One dimensional scattering of a two body interacting system by an infinite wall

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Abstract

The one-dimensional scattering of a two body interacting system by an infinite wall is studied in a quantum-mechanical framework. This problem contains some of the dynamical features present in the collision of atomic, molecular and nuclear systems. The scattering problem is solved exactly, for the case of a harmonic interaction between the fragments. The exact result is used to assess the validity of two different approximations to the scattering process. The adiabatic approximation, which considers that the relative co-ordinate is frozen during the scattering process, is found to be inadequate for this problem. The uncorrelated scattering approximation, which neglects the correlation between the fragments, gives results in accordance with the exact calculations when the scattering energy is high compared to the oscillator parameter.

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I. INTRODUCTION

Recently, important efforts in the fields of molecular, atomic and nuclear physics have been devoted to the analysis of collision processes involving composite quantum systems. Despite the peculiarities of the different fields, the theoretical description of the collision has several common features. R-matrix theory [1] is used for re-arrangement collisions, when several electrons or nucleons may be exchanged between the colliding systems. Coupled channels calculations [1, 2] are used to describe excitation and dissociation in atomic, molecular and nuclear systems. The "adiabatic" or "sudden" approximation is often invoked in molecular and nuclear collisions, because it simplifies significantly the description of the scattering process, by considering that some of the relevant co-ordinates are effectively frozen during the scattering process. Also, the description of the collision of atomic and molecular beams with surfaces requires coupled channels descriptions, but the combined difficulties of the atom-surface interactions and molecular vibrations makes the "sudden" approximation almost essential for its solution [2].

In the case of atomic and molecular physics, one-dimensional atom-molecule collision reactions have been studied in detail by solving the Schrödinger equation [3]. In particular, collisions between an atom and a diatomic molecule represented by harmonic [4], an-harmonic [5] and Morse oscillators [6] have been analysed with different degrees of approximation. Diverse computational methods have been also implemented to study three-dimensional molecular and atomic collisions [7]. Moreover, in some recent papers algebraic approaches have been proposed for describing one- and three-dimensional atom-molecule collision processes [8, 9].

In the field of nuclear physics, much of the interest in recent years has been focused on the study of the properties of halo nuclei, weakly bound systems characterised by the existence of one or two particles (generally neutrons) with a high probability of being at distances larger than the typical nuclear radius. Different approaches have been used in the analysis of reactions involving halo nuclei. The adiabatic approximation [10–13] assumes that, for sufficiently high scattering energies, the internal Hamiltonian is accurately represented by its corresponding eigenvalue for the ground state. The sudden approximation [14–17] relies on two main assumptions: i) the impulse approximation, i.e., the multiple scattering expansion for the T-matrix is approximated by the sum on the individual T-matrices for the scattering of the separated constituents, and ii) only one of the particles of the pro-

jectile interacts with the target. In the high energy regime, the Glauber approach [18], which combine eikonal dynamics with the adiabatic approximation, provides a simple tool to analyse reactions involving halo nuclei. We have recently developed an alternative approach to the description of weakly bound systems. The approach, called "Uncorrelated Scattering Approximation" (USA) [19, 20], is based on the fact that, for a weakly bound projectile, the correlations between the constituents are weak and so, to some extent, they are expected to evolve independently in the strong field of a heavy target. Thus, the three body S-matrix can be expressed in terms of the individual two body S-matrices for the scattering of the constituents. In this framework, the scattering observables of the process are given in terms of two body constituent-target observables. This model has been applied to describe elastic scattering and break-up of deuterons on heavy targets, with encouraging results. The Uncorrelated Scattering Approximation has certain relation with the R-matrix approach. In a R-matrix calculation of deuteron scattering, the wave-function within the range of the target interaction is given in terms of products of single-particle (protons and neutrons) wave-functions with the proper boundary conditions, provided the interaction between the fragments of the projectile is neglected. These single-particle wave-functions should be matched with the proper asymptotic wave-functions. In the USA calculation, the incident wave is expanded in terms of products of fragment-target wave-functions, which then scatter independently from the target.

The objective of this work is to investigate the scattering of a composite system from a target with interactions which have a very short range compared not only with the size of the system, but also with the associated wave-length of the projectiles. For that purpose, we consider the case of two particles, interacting through a harmonic oscillator potential, which collide with an infinite wall. We develop two different methods to solve the problem exactly, obtaining the wave-function as well as the S- matrix, or reflection coefficients, which give the probability amplitudes for the excitation of the different oscillator states. We compare the exact results with the ones obtained using the adiabatic approximation, and the uncorrelated scattering approximation.

The model discussed here does not pretend to be a realistic representation of any specific molecular, atomic or nuclear system. However, it has the virtue that the only length scale is the oscillator length a_0, while the only energy scale is the oscillator parameter $\hbar\omega$. Then, the results obtained, which are expressed in terms of r/a_0 and $E/\hbar\omega$, can be applied in principle
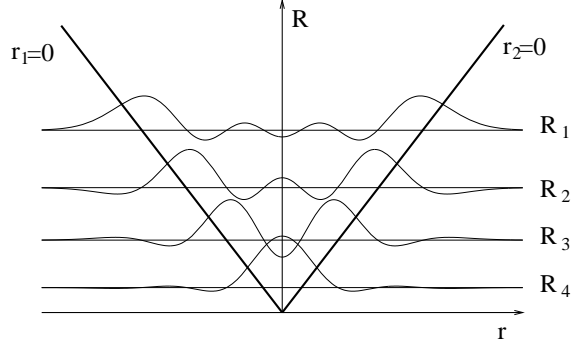
FIG. 1: Schematic plot representing the scattering problem in the (r, R) plane. The waves represent the SCLS associated with a basis with $N = 8$ HO states. Each one of these SCLS has been plotted at the center of mass distance at which it is supposed to be scattered by the wall, according to the formalism described in section II B.

to arbitrary energy and length scales, which may be nuclear, atomic or molecular. This fact makes the model attractive as a bench-mark to test the validity of the approximations which are used for the description of composite systems.

One aspect of the model which seems odd is the infinite nature of the harmonic oscillator interaction between the fragments. This would prevent dissociation in the case of molecules, ionization in the case of atoms or break-up for nuclei. On the other hand, the harmonic oscillator basis is complete, and thus the results of the model incorporate effects on the scattering due to coupling to all possible, open or closed, states.

The paper is organised as follows: in section II we describe the problem to be solved. Two different approaches to extract the exact solutions are developed. In section III we derive the S-matrix in the adiabatic model approach. In section IV we present the Uncorrelated Scattering Approximation. In section V we apply it to evaluate the scattering coefficients and compare with the exact solution. Section VI is devoted to summary and conclusions.

II.   STATEMENT OF THE PROBLEM AND EXACT SOLUTION

Let us consider the scattering of a two-particle bound system by the short range potential due to a heavy target, placed at the origin of coordinates.

The Hamiltonian for the system may be written in terms of the coordinates of the two particles (r_1, r_2) and their momenta (p_1, p_2) as
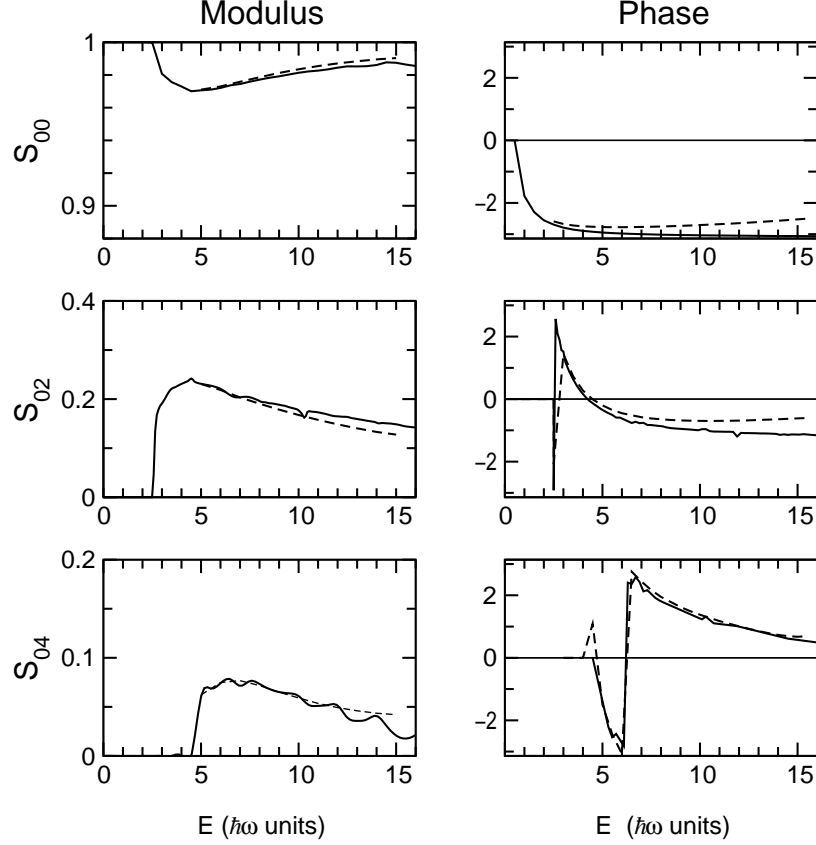
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FIG. 2: S-matrix elements versus the scattering energy for the HO states $n =0$, 2 and 4. The solid and dashed lines correspond to the exact calculation using the methods of sections II A and II B, respectively. A basis space with 15 even parity HO states was used for the calculations.

$$\hat{H} = \hat{h}_1 + \hat{h}_2 + v(r_1 - r_2) \tag{1}$$

$$\hat{h}_i = \frac{\hat{p}_i^2}{2m_i} + v_i(r_i) \tag{2}$$

where m_i are the masses of the constituents, $v_i(r_i)$ is the potential exerted by the target on each particle and $v(r_1 - r_2)$ represents the binding interaction.

Alternatively, it can be expressed in terms of the relative (r) and centre of mass coordinate (R):

$$\hat{H} = \hat{H}_r + \hat{H}_R + v_1(R + \alpha_2 r) + v_2(R - \alpha_1 r), \tag{3}$$

$$\hat{H}_r = \frac{\hat{p}_r^2}{2\mu} + v(r) \tag{4}$$

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$$\hat{H}_R = \frac{\hat{P}_R^2}{2M} \tag{5}$$

where M is the total mass, $\alpha_i = m_i/M$ $(i = 1, 2)$, and $\hat{H}_r$ is the internal Hamiltonian. Here, μ represents the reduced mass of the two-particle system and $r = r_1 - r_2$ is the relative coordinate.

