scale transformation [11–13], which is such that converts the ground-state wave function of the weakly bound composite object $\psi_B(x)$ into a harmonic oscillator wave function $\phi_0^{HO}(s)$ [9,10]. The function $s(x)$, which defines the local scale transformation, is given, for a one-dimensional problem, by

$$\int_{-\infty}^{x} |\psi_B(x')|^2 dx' = \int_{-\infty}^{s} |\phi_0^{HO}(s')|^2 ds' = \frac{1+\mathrm{erf}(s)}{2}. \tag{1}$$

Then, one generates a set of orthogonal wave functions $\phi_n^{\mathrm{THO}}(x) = H_n(s(x))\psi_B(x)$, 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. Then, one takes a finite basis, which is uniquely determined by the number $N+1$ of THO states considered, and diagonalizes the Hamiltonian in this basis. The resulting eigenstates and eigenvalues are taken as representatives of the continuum. We showed that, as the number of states in the THO basis increases, the eigenstates appear more densely packed close to the breakup threshold, although there are eigenstates that appear at higher energies. Besides, we demonstrated that global structure magnitudes related to the coupling to the continuum, such as sum rules, were very accurately described using relatively small THO bases. Our purpose in this paper is to study the adequacy of the THO

basis to describe the effect of the continuum in the scattering processes. We make use of the semiclassical approximation in which the relative motion of projectile and target is described by classical trajectories. This approach is valid when the wavelength associated to the relative motion is small compared to the range of the interaction [14]. This is the case for collisions of heavy nuclei, atoms, and molecules on a wide range of energies.

In this paper we make use of the THO basis to describe the effect of coupling to the continuum in a model one-dimensional problem. In Sec. II we present the model Hamiltonian, we introduce the semiclassical approximation to describe the scattering, and formulate the adiabatic and sudden approximations, which allow for an exact solution. In Sec. III we present the scattering calculation in the THO basis, and investigate the convergence of elastic and breakup probabilities as the number of states in the THO basis is increased. In Sec. IV we investigate the effect of including or neglecting the effect of continuum-to-continuum coupling. Sec. V is for the summary and conclusions.

II. ONE-DIMENSIONAL SCATTERING MODEL

In this work we discuss the application of the THO basis to a scattering problem. We consider a one-dimensional composite object, characterized by two particles with masses m_1, m_2, and coordinates x_1 and x_2. Their reduced mass is $\mu = m_1 m_2/(m_1+m_2)$ and the total mass is $M = m_1 + m_2$. The relative coordinate is $x = x_1 - x_2$, and the center of mass coordinate is $X = (m_1 x_1 + m_2 x_2)/M$. The corresponding Hamiltonian is given by

$$h = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + v_B(x), \tag{2}$$

where the x is the relative coordinate and $v_B(x)$ is the interaction that binds the particles. Initially, the composite object is in its ground state $\psi_B(x)$, which is an eigenstate of h corresponding to an energy e_B. This object collides with a massive particle, or wall. The interaction of the system with the wall is given by a function $V(X,x)$, which depends on the center of mass as well as on the internal coordinate. If the particles interact independently with the wall, then $V(X,x) = V_1(x_1) + V_2(x_2)$, but this will not be true in general, if there are polarization effects. Thus, the complete Hamiltonian can be written as

$$H = -\frac{\hbar^2}{2M}\frac{d^2}{dX^2} + V(X,x) + h. \tag{3}$$

The x dependence of the interaction $V(X,x)$ can be expanded in terms of a family of orthogonal polynomials $P_m(x)$, where m represents the order of the polynomial. These polynomials are orthogonal with respect to the weight function given by $\psi_B(x)^2$, so that

$$\int dx\, \psi_B(x)^2 P_m(x) P_n(x) = \delta(n,m). \tag{4}$$

Explicit expressions for the first few polynomials are, in terms of the expectation values of x^n in the ground state, and assuming that $\psi_B(x) = \psi_B(-x)$,

$$P_0(x) = 1, \tag{5}$$

$$P_1(x) = \frac{x}{\sqrt{\langle x^2\rangle}}, \tag{6}$$

$$P_2(x) = \frac{x^2 - \langle x^2\rangle}{\sqrt{\langle x^4\rangle - \langle x^2\rangle^2}}. \tag{7}$$

Thus, the interaction can be expanded as

$$V(X,x) = \sum_m V_m(X) P_m(x), \tag{8}$$

$$V_m(X) = \int dx\, \psi_B(x)^2 P_m(x) V(X,x). \tag{9}$$

It should be noticed that the first term in this expansion, which is independent of the internal variable x, corresponds to the expectation value of the interaction $V(X,x)$ in the ground state of the composite object, which is the folding potential. This is given by

$$V_f(X) = V_0(X) = \int dx\, \psi_B(x)^2 V(X,x). \tag{10}$$

The other terms give rise to the tidal forces, which can induce the excitation of the composite object during the collision. For the purpose of this paper, we will consider the case in which the composite object consists on two identical particles. Then, the function $V(X,x)$ is even in x, and only the polynomials of even order contribute to the expansion. Moreover, for the sake of simplicity, we will retain only the terms up to $m = 2$. Thus, we have

$$V(X,x) = V_f(X) + V_2(X) P_2(x). \tag{11}$$

In a semiclassical approach [14], the folding potential determines the trajectory $X(t)$ of the center of mass of the object. The trajectory can be obtained by solving the differential equation

$$\frac{M}{2}\left(\frac{dX(t)}{dt}\right)^2 + V_f(X) = E - e_B. \tag{12}$$

The turning point of the classical trajectory X_0 occurs when $E - e_B = V_f(X_0)$. If the time $t = 0$ is taken when $X(t) = X_0$, then the trajectory $X(t)$ is an even function of the time. The tidal potential, which is responsible for the projectile excitation, is given by

$$V_T(X,x) = V_2(X) P_2(x). \tag{13}$$

In a semiclassical treatment, the trajectory $X(t)$ is used to consider the tidal potential $V_T(X(t),x)$ as a time-dependent operator that acts on the internal coordinate x. Moreover, in the case that we are considering, the dependence in the cen-

ter of mass and relative coordinates factorize, so that the effect of the tidal forces are described by the operator $P_2(x)$, which acts with an intensity $F(t)=V_2(X(t))$. The internal state will evolve satisfying the equation

$$i\hbar\frac{d}{dt}\psi(x,t)=[h-e_B+F(t)P_2(x)]\psi(x,t), \qquad (14)$$

with the boundary condition that for $t\to-\infty$, the wave function is that of the ground state $\psi_B(x)$.

Recapitulating, Eq. (14) represents, within some reasonable approximations, the time evolution of the internal state of a two-particle system that collides with a wall. This equation contains derivatives with respect to t and x, and so it is difficult to solve it exactly. Besides, as the eigenstates of h contain both bound and continuum states, one cannot just project on the eigenstates of h and solve the coupled equations.

We will show in the following section that the THO method provides a finite basis of normalizable states, which allow to find an approximate solution to Eq. (14). Besides, as the number of THO states increases, the relevant scattering magnitudes converge.

We will also consider two dynamical approximations to Eq. (14). The *adiabatic approximation* arises when the characteristic time scale of the interaction, given by the time range of the function $F(t)$, is much longer than the time scale of the internal motion, $\hbar/e_B$. In this limit, the time-dependent wave function can be approximated by the expression

$$\psi_{Ad}(x,t)=N(t)\left[\psi_B(x)-F(t)\frac{1}{h-e_B}P_2(x)\psi_B(x)\right]\times\exp[-i\phi(t)], \qquad (15)$$

where $N(t)$ is a normalization factor, which varies slowly, and the phase $\phi(t)$ satisfies the equation

$$\phi(t)=-\frac{\alpha}{\hbar}\int_{-\infty}^{t}dt'F(t')^2. \qquad (16)$$

The parameter α is the polarizability associated to the operator $P_2(x)$. It is given by the expression

$$\alpha=\langle\psi_B|P_2(x)\frac{1}{h-e_B}P_2(x)|\psi_B\rangle. \qquad (17)$$

It should be noticed that, in the adiabatic approximation, the object always emerges from the scattering process in its ground state. Indeed, the function $F(t)$, which is associated to the couplings, vanishes as $t\to\infty$. The only effect that arises from the coupling is a phase shift in the ground-state wave function. This phase shift is determined by the value of the polarizability α. So, the adequacy of any approximate treatment of continuum discretization can be judged by comparing the value of α obtained from the discretization with the exact value. We will make this comparison in the following section for the THO basis.