We refer to the specific case in which $v_i(r_i)$ corresponds to an infinite wall potential, i.e.:

$$v_i(r_i) = \begin{cases} 0 & r_i > 0 \\ \infty & r_i \leq 0 \end{cases} \tag{6}$$

For negative values of r_1 and r_2 the total wave function must vanish. For positive values, the Hamiltonian comprises two terms: one associated with the internal motion of the projectile ($\hat{H}_r$) and the other describing the centre of mass motion ($\hat{H}_R$).

We take $v(r)$ to be a harmonic interaction. Therefore, the eigenfunctions for the internal Hamiltonian are given by

$$\phi_n(r) = \mathcal{N}_n^{-\frac{1}{2}} \exp\left(-\frac{r^2}{2a_0^2}\right) \mathcal{H}_n\left(\frac{r}{a_0}\right) \; ; \; n = 0, 1, \ldots \tag{7}$$

where $a_0 = \sqrt{\hbar/\mu\omega}$ is the oscillator length, $\mathcal{N}_n$ a normalisation constant and $\mathcal{H}_n$ the Hermite polynomial of order n.

Denoting by N the number of open channels, the total wave function will be then expanded in terms of eigenstates of the Hamiltonian as follows:

$$\Psi(r, R) = \frac{1}{\sqrt{v_0}}\phi_0(r)e^{-iK_0R} - \sum_{m=0}^{N-1} \frac{S_{0m}}{\sqrt{v_m}}\phi_m(r)e^{iK_mR} - \sum_{m=N}^{\infty} F_{0m}\phi_m(r)e^{-|K_m|R}. \tag{8}$$

In this expression K_m represents the centre of mass momentum associated with the internal state m and $v_m = \hbar K_m/M$ its velocity. Energy conservation applied to the whole system leads to the constrain

$$\frac{(\hbar K_m)^2}{2M} + \epsilon_m = E, \tag{9}$$

where ϵ_m is the eigenvalue corresponding to the internal state $\phi_m(r)$.

The first term in (8) represents an incoming wave, normalised to unit flux, coming from $R = +\infty$. The second term contains the set of scattered waves travelling in the positive R direction corresponding to open channels, i.e., $\epsilon_m < E$. The coefficients S_{nm} are the
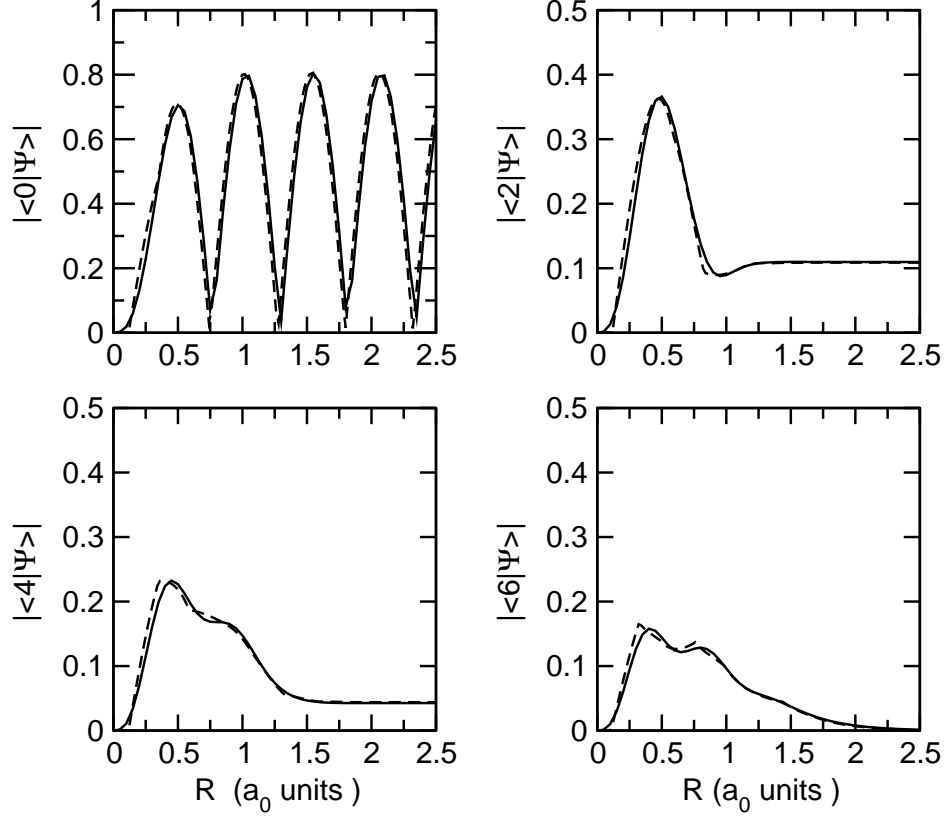
FIG. 3: Projection of the total wave functions on the internal eigenstates n=0, 2, 4 and 6, for the scattering energy $E = 5\,\hbar\omega$. The solid line corresponds to the exact calculation by direct application of the boundary conditions, whereas the dashed line corresponds to the exact calculation in the CLS approach.

S-matrix elements or, strictly speaking, reflection coefficients. Then, S_{0m} represents the amplitude probability of populating the state m during the collision starting from a wave function in its ground state. The last term in (8) contains the contribution to the wave function due to the (infinite) set of closed channels, for which $\epsilon_m > E$. For these states, the associated momentum K_m is a pure imaginary quantity, and the centre of mass motion is described by an exponential decaying behaviour. Therefore, they do not contribute to the asymptotic wave function and so they do not give direct contribution to the outgoing flux. Although they are usually ignored in practical calculations, the peculiarity of the infinite potential requires however the inclusion of these states in order to describe correctly the wave function in all the space.

In this problem there is no transmitted wave due to the presence of the wall and so the S-matrix should fulfil unitarity. Therefore, the ingoing and outgoing flux must be equal:

$$\sum_{m=0}^{N-1} |S_{nm}|^2 = 1, \tag{10}$$

where the sum extends to the set of open channels.

The coefficients S_{nm} and F_{nm} are determined by imposing the boundary conditions at $r_i = 0$. For the infinite wall the wave function must vanish at $r_1 = 0$ and $r_2 = 0$ which, in terms of r and R means

$$\Psi(r, R = +\alpha_1 r) = 0 \quad (r > 0),$$

$$\Psi(r, R = -\alpha_2 r) = 0 \quad (r < 0). \tag{11}$$

In what follows we present two alternative methods to solve *exactly* this problem.

A.   Exact solution by direct application of the boundary conditions

As described above the exact solution of the scattering problem of a two-body projectile by a rigid wall is accomplished by applying the boundary conditions (11) to the general solution (8). For simplicity we assume that the system is initially in its ground state. The first condition in (11) leads to the following equation for the scattering coefficients:

$$\frac{1}{\sqrt{v_0}} e^{-iK_0\alpha_1 r}\phi_0(r) - \sum_{n=0}^{N-1} \frac{S_{0n}}{\sqrt{v_n}} e^{iK_n\alpha_1 r}\phi_n(r) - \sum_{n=N}^{\infty} F_{0n}e^{-|K_n|\alpha_1 r}\phi_n(r) = 0 \, ; \, r > 0. \tag{12}$$

The second condition in (11) leads to a similar equation (with α_2 instead of α_1) which holds for $r < 0$. In particular, we have performed calculations for the particular case of equal masses, i.e., $\alpha_1 = \alpha_2 = \frac{1}{2}$, for which both equations are identical, due to the symmetry of the problem under the exchange of r_1 and r_2. In the remaining of this section we restrict to this particular case.

In order to transform eq. (12) into an ordinary algebraic equation, we require that

$$\int_0^{+\infty} \left| \Psi(r, R = \frac{1}{2}r) \right|^2 dr = 0, \tag{13}$$

which gives for the scattering coefficients the relation:

$$\frac{1}{2} - \sum_n (C_{0n}a_{0n} + C_{0n}^* a_{0n}^*) + \sum_{n,m} C_{0n}C_{0m}^* b_{nm} = 0, \tag{14}$$

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where

$$C_{0n} = \begin{cases} \sqrt{\frac{v_0}{v_n}} S_{0n} \; ; \; n < N \\ \sqrt{v_0} F_{0n} \; ; \; n \geq N \end{cases} \tag{15}$$

and

$$a_{0n} = \int_0^\infty \phi_0^*(r)\phi_n(r)e^{i(K_n+K_0)\frac{1}{2}r} \; ; \; n < N, \tag{16}$$

$$b_{nm} = \int_0^\infty \phi_n^*(r)\phi_m(r)e^{i(K_m-K_n)\frac{1}{2}r} \; ; \; n,m < N. \tag{17}$$

The expressions for a_{0n} and b_{nm} for $n,m \geq N$ are obtained substituting $\pm iK_n$ for $-|K_n|$.

Differentiating eq. (14) with respect to C_{0n}^* we get the following linear system in the variables C_{0n}:

$$\sum_{m=0}^\infty C_{0m}b_{nm} = a_{0n}^*, \quad n = 0, \ldots, \infty. \tag{18}$$

For practical calculations the resolution of this system requires the truncation of the sum at some finite value of m. It should be noticed that in order to achieve convergence for the S-matrix elements one is forced to include in the calculation several closed channels. Otherwise, the boundary conditions (11) are not accurately fulfilled.

B. Exact solution using a discrete basis

In this section we present an alternative method to obtain the exact solution of the problem stated above. The method relies on the introduction of a new basis of states which are particular linear combinations of the internal wave functions. The new functions have the property of being highly localised in configuration space. As we shall see this peculiarity allows to apply more easily the boundary conditions.

We start with a truncated basis of N eigenstates for the internal Hamiltonian that we denote by $\{|Nn\rangle; n = 1, \ldots, N-1\}$. Thus, according to our previous notation, $\langle r|Nn\rangle = \phi_n(r)$.

In the appendix we show how these states can be decomposed in terms of configuration localised states (CLS) as

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$$|Nn\rangle = \sum_{s=1}^{N} \langle CLS; Ns|Nn\rangle \, |CLS; Ns\rangle \qquad (19)$$

In this expression the ket $|CLS; Ns\rangle$ represents a configuration localised state. Explicit expressions for the CLS associated with the HO wave functions can be found in the appendix and in Ref. [22]. The function $\langle r|CLS; Ns\rangle$ has the property of being highly localised around $r = r_s$, the s-th zero of the eigenfunction $\langle r|N\,N\rangle$.