The *sudden approximation* is opposite to the adiabatic one. It arises when the time scale of the interaction is much shorter than that of the internal motion. Thus, the internal coordinates are effectively frozen during the scattering. The sudden approximation is obtained by ignoring the term $h-e_B$ in Eq. (14). That allows to integrate with respect to the time variable, to give

$$\psi_{Su}(x,t)=\psi_B(x)\exp[-i\phi(t)P_2(x)], \qquad (18)$$

where the phase $\phi(t)$ is given by

$$\phi(t)=\frac{1}{\hbar}\int_{-\infty}^{t}dt'F(t'). \qquad (19)$$

In the sudden approximation the object emerges from the scattering process in a state whose density distribution is the same as that of the ground state. However, it can be quite different from the ground state because the additional phase depends on the variable x. The probability amplitude for remaining in the ground state is given by

$$\langle\phi_B|A(\Phi)|\phi_B\rangle=\int dx\psi_B(x)^2\exp[-i\Phi P_2(x)], \qquad (20)$$

where $\Phi=\phi(\infty)$. If the configuration space is restricted, by means of some continuum discretization procedure, the expression above will be modified. In the following section we will evaluate the convergence of the elastic amplitudes in the THO basis, as a function of Φ. Note that the Φ, which is associated to the integral of the coupling potential along the trajectory, is a dimensionless parameter that measures the importance of the coupling. Small values of Φ indicate that the elastic scattering dominates, while large values of Φ imply that excitation dominates.

III. SCATTERING CALCULATIONS IN THE THO BASIS

We make use of the THO basis to expand the wave function $\psi(x,t)$. The THO basis [9] is obtained from the ground-state wave function by the expression

$$\phi_n^{\mathrm{THO}}(x)=H_n(s(x))\psi_B(x), \qquad (21)$$

where $H_n(s)$ is a properly normalized Hermite polynomial, and $s(x)$ is given by Eq. (1). For these calculations, the binding interaction has been taken as a Pöschl-Teller potential [15], given by

$$v_B(x)=v_0/\cosh^2(\beta x). \qquad (22)$$

The potential depth $v_0=-\hbar^2\beta^2/\mu$ is taken so that it only accommodates one bound state, which has an energy $e_B=-\hbar^2\beta^2/2\mu$, and that is given by the analytic wave function

$$\psi_B(x)=\mathcal{N}/\cosh(\beta x). \qquad (23)$$

We can use the THO basis (21), with $n=0,\ldots,N$, to diagonalize the Hamiltonian h. This gives rise to $N+1$ eigenstates $\psi_j^h(x)$, whose corresponding eigenvalues are e_j, for $j=0$ to N. The state with $j=0$ is precisely the ground

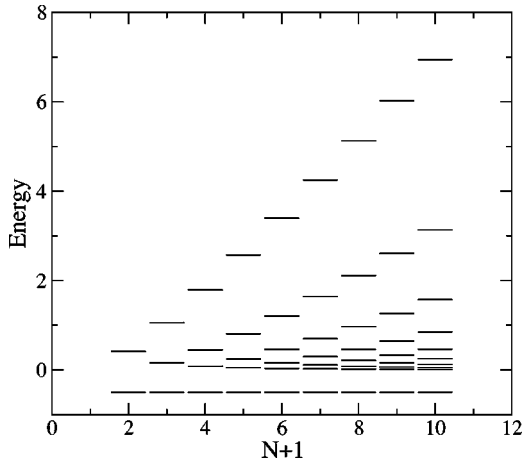

FIG. 1. Energy eigenvalues of the Hamiltonian of the composite object as a function of the number of states, $N+1$, in the THO basis. Energies are given in units of $(\hbar^2\beta^2/\mu)$.

state $\psi_B(x)$, which coincides with $\phi_0^{\mathrm{THO}}(x)$. The other states are normalizable states, which represent the continuum in the THO basis.

In Fig. 1 we present the values of the energies e_i obtained from the diagonalization of the internal Hamiltonian in the THO basis as a function of the number of states included in the THO basis. The energy scale is in units of $\hbar^2\beta^2/\mu$, so that the bound state has $e_B=-1/2$. In Fig. 2 we present the ten eigenfunctions of h constructed from the THO basis with $N+1=10$ (nine continuum states plus the bound ground state). We only had to include the wave functions with positive parity, which are the ones connected by the interaction.

The matrix elements of the interaction are proportional to the matrix elements of the operator $P_2(x)$. These matrix elements can be calculated in the THO basis as

$$\langle \phi_n^{\mathrm{THO}}|P_2|\phi_m^{\mathrm{THO}}\rangle = \int dx\,\psi_B(x)^2 H_n(s(x))P_2(x)H_m(s(x)). \tag{24}$$

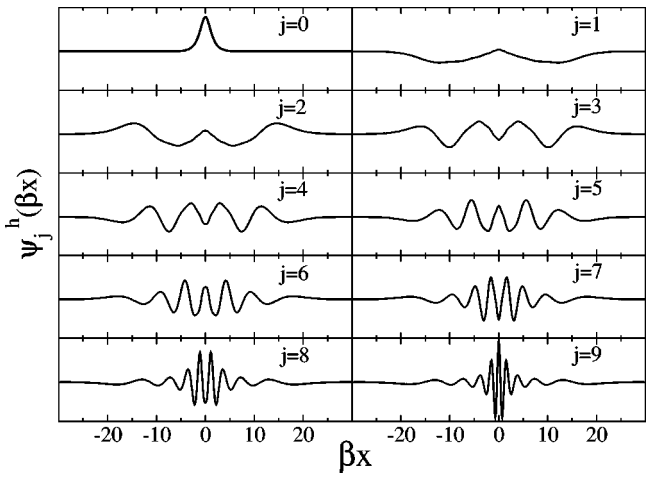

FIG. 2. Wave functions of the composite object in the THO basis with $N+1=10$, expressed as a function of βx (dimensionless).

TABLE I. Convergence of the polarizability α, in units of $(2\mu/\hbar^2\beta^2)$, as a function of the number of positive parity continuum states in the THO basis.

N	α
1	0.52155
2	0.70895
3	0.71720
4	0.71721
5	0.71721
Exact	0.71721

From this matrix, one can also calculate the matrix elements of P_2 in the basis of eigenstates of the Hamiltonian $|\psi_j^h\rangle$. Note that one can diagonalize the operator $P_2(x)$ in the THO basis. Let us label the eigenstates by $|\psi_k^{P_2}\rangle$ and the eigenvalues $P_2(k)$.

We will study the adequacy of the THO basis to describe the polarizability α. As we have argued in the preceding section, this is relevant to the description of the scattering process in the adiabatic limit. In the THO basis, the expression for the polarizability is

$$\alpha(\mathrm{THO}) = \sum_{j\neq 0} \frac{\langle \psi_B|P_2|\psi_j^h\rangle\langle\psi_j^h|P_2|\psi_B\rangle}{e_j - e_B}. \tag{25}$$

In Table I we present the convergence of this magnitude, expressed in units of $|e_B|^{-1}$, as a function of the number of THO states. As we can see, the convergence is very fast.

We will next consider the THO basis to describe the elastic scattering amplitudes in the sudden approximation. The expression corresponding to Eq. (20) in the THO basis can be formulated using the eigenstates of the operator $P_2(x)$ as

$$\langle \phi_B|A(\Phi)|\phi_B\rangle = \sum_k \langle \psi_B|\psi_k^{P_2}\rangle^2 \exp[-i\Phi P_2(k)]. \tag{26}$$

The probability of remaining in the ground state is given by the square of this amplitude. The results are plotted in Fig. 3, as a function of Φ. They indicate that the number of THO states needed to obtain the full sudden calculation increases as the coupling strength Φ increases.

We finally consider the general case, in which we do not make use of the adiabatic or sudden approximations. For the purpose of the calculations, we assume that the folding potential can be approximated by an exponential form, for distances beyond the turning point

$$V_F(X) = V_F(X_0)\exp[-(X-X_0)/a]. \tag{27}$$

It is straightforward to obtain the trajectory in this case. In terms of the variable $y=(X-X_0)/a$, one gets

$$\tanh(vt/2a) = \pm\sqrt{1-\exp[-y(t)]}, \tag{28}$$

where $v=\sqrt{2(E-e_B)/M}$ is the asymptotic velocity. In this equation, $t=0$ corresponds to the distance of closest ap-