The problem is significantly simplified in the case of fragments of equal masses. Parity conservation guarantees that only states with the same parity as the incident wave function will be populated in the process. This allows to work in the subspace: $\{\phi_n(r); n = 0, 2, \ldots, N-2\}$ (for simplicity of the notation, and without loss of generality, we take N even). These functions are symmetric with respect to their natural variable, r. From this set of $\frac{N}{2}$ states it is possible to construct, by means of a transformation similar to (19), a set of *symmetric configuration localised states* (SCLS), which are also even functions with respect to the variable r. We denote this new set of states by $\{|SCLS; Ns\rangle; s = 1, \ldots, \frac{N}{2}\}$, where the index s runs over the positive zeros of $\mathcal{H}_N(x)$. The details of its derivation are presented in the appendix. The state $\langle r|SCLS; Ns\rangle$ has the property of being localised around the points $r = r_s = \pm x_s a_0$, where x_s is the $s-$th positive zero of the Hermite polynomial $\mathcal{H}_N(x)$. In the treatment that follows we make extensive use of this remarkable signature.

The boundary condition due to the wall requires that the total wave function vanishes for $r_1 = 0$ and $r_2 = 0$ or, in terms of coordinates r and R, along the lines $R = r/2$ ($r > 0$) and $R = -r/2$ ($r < 0$) in the $(R,\, r)$ plane. At each value of R a reflected wave is generated, interfering with the other outgoing waves to construct the total scattered wave. This picture is simplified working in terms of SCLS. The part of the wave function associated to the state $\langle r|SCLS; Ns\rangle$ is peaked around $r = \pm r_s$ and, therefore, it will be mainly scattered around $R = R_s = |r_s|/2$. In the limit case $N \to \infty$, $\langle r|SCLS; Ns\rangle$ becomes a delta function in r and the associated wave is exactly scattered at $R = R_s$. Moreover, continuity of the wave function implies that a reflected wave, affected by a phase factor $-\exp(-2iK_oR_s)$, is generated at this point. Obviously, this is not exactly our situation as, in practise, N is always finite and so our localised states have a finite dispersion around r_s. However, we can make this dispersion as small as required by increasing the number of states.

Consequently, the process is considered as a distribution of localised states that are

reflected at some definite *barriers* in the R direction. The total scattered wave is given by the superposition of the reflected waves. To make the treatment clearer, we divide the R axis in $\frac{N}{2}$ regions, delimited by the values of R_s. We order the zeros of the Hermite polynomial $\mathcal{H}_N$ in such way that $R_1 > R_2 > \ldots > R_{N/2}$. Let us introduce an index i to label each region $(i = 1, \ldots, \frac{N}{2})$, such that $i = 1$ corresponds to the asymptotic region, i.e., $R > R_1$, before any localised state has been reflected. In this region the basis space associated with the internal motion is described in terms of the first $\frac{N}{2}$ HO eigenfunctions with positive parity. Alternatively, it can be described in terms of $\frac{N}{2}$ symmetric localised states.

At $R = R_1$ the SCLS corresponding to $s = 1$ is reflected and removed from the incident wave function, while the rest of SCLS remain unaltered. Therefore, in the region $i = 2$ the basis is limited to the subspace spanned by the remaining $\frac{N}{2} - 1$ states $(s = 2, ..., \frac{N}{2})$. Subsequently, our original set of states are no longer eigenstates of the Hamiltonian in this region. Instead, a new family of $\frac{N}{2} - 1$ eigenstates must be calculated, by diagonalizing the Hamiltonian in the basis constituted by the remaining $\frac{N}{2} - 1$ localised states.

The method is schematically illustrated in Fig. 1. The picture represents the scattering problem in the (r, R) plane. The total wave function travels in the R direction (vertical axis) and must vanish along the lines $r_1 = 0$ and $r_2 = 0$, which have been also plotted for reference. The case with $N = 8$ has been considered, in which the incoming wave is decomposed in a set of four SCLS. Each one of these SCLS is consider to scatter at a definite barrier in the R axis, labelled from R_1 to R_4. Note that they partially extend to the forbidden region $(r_i < 0)$, which is a consequence of the truncation of the HO basis.

Let us specify explicitly the boundary condition at $R = R_i$. This barrier separates regions i and $i + 1$. The eigenstates corresponding to region i will be denoted by $\{|N^{(i)}\, m\rangle;\ m = 0, ..., N^{(i)} - 1\}$ where $N^{(i)} = \frac{N}{2} - i + 1$ is the number of states in region i. The total wave function is then expanded in each region in terms of the corresponding eigenstates. For region i, corresponding to the interval $R_{i-1} > R > R_i$, we have:

$$|\Psi^{(i)}(E)\rangle = \sum_{m=0}^{N^{(i)}-1} \left(A_m^{(i)} e^{-iK_m^{(i)}R} - B_m^{(i)} e^{+iK_m^{(i)}R} \right) |N^{(i)}\, m\rangle, \tag{20}$$

where $A_m^{(i)}$ $(B_m^{(i)})$ are the coefficients of the incoming (outgoing) waves. Energy conservation requires, in analogy with (9),
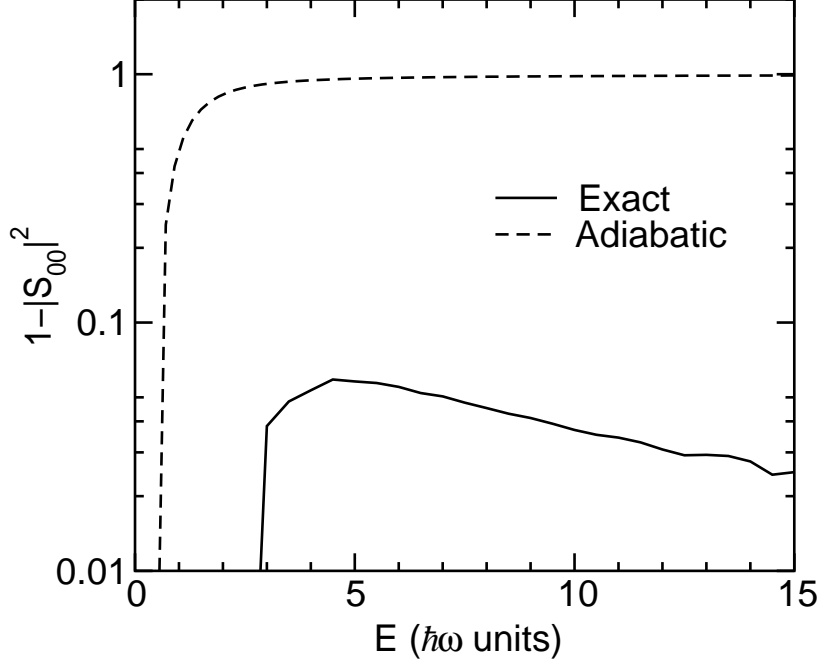
FIG. 4: Representation of the quantity $1 - |S_{00}|^2$ versus the scattering energy for the exact calculation (solid line) and the adiabatic model (dashed line).

$$\frac{(\hbar K_m^{(i)})^2}{2M} + \epsilon_m^{(i)} = E, \tag{21}$$

where $\epsilon_m^{(i)}$ is the m-th eigenvalue of the Hamiltonian in region i and $K_m^{(i)}$ its corresponding centre of mass momentum.

Similarly, for region $i+1$ the wave function will be written as

$$|\Psi^{(i+1)}(E)\rangle = \sum_{n=0}^{N^{(i+1)}-1} \left(A_n^{(i+1)} e^{-iK_n^{(i+1)}R} - B_n^{(i+1)} e^{+iK_n^{(i+1)}R} \right) |N^{(i+1)}\, n\rangle. \tag{22}$$

At $R = R_i$ the part of the wave function associated with the localised state $s = i$ is reflected by the wall. Therefore, continuity of the wave function requires that

$$\langle SCLS; N\, i|\Psi^{(i)}(E)\rangle\Big|_{R_i} = 0. \tag{23}$$

By contrast, the rest of localised states are unaffected by this barrier, so we may require continuity of the wave function and its derivative for the components $s > i$:

$$\langle SCLS; N\, s|\Psi^{(i)}(E)\rangle\Big|_{R=R_i} = \langle SCLS; N\, s|\Psi^{(i+1)}(E)\rangle\Big|_{R=R_i} \tag{24}$$
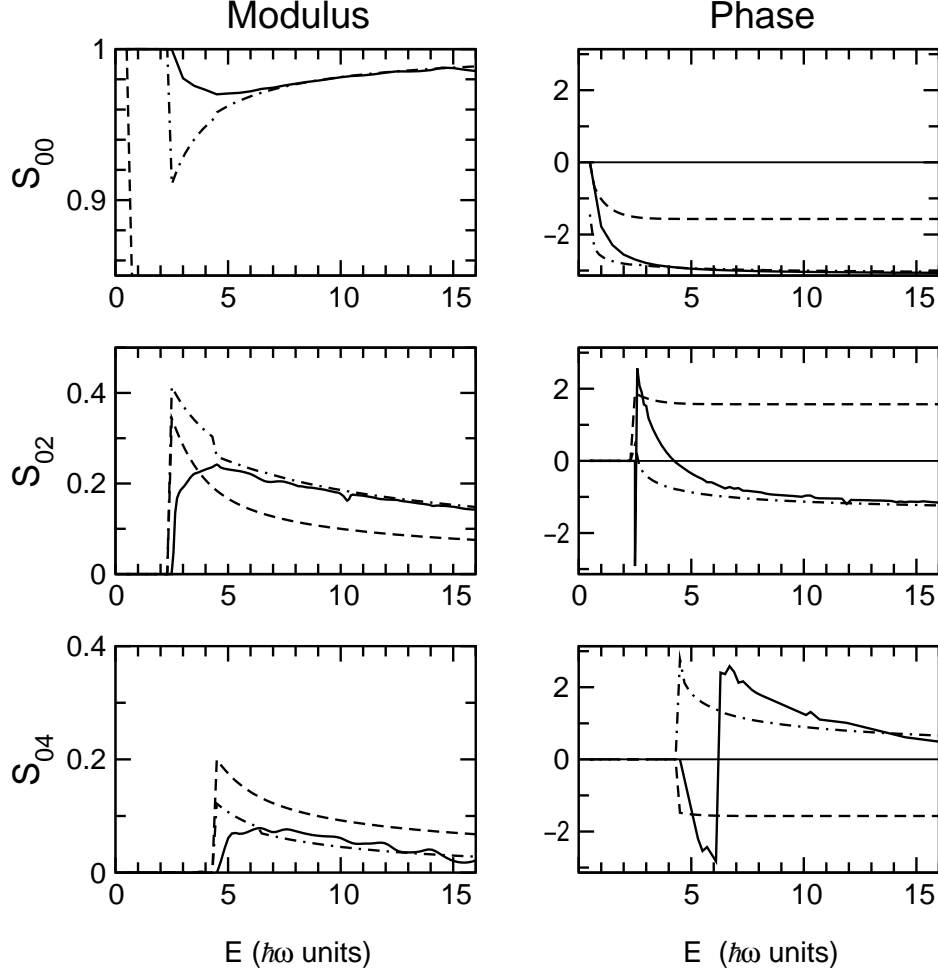
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FIG. 5: S-matrix coefficients for the ground and first excited states. The solid line is the exact calculation. The dot-dashed line corresponds to the USA model, with the prescription (47) for the phases. The dashed line corresponds to the adiabatic model.