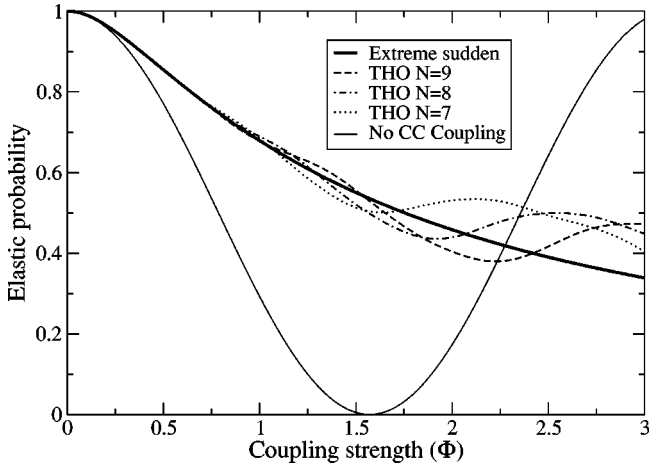

FIG. 3. Ground-state probability in the sudden limit as a function of the parameter Φ (dimensionless). The thick full line is the full sudden result. The dashed lines correspond to the THO discretization, for several numbers of states. The thin full line is the sudden calculation excluding continuum-to-continuum coupling.

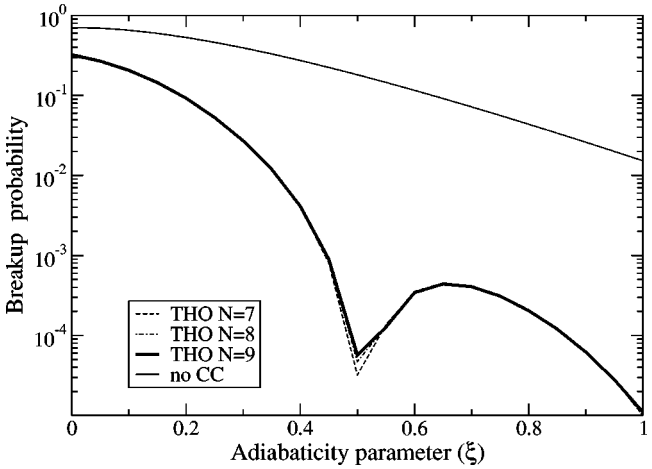

FIG. 4. Breakup probability as a function of the adiabaticity parameter ξ (dimensionless), for a fixed value of the coupling parameter $\Phi=1$. Lines corresponding to those marked in the legend box as THO are the full THO results for different numbers of states included in the basis. The thin full line is the converged result excluding continuum-to-continuum coupling.

proach, $y=0$. It should be noticed that the depth of the potential V_F only determines the distance of closest approach. The trajectory, measured with respect to X_0, only depends on the range a.

We will also assume that the coupling term is also exponential, with the same range as the folding potential. Then,

$$V_2(X)=V_2(X_0)\exp[-(X-X_0)/a]. \tag{29}$$

If this is expressed in terms of the time, one gets

$$F(t)=V_2(X(t))=V_2(X_0)\cosh^{-2}(vt/2a). \tag{30}$$

From this expression, one gets that the characteristic time of the collision is given by $T_c=a/v$. This time is to be compared with a characteristic time for the internal motion, which is $T_i=\hbar/|e_B|$. So, we define an adiabaticity parameter $\xi=T_c/T_i$. Small values of ξ correspond to the sudden limit, and large values to the adiabatic limit. Besides, we will define a dimensionless time $\tau=t/T_i$. The value of Φ for $F(t)$ is $4V_2(X_0)a/(\hbar v)$. Thus, we can write the interaction, in terms of suitable dimensionless parameters, as

$$F(\tau)=\frac{\Phi|e_B|}{4\xi}\cosh^{-2}[\tau/(2\xi)]. \tag{31}$$

With this expression, the equation of the evolution can be written as

$$i\frac{d}{d\tau}\psi(x,\tau)=\left[\frac{h-e_B}{|e_B|}+\frac{\Phi}{4\xi}\cosh^{-2}[\tau/(2\xi)]P_2(x)\right]\psi(x,\tau). \tag{32}$$

We expand the function in terms of the eigenstates of h in a THO basis. This gives

$$\psi(x,\tau)=\sum_{j=0}^{N} c_j(\tau)\psi_j^h(x)\exp[-i\tau(e_j-e_B)/|e_B|]. \tag{33}$$

Substituting this expansion in the previous equation, and projecting with $\psi_i^h(x)$ one gets,

$$i\frac{d}{d\tau}c_i(\tau)=\sum_{j=0}^{N}\frac{\Phi}{4\xi}\cosh^{-2}[\tau/(2\xi)]\langle\psi_i^h|P_2|\psi_j^h\rangle c_j(\tau) \times\exp[-i\tau(e_j-e_i)/|e_B|], \tag{34}$$

with the boundary condition that, for $\tau\to-\infty$, only $c_0(\tau)=1$ and the other components vanish.

The probability of remaining in the ground state, after the scattering, is given by $|c_0(\infty)|^2$. This value depends on the parameter Φ, which measures the coupling strength, and the parameter ξ, which measures the degree of adiabaticity. In Fig. 4 we represent the value of the ground-state probability versus ξ, for a fixed value of the coupling strength parameter $\Phi=1$, calculated in the THO basis. We see that the results converge rapidly as the number of THO states increases. Only when the adiabaticity parameter is very small ($\xi<0.1$) the convergence is not so fast. We have performed calculations for other values of the coupling strength, and we find that the convergence of the THO scattering calculations is very good except for the cases in which both the coupling strength is large and the adiabaticity parameter is small, this is, for strong coupling very close to the sudden limit.

We have evaluated the average value of the energy of the breakup states that are produced after the scattering process, weighted by the corresponding excitation probabilities. The results in Fig. 5 show that the average excitation energy increases as one goes to the sudden limit. That indicates that one should be careful when applying the sudden approximation, which implies neglecting the excitation energy, even in cases in which the adiabaticity parameter is small. We find that the convergence of the THO calculation is satisfactory,

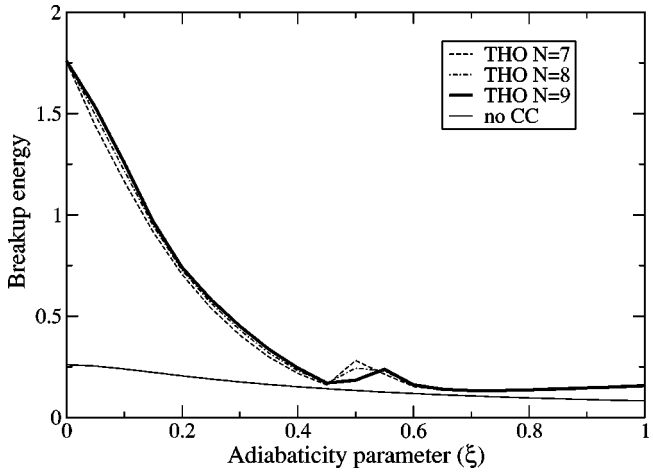

FIG. 5. Average of the energy of the breakup states, in units of $(\hbar^2\beta^2/\mu)$, as a function of the adiabaticity parameter ξ (dimensionless), for a fixed value of the coupling parameter $\Phi=1$. The lines correspond to the THO discretization, for several numbers of states. The thin line is the converged result excluding continuum-to-continuum coupling.

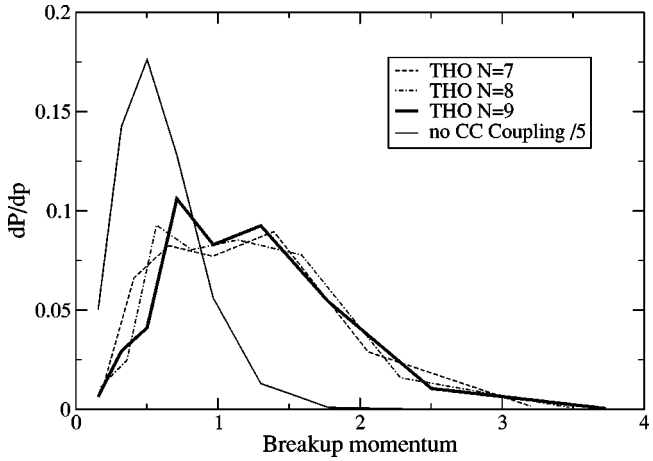

FIG. 6. Probability of excitation to the continuum, in units of $(\hbar\beta)^{-1}$, as a function of the breakup momentum, in units of $(\hbar\beta)$, for different numbers of states in the THO basis. The coupling strength is $\Phi=1$ and the adiabaticity parameter is $\xi=0.15$. The thin line is the converged result excluding continuum-to-continuum coupling.

except for $\xi\approx 0.5$. There the breakup probabilities are very small, and this induces uncertainties in the evaluation of the average energy.