$$\left[\frac{d}{dR}\langle SCLS; N\, s|\Psi^{(i)}(E)\rangle\right]_{R=R_i} = \left[\frac{d}{dR}\langle SCLS; N\, s|\Psi^{(i+1)}(E)\rangle\right]_{R=R_i}. \tag{25}$$

Equations (23) to (25) give rise to a set of $2\left(\frac{N}{2}-i\right)+1$ conditions for the scattering coefficients $A_n^{(i)}$ and $B_n^{(i)}$ ($n=0,\ldots,N^{(i)}-1$). When applied to all regions a total of $\left(\frac{N}{2}\right)^2$ equations with $\frac{N}{2}(\frac{N}{2}+1)$ coefficients is obtained. From these, the $\frac{N}{2}$ coefficients $A_n^{(0)}$ are known, as they are determined by the initial conditions. Therefore, there remain $\frac{N}{2}(\frac{N}{2}+1)-\frac{N}{2}=\left(\frac{N}{2}\right)^2$ coefficients to be determined, that coincides with the number of equations. Thus, the resolution of the problem reduces to the calculation of the inverse of a $\left(\frac{N}{2}\right)^2\times\left(\frac{N}{2}\right)^2$ matrix. This can be a slow computational task when N takes large values. This drawback has led us to adopt an alternative method that avoids this sort of calculations,

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speeding significantly the computational time. For its application, it is convenient to define a generalised "S-matrix" for region i as:

$$B_n^{(i)} = \sum_{n'} \sqrt{\frac{K_{n'}^{(i)}}{K_n^{(i)}}} S_{n'n}^{(i)} A_{n'}^{(i)}. \tag{26}$$

For region $i = 1$ this definition gives just the usual S-matrix. The factor $\sqrt{K_{n'}^{(i)}/K_n^{(i)}}$ has been introduced to ensure unitarity.

Substituting this expression into equations (23) to (25) we get a set of $2\left(\frac{N}{2} - i\right) + 1$ equations relating the S-matrix elements of $S^{(i)}$ and $S^{(i+1)}$. Then, instead of solving the system of equations as a whole, we perform an iterative calculation in which the S-matrix for each region is determined in terms of the S-matrix for the neighbouring region. The starting point is the region $i = \frac{N}{2}$, for which the S-matrix is known. In this region there is only one state left, which is completely reflected at $R_{N/2}$. The S-matrix in this case is just the phase factor: $S^{(\frac{N}{2})} = \exp\left(-2iK_1^{(\frac{N}{2})} R_{N/2}\right)$. From this, we can determine the S-matrix for region $\frac{N}{2} - 1$, and so on. Finally, we obtain the S-matrix, $S^{(1)}$, in terms of $S^{(2)}$. Taking into account (26) and the fact that $A_n^{(1)}$ are given by the initial conditions, it is possible to determine the coefficients $B_n^{(1)}$. One can derive also an iterative procedure to determine the coefficients $A_n^{(i)}$ for all regions in terms of the corresponding S-matrices.

C. Discussion of the exact results

In order to compare both treatments we have plotted in figure 2 the S-matrix coefficients S_{00}, S_{02} and S_{04}, as a function of the scattering energy. The energy scale is in units of $\hbar\omega$. A basis space with 15 even parity HO states was used for the calculation. The figure shows a good agreement between both treatments, specially at low scattering energies. As the scattering energy increases, the effect of the truncation of the basis becomes more important and both calculations differ slightly. Notice that this discrepancy appears to be more evident for the phase of the S-matrix elements. Nevertheless, this difference between both calculations is reduced as the number of basis states is increased.

We notice that, as expected, the elastic coefficient is identically one for scattering energies below $\frac{5}{2}\hbar\omega$. This corresponds to the energy of the first excited state that is suitable to be populated. Accordingly, the inelastic coefficients, $S_{02}, S_{04}, \dots$ are identically zero below this

threshold. For scattering energies higher than $\frac{5}{2}\hbar\omega$, the modulus of the elastic coefficient is less than one and the rest of the coefficients are non zero. Note that the modulus of S_{00} presents a minimum at $E = 5\,\hbar\omega$, indicating a maximal loss of flux from the elastic channel to other channels at this energy. For higher scattering energies the modulus of elastic scattering coefficient tends gradually to unity.

We have also compared the wave functions in both approaches. In our problem the wave function is a complex quantity depending on two variables, r and R. For the exact direct calculation the wave function is given by (8), where the scattering coefficients are calculated by imposing the boundary conditions (11). It must be noticed, however, that this expression only holds for r_1, $r_2 \geq 0$ or, equivalently, for $-2R < r < 2R$. Outside this range, the total wave function must be identically zero. The projection of the wave function on a state $|N\,n\rangle$ is calculated as

$$\Psi_n(R) \equiv \langle N\,n|\Psi\rangle = \int_{-2R}^{2R} dr\phi_n^*(r)\Psi(r,R). \tag{27}$$

For large values of R (compared to the spatial extension of the internal wave function) the integral can be extended to the interval $(-\infty,\infty)$ and the projection above is directly related to the corresponding S-matrix element:

$$\Psi_n(R) \approx \int_{-\infty}^{\infty} dr\phi_n^*(r)\Psi(r,R) = \frac{1}{\sqrt{v_0}}\delta_{n0}e^{-iK_0R} - \frac{1}{\sqrt{v_n}}S_{0n}e^{iK_nR}; \quad (R \gg a_0). \tag{28}$$

In the analysis based on CLS, the total wave function is given in terms of a piecewise function of R, according to (20). For a certain region i, this wave function is written as a superposition of the eigenstates of the Hamiltonian in this region. These eigenstates travel freely between the consecutive barriers R_i and R_{i+1}. Thus, the projection on a state $|Nn\rangle$ for a value of R belonging to a region i reads

$$\Psi_n^{(i)}(R) = \langle N\,n|\Psi^{(i)}\rangle = \sum_{m=0}^{N^{(i)}-1} \left(A_m^{(i)}e^{-iK_m^{(i)}R} - B_m^{(i)}e^{+iK_m^{(i)}R} \right) \langle N\,n|N^{(i)}\,m\rangle. \tag{29}$$

We notice that, except for the incoming region ($i = 1$), the states $|N\,n\rangle$ and $|N^{(i)}\,m\rangle$ are eigenstates belonging to different Hamiltonians and so orthogonality can not be directly applied to them. However, they are both given in terms of the SCLS and so the calculation of their overlap is straightforward.

The results are shown in figure 3, where we present the modulus of the projection of the total wave function on the internal states. The solid line corresponds to the treatment of section II A and the dashed line to the CLS method. These wave functions have been obtained for a scattering energy $E = 5\,\hbar\omega$. The R scale is in units of a_0. As shown in this figure both treatments give almost identical results, the small differences being attributed to the truncation of the infinite basis.

A similar agreement between both approaches is found at other energies, provided that a sufficient number of states is included in each case.

From this picture it becomes apparent the role played by each internal state. The state $n=0$ corresponds to the initial state. Then, the asymptotic wave function contains both incoming and outgoing contributions of this state. This is reflected in the characteristic interference pattern of the curve $|\langle N\,0|\Psi\rangle|$. At this scattering energy, the states $n=2$ and $n=4$ are open channels, and so they give a non vanishing contribution to the asymptotic scattered wave. In fact, the curves tend to a constant value for large distances which, according to (28), is proportional to the corresponding coefficient S_{0n}. By contrast, the state $n=6$ is closed. Its exponential decaying tail reflects the fact that this state does not contribute *directly* to the asymptotic wave function, but it does give a non negligible contribution to the total wave function in the vicinity of the wall. As mentioned before, the inclusion of these states is essential in order to reproduce accurately the boundary conditions and to achieve convergence for the S-matrix elements. Then, they indirectly affect the wave function in all the space.

The approach based on CLS presents some advantages compared to the treatment described in section II A. It allows to evaluate all the matrix elements S_{nm}, $n, m = 0, \ldots, N-1$ in a single calculation, i.e., the initial state does not need to be specified. By contrast, in the previous approach a new calculation is required for each initial state.

Moreover, the method based on the CLS preserves the general properties of the S-matrix for any value of N. In particular, conditions (23) and (25) ensure that the total flux is conserved at each barrier. As a relevant consequence, the resulting S-matrix fulfils unitarity, regardless of the number of initial states chosen for the basis.

III. THE ADIABATIC MODEL

We derive in this section an expression for the S-matrix in the adiabatic approximation [10]. The standpoint of the approach is that a fundamental distinction is made between the two relevant coordinates of our problem, namely, the centre of mass coordinate, R, and the internal variable, r. The former is identified as a high-energy (*fast*) variable and the latter as a low-energy (*slow)* variable.

In this dynamical regime, it is expected that the excitation energies ϵ_n associated with those excited states which are significantly populated, are such that $\epsilon_n \ll E$, where E is the incident energy of the projectile. Under this assumption it seems reasonable to replace the internal Hamiltonian by a representative constant. By choosing this constant as ϵ_0, the ground state energy, it is also guaranteed that the solution of the resulting approximate three-body equation satisfies the correct incident wave boundary condition.

Then, applying this approximation to the Hamiltonian (3) the Schrödinger equation reads:

$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dR^2} + v_1(R + \frac{1}{2}r) + v_2(R - \frac{1}{2}r) + \epsilon_0 - E \right] \Psi^{ad}(R,r) = 0. \tag{30}$$

Note that this approximate Schrödinger equation is independent of the relative momentum between the fragments. Then, its conjugate coordinate, r, is a constant of motion, remaining *frozen* during the collision. Thus, eq. (30) has to be solved for all values of a fixed separation r.

In the case of a rigid wall potential, v_1 and v_2 are zero for positive values of r_1 and r_2, respectively. Therefore, in this case the solution of eq. (30) is given by the plane wave, $\exp(-iK_0R)$, multiplied by an arbitrary function of r. The most general solution verifying the boundary incident condition at infinity can be written as

$$\Psi^{ad}(r, R) = \phi_0(r)e^{-iK_0R} - S(r)\phi_0(r)e^{iK_0R}. \tag{31}$$

where $\phi_0(r)$ is the ground state wave function and $S(r)$ is a function determined by imposing the boundary condition at the wall. This requires that the wave function vanishes at $R = |r|/2$. Then

$$S(r) = e^{-iK_0|r|}. \tag{32}$$

The scattering coefficients defined by eq. (8) can be obtained by projecting the wave function (31) onto the basis states $\{\phi_n(r)\}$. This gives rise to the following simple expression:

$$S_{0n} = \int_{-\infty}^{+\infty} \phi_n^*(r)S(r)\phi_0(r)dr. \tag{33}$$

We notice that in this expression no distinction is made between open and closed channels. Actually, the approximation treats the full excitation spectrum of the internal Hamiltonian as being degenerate in energy with the ground state. As a consequence, unitarity of the adiabatic S-matrix is only achieved when summing over the infinite set of eigenstates.

In what follows we show that the adiabatic approximation is not adequate for the problem treated in this work. In Fig. 4 the quantity $1-|S_{00}|^2$ is plotted versus the collision energy for the exact (solid line) and adiabatic (dashed line) calculations. This quantity can be interpreted as an excitation probability. The adiabatic prediction completely disagrees with the exact calculation, indicating that the assumptions involved in the adiabatic approximation are not adequate for this problem. We attribute this failure to the fact that, as revealed by the exact calculation, many internal states participate in this process.

This is probably due to the peculiarities of an infinite zero-range interaction. In this case, the momentum transferred to each particle by the wall is twice the incident momentum and so, when increasing the scattering energy, the expected excitation energy increases. During the collision time, i.e., while one particle has collided with the wall, but the other still has not, the internal motion of the projectile is strongly excited. Then, the assumption of the adiabatic model, i.e., to consider the whole spectrum to be degenerated with the ground state, does not work properly in this case. After the collision, that is, when both particles have collided with the wall, the centre of mass momentum is reversed and the final excitation energy is small. Thus, this model represents a case in which, although the final excitation of the projectile is small, the adiabatic approximation is inadequate, because during the collision the internal motion is strongly excited.

From this discussion we conclude that one should be very careful in applying the adiabatic approximation when dealing with strong, short-range interactions. In the next section we develop a new method to treat this type of situations.

IV. UNCORRELATED SCATTERING APPROXIMATION (USA)

The main goal of this section is to derive an approximated expression for the S-matrix corresponding to the one dimensional scattering of a two particle system in terms of the constituent-target scattering amplitudes. The results presented here are not restricted to the case of an infinite potential. Thus, we start with a general derivation of the model ant later we particularize the results to the problem of a wall potential in order to compare with the exact solution.

There are two opposite effects acting on a projectile in the process of the collision. The first one is the binding potential $v(r)$ that tends to keep the system bound. The second one is the interaction with the target which, apart from governing the motion of the projectile centre of mass, is the responsible for exciting or breaking the system. The relative importance of these two effects depends importantly on the separation between the projectile and the target. In particular, for sufficient large distances between them the dominant interaction is clearly the mutual interaction between the constituents. Thus, it seems reasonable to approximate the projectile-target potential by an average (folding) potential at sufficiently large distances. By contrast, when the bound projectile is close enough to the target the dynamical evolution of the projectile is mainly governed by the target interaction. In this case it is reasonable to neglect the correlations between the fragments.

Let us introduce a characteristic centre of mass distance R_0 separating these two regions. For distances $R \gg R_0$, referred as the "asymptotic region" and denoted by the index I, we adopt an approximate Hamiltonian in which the interaction with the target is neglected

$$\hat{H} \approx \hat{H}_r + \hat{H}_R \equiv \hat{H}_I, \tag{34}$$

where $\hat{H}_r$ is the internal Hamiltonian (4) and

$$\hat{H}_R = \frac{\hat{P}_R^2}{2M} + V_F(R) \tag{35}$$

with $V_F(R)$ representing the folding potential between the projectile and target.

Asymptotically, the eigenstates of $\hat{H}_I$ are just the product of the eigenstates of the internal Hamiltonian $\hat{H}_r$ times a plane wave in R, subject to the restriction (9). As mentioned before, there is only contribution to the asymptotic wave function coming from the open channels. Denoting by N the number of these states, we restrict the basis space to the set

$\{|Nn\rangle; n = 0, 1, \dots, N-1\}$. Then, the total wave function corresponding to an incoming wave in an internal state n will be written in the asymptotic region as

$$|\Psi_{I,n}(E)\rangle \rightarrow \frac{1}{\sqrt{v_n}} e^{-iK_n R} |Nn\rangle - \sum_{m=0}^{N-1} \frac{S_{nm}}{\sqrt{v_m}} e^{iK_m R} |Nm\rangle. \tag{36}$$

For distances $R \ll R_0$, in what we call "interaction region" (denoted by II), the Hamiltonian (1) is approximated by

$$\hat{H} \approx \hat{h}_1 + \hat{h}_2 + \bar{v} \equiv \hat{H}_{II}, \tag{37}$$

where $\bar{v}$ is a constant that substitutes $v(r)$.

The eigenfunctions of $\hat{H}_{II}$ can be expanded in terms of the product of eigenfunctions of the Hamiltonians $\hat{h}_1$ and $\hat{h}_2$. An eigenstate of $\hat{h}_i$ corresponds to the distorted wave for the scattering of a particle under the potential $v_i(r_i)$:

$$\hat{h}_i |\chi_i(k_i)\rangle = E_i |\chi_i(k_i)\rangle; \quad (i = 1, 2), \tag{38}$$

where k_i is the asymptotic incident momentum for the constituent i, and $E_i = (\hbar k_i)^2 / 2m_i$. Asymptotically this distorted wave behaves as

$$|\chi_i(k_i)\rangle \rightarrow |k_i\rangle - S_i(k_i)|-k_i\rangle; \quad (i = 1, 2), \tag{39}$$

where $\langle r_i | k_i \rangle = \exp(-ik_i r_i)/\sqrt{2\pi}$ is a plane wave with momentum k_i and $S_i(k_i)$ is the constituent-target S-matrix for the scattering energy E_i. Note that, in the case of the infinite wall, this expression is valid for all values of $r_i \geq 0$.

Thus, the eigenstates of the Hamiltonian $\hat{H}_{II}$, corresponding to the asymptotic momenta k_1 and k_2, can be expressed as products of the form

$$|\psi(k_1, k_2)\rangle \propto |\chi_1(k_1)\rangle |\chi_2(k_2)\rangle. \tag{40}$$

where

$$\frac{\hbar^2 k_1^2}{2m_1} + \frac{\hbar^2 k_2^2}{2m_2} + \bar{v} = E. \tag{41}$$

According to (39), the asymptotic expansion of the eigenfunction (40) contains an incoming wave, $|k_1\rangle |k_2\rangle$, an scattered wave, $S_1(k_1)S_2(k_2)|-k_1\rangle|-k_2\rangle$, and two cross terms

mixing ingoing and outgoing contributions, namely $S_1(k_1)|-k_1\rangle|k_2\rangle$ and $S_2(k_2)|k_1\rangle|-k_2\rangle$. In practise, these last two terms do not contribute to the incoming nor the scattered wave function at large distances. This can be verified by considering an incoming wave packet in k_1 and k_2. The superposition of states of the form $|k_1\rangle|-k_2\rangle$ or $|-k_1\rangle|k_2\rangle$ contains an incoming part which vanishes for $t \to +\infty$, and an outgoing part which cancels for $t \to -\infty$. Then, these cross terms can be omitted as far as the asymptotic behaviour concerns. As we will show later, the use of MLS allows to demonstrate that these terms do not contribute to the wave function at large distances in a time-independent formalism. The form of the scattered wave, $S_1(k_1)S_2(k_2)|-k_1\rangle|-k_2\rangle$, indicates that the S-matrix for an incoming wave with definite values of k_1 and k_2, denoted $S(k_1, k_2)$, appears to be the product of the individual S-matrices for the constituents, i.e., $S(k_1, k_2) = S_1(k_1)S(k_2)$. This S-matrix is unitary, provided the individual S-matrices are unitary, i.e., $|S_i(k_i)| = 1$. This condition is satisfied for the infinite potential, but it also holds for any other situation for which the transmission coefficient is zero.

Therefore, the scattering problem for the Hamiltonian $\hat{H}_{II}$ corresponding to a situation characterised by an incoming wave with definite values of the energies of the constituents can be easily solved. However, our physical initial state is not characterised by the individual energies of the two particles, but by a certain internal state of the projectile and the energy of the collision. The general solution in the interaction region for a total energy E will be a certain superposition of eigenstates (40), verifying (41) and the adequate asymptotic boundary conditions. These boundary conditions require that the wave function in region II matches smoothly with the asymptotic wave function of eq. (36). One possible way to proceed might be to expand the total wave function in each region in terms of the eigenstates of the approximated Hamiltonian for that region. The coefficients of the expansion are determined by imposing the continuity of the wave function and its derivative at the matching radius R_0. Apart from the complexity of the calculation, this method has the problem that incoming waves coming from the asymptotic region do not match exactly with incoming waves of the interaction region, due to the discontinuity of the Hamiltonian at R_0. As a result, part of the incoming flux is reflected at R_0 and spurious outgoing waves are generated. To overcome this difficulty we proceed on a different way. In order to avoid the unphysical reflections we relax the meaning of the matching radius R_0. We assume that the Hamiltonian $\hat{H}_I$ is smoothly transformed into $\hat{H}_{II}$ in a finite transition region around R_0.

Although we do not make an explicit description of this transition region in our model, we include its effect by requiring that the wave function passes from one region to the other without loss of flux.

Let us consider the incoming part of the general solution (36):

$$|\Psi_{I,n}^{(in)}(E)\rangle \rightarrow \frac{1}{\sqrt{v_n}}e^{-iK_nR}|Nn\rangle. \tag{42}$$

In order to match this wave function with the inner wave solution it is convenient to express the internal states in terms of a basis of Momentum Localised States (MLS). These are obtained from the original basis by diagonalizing the momentum operator in the set of internal states. Due to the truncation of the original basis the MLS do not have a definite value of the internal momentum q but, provided the number of states N is large, their momentum distribution is highly localised around a certain value. The two basis of states are connected by an orthogonal transformation (see appendix) and so, the incoming state can be rewritten as

$$|\Psi_{I,n}^{(in)}(E)\rangle \rightarrow \frac{1}{\sqrt{v_n}}e^{-iK_nR}\sum_{s=1}^{N}\langle MLS; Ns|Nn\rangle\,|MLS; Ns\rangle. \tag{43}$$

where $|MLS; Ns\rangle$ denotes a MLS and $\langle MLS; Ns|Nn\rangle$ are the transformation coefficients. The function $\langle q|MLS; Ns\rangle \equiv \tilde{\varphi}_s(q)$ has the property of being highly localised around $q = q_s$, the s-th zero of the eigenfunction $\langle q|N\,N\rangle$.