We have investigated the breakup probability distribution obtained making use of the THO discretization. We have calculated approximately the differential probability of excitation as a function of the relative momentum of the breakup fragments. The evaluation of this function requires to estimate the interval that corresponds, in the true continuum, to each eigenstate of the internal Hamiltonian in the THO basis. The average momentum of our continuum states can be obtained in terms of the energy by means of $p_i^2/2\mu=e_i$. A simple interpolation procedure yields the range in terms of the momenta of the neighboring states,

$$\Delta_i=\frac{1}{2}p_{i+1}-\frac{1}{2}p_{i-1}, \quad 2<i<N, \tag{35}$$

$$\Delta_1=\frac{1}{2}p_2, \tag{36}$$

$$\Delta_N=-2p_{N-1}+\frac{3}{2}p_N+\frac{1}{2}p_{N-2}. \tag{37}$$

Thus, we can express the differential excitation probability at energies close to the THO eigenvalues by

$$\left(\frac{dP}{dp}\right)_{p=p_j}=\frac{P_j}{\Delta_j}. \tag{38}$$

In Fig. 6 we present the breakup probability distribution obtained in THO calculations using different number of states. The coupling parameter is taken as $\Phi=1$ as in the preceding calculation. The adiabaticity parameter is taken as $\xi=0.15$, which correspond to an intermediate situation between the adiabatic and sudden limits. We can see that there is a reasonable convergence of the calculations with different number of states. We have also performed calculations with different values of the coupling strength and the adiabaticity parameter. We find that larger coupling strength increases the breakup, but does not modify the form of the momentum distribution of the fragments. However, larger adiabaticity parameters (corresponding to slower collisions) move the momentum distribution to smaller values. The structure of the breakup distribution shows a single maximum at certain momentum distribution, with the exception of certain values of the adiabaticity parameter for each coupling strength, for which the breakup probability is very small, and the distributions shows two maxima.

IV. EFFECT OF CONTINUUM-TO-CONTINUUM COUPLING IN THE THO BASIS

Having established that the THO basis is an adequate method to describe the continuum of breakup states, we want to assess the question of whether the continuum-to-continuum coupling is important. For that, we have performed calculations in the THO basis where we have ignored continuum-to-continuum coupling, both diagonal and nondiagonal. Our first observation is that the calculation in the THO basis converges much faster in the cases in which continuum-to-continuum coupling is neglected. Usually, it is enough to introduce 3 or 4 continuum states in the THO basis to get convergence. In Fig. 3 we have presented the exact sudden result excluding continuum-to-continuum coupling. We have presented in Figs. 4, 5, and 6 the calculations with nine continuum states in the THO basis, which practically coincide with the calculations with 7 or 8 continuum states.

It should also be noticed that, comparing the calculations in Fig. 3, the breakup probability is considerably enhanced when continuum-to-continuum coupling is neglected. This is due, in our calculations, to the properties of the operator

$P_2(x)$ in the tidal potential. The expectation value of this operator vanishes for the ground state. However, for continuum states, with a large spatial extension, the expectation value is positive, and hence the tidal potential has a repulsive effect in these states, and this decreases the probability of breakup.

We have observed that this effect does not only occur in the sudden limit. For finite values of the adiabaticity parameter, the calculations that ignore continuum-to-continuum coupling give in general larger breakup probabilities. This is shown in Fig. 4. This effect is more acute as the coupling strength is larger. For weak coupling strength $\Phi \ll 1$, the effect of continuum-to-continuum coupling gets smaller.

We have also investigated the energy distribution of the breakup states obtained in calculations that ignore continuum-to-continuum coupling. As it is shown in Fig. 5, the average energy of the breakup states is lower in the calculations that neglect continuum-to-continuum coupling. Besides, as the collision is faster (adiabaticity parameter smaller) the increase in the excitation energy is smaller than when continuum-to-continuum coupling is considered.

The momentum distribution of the breakup fragments is also very different in the calculations neglecting continuum-to-continuum coupling, as it is shown in Fig. 6. These calculations give much larger breakup probabilities, which are concentrated on small values of the fragment momenta.