As noted before, the eigenstates of the approximated Hamiltonian in the interaction region are characterized by the energies of the two particles. These energies are directly related to their incident momenta. Equivalently, they can be characterised by the asymptotic values of the internal momentum q and the centre of mass momentum K. In our approach, the internal eigenstates will be approximated in region II by the discrete basis of MLS. The incoming wave function for the interaction region is then expressed at large distances as

$$|\Psi_{II,n}^{(in)}(E)\rangle \rightarrow \sum_{s=1}^{N} A_s^{(n)}e^{-i\tilde{K}_sR}|MLS; Ns\rangle \tag{44}$$

with the centre of mass momentum $\tilde{K}_s$ defined by the relation

$$\frac{\hbar^2 q_s^2}{2\mu} + \frac{\hbar^2 \tilde{K}_s^2}{2M} + \bar{v} = E. \tag{45}$$

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The coefficients $A_s^{(n)}$ are determined in order the waves (36) and (44) match smoothly. In particular, we impose the incoming flux to be conserved in the transition. This can be achieved by taking

$$A_s^{(n)} = \frac{1}{\sqrt{\tilde{v}_s}} e^{-i\delta_{ns}} \langle MLS; Ns|Nn \rangle, \tag{46}$$

with $\tilde{v}_s = \hbar \tilde{K}_s/M$ and $\delta_{ns} = \gamma_n - \chi_s$. The phases γ_n and χ_s must be real numbers to preserve the incoming flux.

In order to evaluate the phases γ_n and χ_s, we impose the two incoming solutions to have the same phase at R_0. This is achieved by taking $\gamma_n = K_n R_0$ and $\chi_s = \tilde{K}_s R_0$, which leads to

$$\delta_{ns} = (K_n - \tilde{K}_s)R_0. \tag{47}$$

Once the coefficients $A_s^{(n)}$ are known, the total wave function in the interaction region is completely determined. It can be expressed in terms of the distorted waves for each one of the constituents. To this end, we rewrite expression (44) as

$$|\Psi_{II,n}^{(in)}(E)\rangle \rightarrow \sum_{s=1}^{N} A_s^{(n)} e^{-i\tilde{K}_s R} \int_{-\infty}^{\infty} dq |q\rangle \tilde{\varphi}_s(q) =$$
$$= \sum_{s=1}^{N} A_s^{(n)} \int_{-\infty}^{\infty} dq \, \tilde{\varphi}_s(q) |k_1^s(q)\rangle |k_2^s(q)\rangle, \tag{48}$$

where we have introduced the momenta $k_1^s(q) = \frac{m_1}{M}\tilde{K}_s + q$ and $k_2^s(q) = \frac{m_2}{M}\tilde{K}_s - q$. The scattering wave function corresponding to an incoming plane wave $|k_i^s(q)\rangle$ is given by the distorted wave $|\chi(k_i^s(q))\rangle$. Then, the total wave function in region II, including both the incoming and scattered wave reads

$$|\Psi_{II,n}(E)\rangle = \sum_{s=1}^{N} A_s^{(n)} \int_{-\infty}^{\infty} dq \, \tilde{\varphi}_s(q) |\chi_1(k_1^s(q))\rangle |\chi_2(k_2^s(q))\rangle. \tag{49}$$

Taking into account the asymptotic behaviour of the distorted waves, (39), this wave function can be written beyond the range of the potentials as

$$|\Psi_{II,n}(E)\rangle \rightarrow \sum_{s=1}^{N} A_s^{(n)} \int_{-\infty}^{\infty} dq \, \tilde{\varphi}_s(q) \Big\{ |k_1^s(q)\rangle |k_2^s(q)\rangle$$

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$$- \ S_1(k_1^s(q)| - k_1^s(q)\rangle)|k_2^s(q)\rangle - S_2(k_2^s(q)|k_1^s(q)\rangle)| - k_2^s(q)\rangle$$

$$+ \ S_1(k_1^s(q)S_2(k_2^s(q)| - k_1^s(q)\rangle)| - k_2^s(q)\rangle\} \tag{50}$$

Assuming that the individual S-matrices, S_1 and S_2, are smooth functions of the energy in the region where the integrand takes significant values, they can be evaluated at k_1^s and k_2^s, respectively. Also, it is convenient to express the products of planes waves in terms of the relative and centre of mass momenta. Considering the case of equal masses we can use the expressions $k_1^s(q)r_1 + k_2^s(q)r_2 = \tilde{K}_s R + qr$ and $k_1^s(q)r_1 - k_2^s(q)r_2 = \frac{1}{2}\tilde{K}_s r + 2qR$. Then one can perform explicitly the integration with respect to q, to obtain

$$\Psi_{II,n}(r, R) \ \to \ \sum_{s=1}^{N} A_s^{(n)}\Big\{ e^{-i\tilde{K}_s R}\varphi_s^*(r) + S_1(k_1^s)S_2(k_2^s)e^{i\tilde{K}_s R}\varphi_s(r)$$

$$- \ S_1(k_1^s)e^{i\frac{1}{2}\tilde{K}_s r}\varphi_s(2R) - S_2(k_2^s)e^{-i\frac{1}{2}\tilde{K}_s r}\varphi_s^*(2R)\Big\}$$

$$\tag{51}$$

where $\varphi_s(r)$ is the Fourier transform of $\tilde{\varphi}_s(q)$. This wave function can be interpreted as follows. The incoming wave is decomposed as products of MLS, $\varphi_s(r)$, describing the internal evolution, times an incoming plane wave describing the centre of mass motion, $e^{-i\tilde{K}_s R}$. This wave scatters by the target giving rise to three terms. The second term in (51) is just the conjugate of the incident wave, times the product of the S-matrices of the constituents. The remaining two terms comprise the product of the function $\varphi_s(2R)$, or its conjugate, times a plane wave in the variable r. As it can be easily verified, the function $\varphi_s(2R)$ vanishes for large values of R and so, these two terms do not contribute to the asymptotic wave function. Actually, these terms containing only one of the involved S-matrices can be physically regarded as the situation in which only one of the particle has scattered and the other has not yet. This is consistent with the fact that they both cancel at large distances. However, we remark that these vanishing terms are essential in order to reproduce the wave function at small distances. In this sense, it is also interesting to note that the wave function (51) retains components associated to closed channels, even when they are explicitly omitted in the asymptotic region, according (36). As noted in section II, in the case of the wall potential the inclusion of these states is essential in order to reproduce the boundary conditions. For this particular problem, expression (51) is valid for all the interaction region and, as can be easily verified, it identically fulfils the boundary conditions, vanishing for

$r = \pm 2R$.

Thus, we can conclude that an incoming MLS scatters with the product of the S-matrices of the fragments. This result is consistent with our previous discussion in which, using wave packet arguments, we concluded that the S-matrix is given by the product of the S-matrices of the fragments in the basis characterised by the momenta of the two particles. We now see that this property also holds for the MLS basis which, in a sense, can be described as a wave packet of plane waves in terms of q, centred around q_s.

Therefore, writing explicitly the value of the coefficients $A_s^{(n)}$ the scattered wave in the interaction region behaves at large distances as

$$|\Psi_{II,n}^{(scat)}(E)\rangle \to \sum_{s=1}^{N} \frac{1}{\sqrt{\tilde{v}_s}} e^{-i\delta_{ns}} \langle MLS; Ns|Nn\rangle \, e^{i\tilde{K}_s R} S_1(k_1^s) S_2(k_2^s)|MLS; Ns\rangle. \qquad (52)$$

By writing the MLS appearing in this expression in terms of the original basis, and imposing the conservation of flux, one can easily obtain the scattered wave in the asymptotic region

$$\begin{aligned}
|\Psi_{I,n}^{(scat)}(E)\rangle \;\to\; &\sum_m \frac{e^{iK_m R}}{\sqrt{v_m}} \Big\{ \sum_{s=1}^{N} e^{-i(\delta_{ns}+\delta_{ms})} \langle Nm|MLS; Ns\rangle \\
&\times\; \langle MLS; Ns|Nn\rangle S_1(k_1^s) S_2(k_2^s) \Big\}|Nm\rangle.
\end{aligned} \qquad (53)$$

The expression between brackets provides the S-matrix element connecting an initial state n with a final state m

$$S_{nm} = -\sum_{s=1}^{N} e^{-i(\delta_{ns}+\delta_{ms})} \langle Nm|MLS; Ns\rangle \, S_1(k_1^s) S_2(k_2^s) \, \langle MLS; Ns|Nn\rangle. \qquad (54)$$

As pointed before, the peculiarities of the problem treated in this work imply that, starting with the system in its ground state, only positive parity states are suitable to be populated. As far as expression (54) concerns, this means that the matrix elements S_{0n}, with n odd, are identically zero.

Under these considerations it is possible to exclude those inhibited states. Then, one is left with a truncated basis of the form $|N\,n\rangle$, where N is now even. Following the arguments above and using the results of the appendix one finally gets the following expression for the S-matrix in the case of equal masses

$$S_{nm} = -\sum_s e^{-i(\delta_{ns}+\delta_{ms})} \langle N\, m|SMLS; N\, s\rangle \langle SMLS; N\, s|N\, n\rangle\, S_1(k_1^s)S_2(k_2^s), \qquad (55)$$

with n and m even and the sum in s restricted to the positive zeros of $\mathcal{H}_N(x)$. The coefficients $\langle SMLS; N\, s|N\, n\rangle$ are equal to $\langle MLS; N\, s|N\, n\rangle$ up to a factor $\sqrt{2}$ (see appendix).

We remark the simplicity of the expression (54) as compared to the exact solution of the problem. Part of the payoff for this simplicity is the existence of two undetermined parameters, $\bar{v}$ and R_0. The optimal value of R_0 is nevertheless constrained by two considerations. On one side, it can not be too large, as at large distances the interaction between the two fragments would dominate over the interaction due to the target, and so ignoring the correlations between the particles for values just below R_0 would not be a good approximation. On other side, the value of R_0 should be large enough to allow us to ignore the interaction with the target for R above R_0. Thus, the matching radius must be about the size of the system. Moreover, $\bar{v}$ must be of the order of the expectation value of $v(r)$ on the ground state.

V.   COMPARISON OF USA AND EXACT CALCULATIONS

In this section we analyse the reliability of USA by comparing its predictions with the exact results. In Fig. 5 the S-matrix coefficients for the USA model (dot-dashed line) with the phases δ_{ns} given by (47) are compared with the exact calculation (solid line) and the adiabatic approach (dashed line). The calculations have been performed using the matching radius $R_0 = 0.6a_0$ and an average potential $\bar{v} = 0$. These values were determined by fitting the elastic S-matrix at high energies, where the model is expected to be more accurate. We notice that for these energy independent parameters a good description of the elastic and inelastic coefficients is achieved for energies above $\sim 6\,\hbar\omega$. By contrast, the adiabatic model does not seem to give a good description of the S-matrix at any scattering energy.

A quantity closely related to the S-matrix coefficients is the *average final excitation energy*. It gives an idea on the degree of excitation of the final system. It has been defined as

$$\langle \epsilon \rangle = \sum_{n=0} (\epsilon_n - \epsilon_0)|S_{0n}|^2, \qquad (56)$$
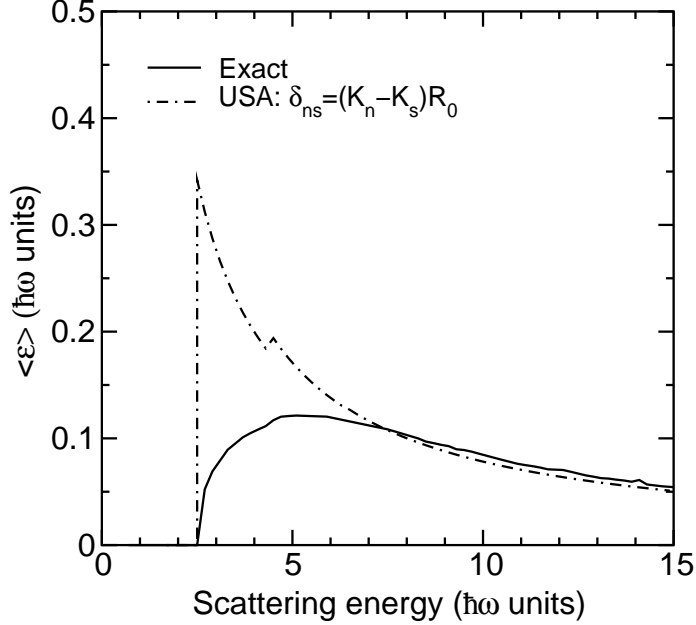
FIG. 6: Average excitation energy. The solid line corresponds to the exact calculation. The dot-dashed line corresponds to the USA with the prescription $\delta_{ns} = (K_n - \tilde{K}_s)R_0$.

where the sum must be extended only to the set of open channels.

In Fig. 6 we show the energy dependence of the average excitation energy, $\langle \epsilon \rangle$. As in the previous case, the USA model (dot-dashed line) agrees well with the exact calculation (solid line) for energies above $6 \, \hbar\omega$. On the contrary, the USA model, as expected, does not describe properly the low energy regime. In particular, a spurious discontinuity is observed for the threshold at $E = \frac{5}{2} \, \hbar\omega$.

In Fig. 7 we compare the wave function given by the USA approach with the exact calculation at $E = 10 \, \hbar\omega$. The curve for the exact calculation has been obtained using expression (27). In the USA model, represented by the dot-dashed line, one has to distinguish the asymptotic and the interaction regions. For the asymptotic wave function, the interaction with the wall is neglected $(v_i(r_i) = 0)$ and so the range of values of r is unrestricted. Then, the projection on a state n is simply given by

$$\Psi_n^{asym}(R) \rightarrow \delta_{n0}\frac{1}{\sqrt{v_0}}e^{-iK_0R} - \frac{S_{0n}}{\sqrt{v_n}}e^{iK_nR}. \tag{57}$$

By contrast, in the interacting region, explicit account is taken for the wall and an expression similar to (27) should be used instead. Thus, the total wave function in II (51) is projected on the different eigenstates, taking into account that the integration is restricted
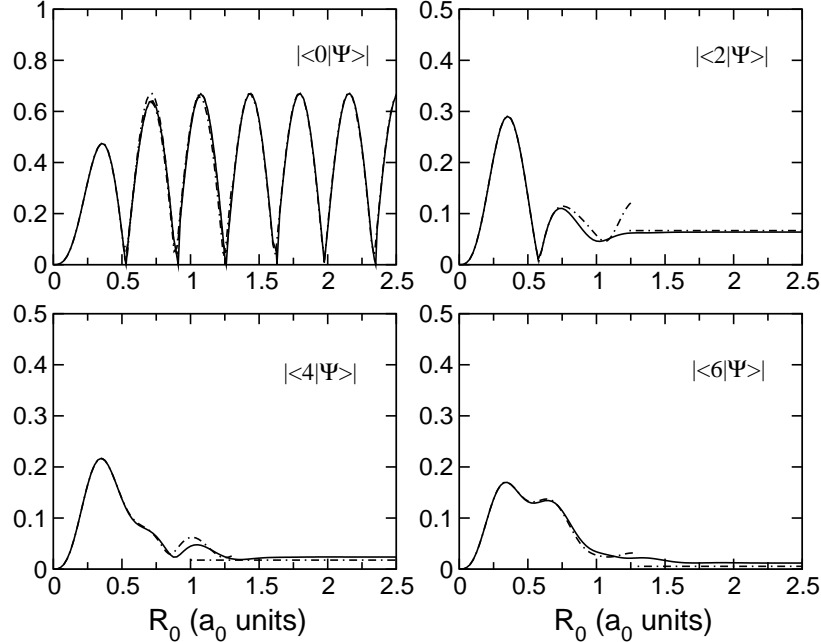
27

FIG. 7: Projection of the total wave function on the internal eigenstates for a scattering energy $E = 10\,\hbar\omega$. The solid line is the exact calculation, the dot-dashed line corresponds to the formula (54), with the prescription $\delta_{ns} = (K_n - \tilde{K}_s)R_0$.

to the interval $|r| < 2R$.

At this collision energy, Fig. 5 indicates that the scattering coefficients are well reproduced by (54) with the phases $\delta_{ns} = (K_n - \tilde{K}_s)R_0$. Then, we have adopted this prescription (with the same matching radius) to describe the approximated wave function at this energy. As can be seen in Fig. 7, the agreement with the exact calculation is quite good for all the states.

As a general rule, our calculations show a better agreement for the elastic and first excited states, and it tends to be worse for excited states of increasing energies. This is expected because within the USA model we restrict the basis to the set of open channels and so, the effect of this truncation becomes more evident as we explore excited states close to the cut off.

We have explored in more detail the limits of the USA model as well as the validity of the prescription (47) for the phases. In order to do that we start from the exact expression of the S-matrix for a fixed collision energy. Making use of (54), we fit the phases γ_n and χ_s appearing in δ_{ns} in order to reproduce the exact calculation. We find that the S-matrices can be accurately fitted for all the scattering energies (even for very small values). Although

these phases, γ_n and χ_s, can not be written exactly as $K_n R_0$ and $\tilde{K}_s R_0$, respectively, one can define effective energy and channel dependent radii so that $R_n = \gamma_n / K_n$ and $R_s = \chi_s / \tilde{K}_s$. In Fig. 8 we plot the values of the quantities R_n versus n and $R_s = \chi_s$ versus the absolute value of q_s, i.e., the internal momentum at which the state $\langle q | MLS; Ns \rangle$ is peaked. The selected collision energies are $E = 9\,\hbar\omega$ and $E = 10\,\hbar\omega$. In both cases we deal with a total of five HO states, namely, the ground state and the first four excited states with even parity. Using the prescription (47) both quantities are just R_0 for all values of n or s. Note that the value of R_s is rather constant and very close to the matching radius used in our calculations, i.e., $R_0 = 0.6 a_0$. This constant value has been also plotted in the figure for reference. The values of R_n are also very close to $R = R_0$ for the lower values of n, but they tend to deviate from our prescription for values of n close to the threshold. It is remarkable that the values of R_n and R_s are mostly independent on the scattering energy and of the individual state considered. This indicates that for scattering energies large compared to $\hbar\omega$, the USA works very well, and the matching radius can be taken as a constant, related to the size of the system, and independent on the energy or the internal state. For lower energies, the USA may still be used, but in this regime the radius R_0 depends on the energy and the state considered.

VI.   CONCLUSIONS

We have formulated a one dimensional problem consisting on the scattering of two particles, interacting with a HO potential, that collide with an infinite potential. This problem contains some of the dynamical features of the scattering of composite systems in atomic, molecular and nuclear physics, which interact with a target through short range interactions.

We have obtained the *exact* solution of the problem using two different procedures. The first one consists of imposing the adequate boundary conditions on the scattering wave function. The second procedure deals with a basis of configuration localized states (CLS), which are wave functions with a strong spatial localisation. Both procedures converge, provided that a sufficiently large basis of states is used. The main characteristic of the exact solution is that, for large scattering energy, the elastic scattering dominates. In order to achieve convergence, the inclusion of closed channels, i.e., states with internal energy larger than the scattering energy, is required. Although these states do not contribute to the S-
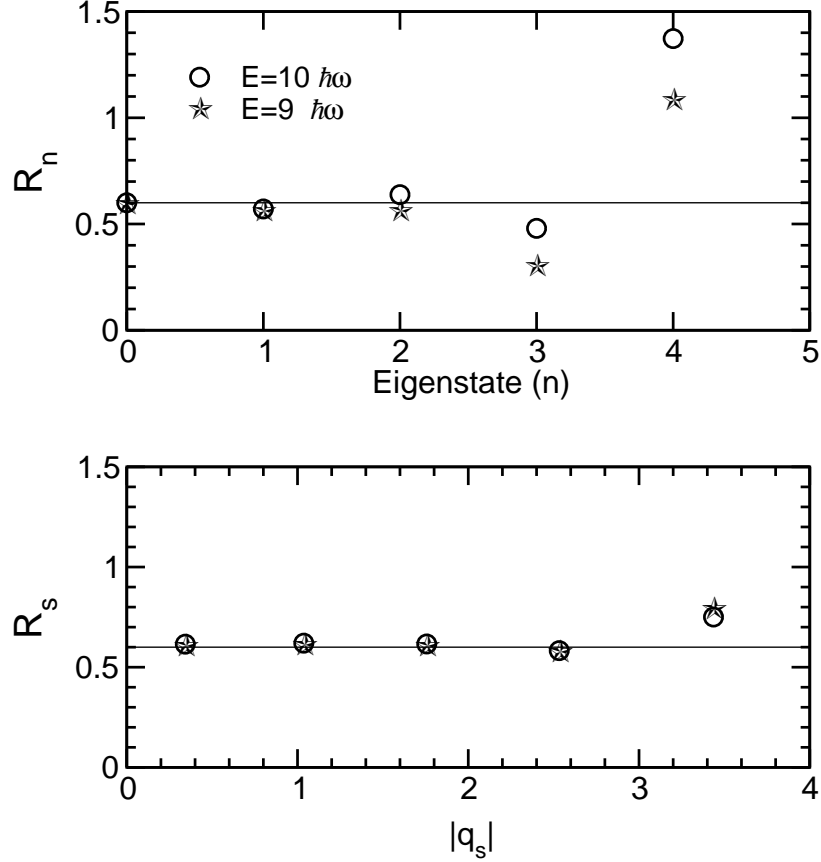
FIG. 8: Behaviour of the ratios $R_n = \gamma_n/K_n$ (upper figure) and $R_s = \chi_s/\tilde{K}_s$ (lower figure) versus the value of n and $|q_s|$, respectively, for the scattering energies $E = 9\,\hbar\omega$ (stars) and $E = 10\,\hbar\omega$ (circles). The phases γ_n and χ_s have been calculated by fitting the S-matrix elements predicted by (54) to the exact calculation.

matrix they must be taken into account in the calculations to obtain accurate results. This fact indicates that for short-range interactions one should be very careful when truncating the basis of states used in continuum discretized calculations.