V. SUMMARY AND CONCLUSIONS

In this work we have made use of a recently proposed method to discretize the continuum of breakup states for weakly bound systems. The method, named THO, provides a basis of normalizable wave functions, which are generated by multiplying the ground state of the composite object by a number $N+1$ of Hermite polynomials on a variable $s(x)$. This variable is obtained as a local scale transformation from the physical variable x. As the number N increases, the basis approaches completeness, and the true continuum of breakup states should be accurately described in terms of the THO basis.

We have investigated the adequacy of the THO basis to describe the effect of the coupling to breakup states on the scattering of a composite object. We have considered a one-dimensional problem in which a composite object, made up of two structureless fragments that are initially bound, collides with a repulsive potential that depends both on the center of mass coordinate and on the relative coordinate of the fragments. This potential is approximated as the sum of a folding potential, which acts on the center of mass coordinate, and determines the classical trajectory, and a tidal potential, which is written as the product of a coupling form-factor times an operator acting on the relative coordinate. As a result of the collision, the composite object can breakup producing fragments with a certain energy distribution. We use a semiclassical approximation, by which the center of mass describes a trajectory that is determined by the folding potential. The evolution of the internal state of the composite system is determined by a time-dependent Schrödinger equation, which is projected on a finite THO basis.

We find that the dynamics of the collision can be characterized within a semiclassical approximation in terms of two dimensionless parameters. One is the coupling strength, which is defined as the time integral of the coupling form-factor along the trajectory and the other is the adiabaticity parameter, which is the ratio of the collision time and the characteristic time for the internal motion.

When the collision is slow, the adiabaticity parameter is large and one is in the adiabatic limit. In this case, the effect of coupling to the continuum is just to induce a phase change in the elastic wave function. The calculations in the THO basis converge very quickly to the exact results in this case.

When the collision is fast, the adiabaticity parameter is small and one is in the sudden limit. In this case, the number of THO states needed to obtain convergence in the elastic probability depends on the value of the coupling strength.

We have performed calculations in intermediate situations, for different values of the coupling strength and the adiabaticity parameters. We find that the convergence in the THO basis is satisfactory, except in situations in which both the coupling strength is large and the adiabaticity parameter small, this is, in situations of strong coupling close to the sudden limit.

We have used the THO basis to evaluate different scattering magnitudes in our model problem. We find that the probability of breakup increases, in general, as the coupling strength increases, and as the adiabaticity parameter decreases. However, there are certain values of the adiabaticity parameter, for each coupling strength, for which the breakup probability gets very small. We find that the THO calculations, with different numbers of states, present consistently this feature.

We have used the THO basis to evaluate the energy distribution of the breakup states. We find that the average excitation energy of the breakup states does not depend very much on the coupling strength, and increases significantly as the adiabaticity parameter decreases. We have also evaluated the energy distribution of the breakup states, finding that the distribution is wider for the lower adiabaticity parameter.

We have investigated the role of continuum-to-continuum coupling in this problem. We find that the THO method converges very fast when continuum-to-continuum coupling is neglected, even in the sudden limit. We find that, when continuum-to-continuum coupling is neglected, the breakup probabilities are, in general, overestimated. Also, the energy distribution of the breakup states becomes narrower. We interpret these results as a consequence that, due to the form of the $P_2(x)$ operator that generates the coupling, the effect of continuum-to-continuum coupling is repulsive for the breakup states, and this reduces the effect of the coupling in the full calculations. We also find that, if continuum-to-continuum coupling is neglected, we do not get the special values of the adiabaticity parameter for which breakup is very small. So, we can conclude that, at least in the scattering problem under discussion, continuum-to-continuum coupling is very important, and that the THO basis is a useful method to study its effect. It should be noticed that both calculations, with continuum-to-continuum coupling and without it, converge satisfactorily in the THO basis.

We conclude that the THO basis is adequate to describe the coupling to breakup states in scattering problems that can be treated within the semiclassical approximation. For a full quantum-mechanical calculation the THO basis provides with a finite set of normalized states that represent the continuum of breakup states. These wave functions are used to evaluate diagonal and transition potentials, which enter in a standard coupled channel calculation. We have already applied this method to describe the scattering of deuterons on heavy targets with satisfactory results [16].

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