We have compared our *exact* results with the adiabatic approach, that considers the relative coordinate frozen during the scattering process. The results disagree completely. This indicates that the adiabatic approximation could be inaccurate when the interactions of the fragments with the target have a very short range. These short range interactions could couple to highly excited internal states for which the adiabatic approximation is not valid. However, it should be reminded that our calculations make use of a sharp infinite wall. Thus, they will be relevant when the range of the interaction is short compared not

only with the size of the projectile but also with the wavelength describing the motion of the fragments with respect to the target.

We have developed a model which describes the scattering of a composite object in terms of the scattering wave functions and the S-matrices of the fragments. The model, that we call Uncorrelated Scattering Approximation (USA), neglects the correlations between the fragments during the scattering. The application of the USA to our model problem gives an expression for the S-matrix of the composite system in terms of the product of the S-matrices of the fragments. Similarly, the scattering wave function is given as a combination of the product of regular wave functions of the fragments. The particular superposition is determined by application of the asymptotic boundary conditions. The application of the USA to our model problem relies on the use of two parameters. The most important one is the distance R_0 at which the asymptotic and uncorrelated wave functions are matched. We have fixed this value to $0.6a_0$, in terms of the oscillator length, for all our calculations. It should be noticed that this parameter has a similar meaning to the matching radius that is used in R-matrix theory. The other parameter is the average potential $\bar{v}$ that replaces the interaction between the fragments. We have set this value to $\bar{v} = 0$.

By considering the matching radius to be energy- and state-dependent, the exact S-matrix and scattering wave functions are accurately reproduced. Moreover, for high scattering energies the elastic and inelastic S-matrices are well reproduced by taking a fixed value of the matching radius.

In general, the agreement with the exact calculation is better for the observables associated with the ground and first excited states and they tend to be worse for states with excitation energies close to the total energy. This is attributed to the fact that for these states the relative velocity between the fragments is small and then the correlations are expected to be more important.

The one-dimensional model presented in this work can be a useful test case to check the validity of different approaches used in the description of the scattering of composite systems. The present choice of a sharp infinite wall for the description of the interaction with the target, and harmonic oscillator for the interactions between the fragments has the advantage that sets $\hbar\omega$ as the unique scale for energies and a_0 as the unique scale for lengths. In this sense, our results, which are expressed in those units, are valid for any value of the mass or harmonic constant. However, the model could be done more realistic, and more

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complicated, by substituting the infinite wall for an exponential function, and substituting the harmonic oscillator by finite potentials.

Acknowledgements

Appendix A

In this work different sets of basis states have been used, based on harmonic oscillator (HO) wave functions. These obey the general form

$$\phi_n(r) = \mathcal{N}_n^{-\frac{1}{2}} \exp\left(-\frac{r^2}{2a_0^2}\right) \mathcal{H}_n\left(\frac{r}{a_0}\right) \ ; \ \ n = 0, 1, \ldots \tag{58}$$

where $a_0 = \sqrt{\hbar/\mu\omega}$ is the oscillator length, $\mathcal{N}_n$ a normalisation constant and $\mathcal{H}_n$ the Hermite polynomial of order n. In all the calculations we restrict the infinite set of states to a finite family of N states, denoted by $\{|N\,n\rangle; n = 0, \ldots, N-1\}$, where $\langle r|N\,n\rangle = \phi_n(r)$.

By diagonalizing the position operator in the truncated basis of HO wave functions, a new set of N states is obtained which have the property of being localised in configuration space. They are called Configuration Localised States (CLS) and are denoted by $\{|CLS; Ns\rangle; s = 1, \ldots, N\}$. These two families of states are related by means of the orthogonal transformation

$$|CLS; Ns\rangle = \sum_{n=0}^{N-1} \langle Nn|CLS; Ns\rangle \, |Nn\rangle \tag{59}$$

For HO wave functions, the state $\langle r|CLS; Ns\rangle$ is localised around $r = a_0 x_s$, where x_s is the s-th zero of the Hermite polynomial $\mathcal{H}_N(x)$. In this case, the transformation coefficients are given by (see [22])

$$\langle Nn|CLS; Ns\rangle = \left[\frac{2^{N-n}}{2N}\frac{(N-1)!}{n!}\right]^{1/2} \frac{\mathcal{H}_n(x_s)}{\mathcal{H}_{N-1}(x_s)}. \tag{60}$$

In analogy with the CLS, it is possible to define internal states localised in momentum space, known as Momentum Localized States (MTS). This is carried out by diagonalizing the momentum operator in the truncated HO basis. Thus, starting with the basis of N states, this procedure provides a new set of N internal states, each one of them is peaked around a certain momentum. As in the case of the CLS there is an orthogonal transformation relating both sets of states:

$$|MLS; Ns\rangle = \sum_{n=0}^{N-1} \langle Nn|MLS; Ns\rangle|Nn\rangle, \tag{61}$$

where $|MLS; Ns\rangle$ represents a MLS. Then $\langle q|MLS; Ns\rangle$ is localised around $q = x_s/a_0$ where, due to the formal analogy of the HO wave functions in momentum and configuration space, $\{x_s\}$ are again the zeros of the Hermite polynomial $\mathcal{H}_N$. This analogy provides also a

simple relation between the transformation coefficients $\langle MLS; Ns|Nn\rangle$ and $\langle CLS; Ns|Nn\rangle$. In this work, we take the internal wave function to be real in configuration space, and so they will be affected by a factor $(-i)^n$ in momentum space. Moreover, we take the CLS to be real functions, so the coefficients $\langle CLS; Ns|Nn\rangle$ are real numbers. Therefore,

$$\langle MLS; Ns|Nn\rangle = (-1)^n \langle CLS; Ns|Nn\rangle. \tag{62}$$

Although the formalisms presented in this work do not require the fragments to have equal masses, we have performed all the calculations for this particular situation. In this case, parity conservation implies that only positive parity states are suitable to be populated during the process. In fact, the coefficients S_{0n} derived from the exact calculations of sections (II A) and (II B) are found to be zero for odd values of n. This is also satisfied by eq. (54), as can be easily verified.

Under these considerations one is allowed to exclude those inhibited states from the beginning. This permits to work with the truncated basis of states: $\{\phi_n(r); n = 0, 2, \ldots, N-2\}$, with N even. This requires, however, some care in the evaluation of the localised states in the new basis. The formalism of CLS can not be directly applied to this set, as many of its properties entails the sum over both even and odd states. The starting point for the construction of the CLS formalism requires a set of functions of the form [22]

$$\psi_m(x) = \langle x|j\, m\rangle = \mathcal{N}_{jm}^{-1/2} F(y)\mathcal{P}_m(y), \quad m = 0, 1, \ldots, j-1, \tag{63}$$

where y is a certain function of r, $\mathcal{N}_{jm}$ a normalisation constant, F an arbitrary function of y and $\mathcal{P}_m$ is a polynomial of order m.

The drawback outlined above can be overcome in the case of HO wave functions by writing the Hermite polynomials in terms of generalised Laguerre functions (see, for instance, Ref. [23]):

$$\phi_{2m}(r) = (-1)^m m! 2^{2m} \mathcal{N}_{2m}^{-\frac{1}{2}} \exp\left(-\frac{r^2}{2a_0^2}\right) \mathcal{L}_m^{(-1/2)}(y), \quad y = \left(\frac{r}{a_0}\right)^2. \tag{64}$$

Then, taking $\mathcal{P}_m(y) \equiv \mathcal{L}_m^{(-1/2)}(y)$, $F(y) \equiv \exp(-y/2)$ and $j \equiv \frac{N}{2}$ we can identify $\psi_m(x) \equiv \phi_{2m}(r)$ ($m = 0, 1, \ldots, \frac{N}{2} - 1$). The set of configuration localised states are now calculated for the new set of functions. It requires the calculation of the roots of the polynomial $\mathcal{L}_{N/2}^{(-1/2)}(y)$ which, attending to (64), are just the square of the zeros of $\mathcal{H}_N(x)$. The new set of localised

states are given by a linear combination of the states $\phi_n(r)$ and so they are even functions with respect to the variable r. Therefore, we call them Symmetric Configuration Localised States, SCLS. The transformation between the set of states (64) and the SCLS is then expressed as

$$|SCLS; Ns\rangle = \sum_{n=0(even)}^{N-2} \langle N\,n|SCLS;\,N\,s\rangle\,|N\,n\rangle, \;\; s = 1, ..., \frac{N}{2}. \tag{65}$$

The state $\langle r|SCLS; Ns\rangle$ is localised around $r = \pm a_0 x_s$ where $\{x_s\}$ are the positive zeros of $\mathcal{H}_N(x)$.

The coefficients $\langle SCLS;\,N\,s|N\,n\rangle$ are found to be equal to those appearing in eq. (59) up to a factor $\sqrt{2}$:

$$\langle SCLS; N\,s|N\,n\rangle = \sqrt{2}\,\langle CLS; N\,s|N\,n\rangle \tag{66}$$

for n even.

As an example, in Fig. 9 the set of HO wave functions $n = 0, 2, 4, 6$ are plotted versus the adimensional variable x (upper figure). The corresponding Symmetric Localised States are also plotted (lower figure) and labelled with the index s ($s = 1, 2, 3, 4$). Notice that each one of these localised states is peaked around two symmetrical points, corresponding to symmetrical roots of the Hermite polynomial $\mathcal{H}_8(x)$.

In a similar way, it is possible to construct Symmetric Momentum Localised States, which are given by means of the transformation

$$|SMLS; Ns\rangle = \sum_{n=0(even)}^{N-2} \langle N\,n|SMLS;\,N\,s\rangle\,|N\,n\rangle, \;\; s = 1, ..., \frac{N}{2}. \tag{67}$$

The state $\langle q|SCLS; Ns\rangle$ is localised around $q = \pm x_s/a_0$ where $\{x_s\}$ are again the positive zeros of $\mathcal{H}_N(x)$. In the case of the HO basis, the transformation coefficients are related to those in configuration space:

$$\langle SMLS; N\,s|N\,n\rangle = \sqrt{2}(-i)^{n/2}\,\langle CLS; N\,s|N\,n\rangle. \tag{68}$$

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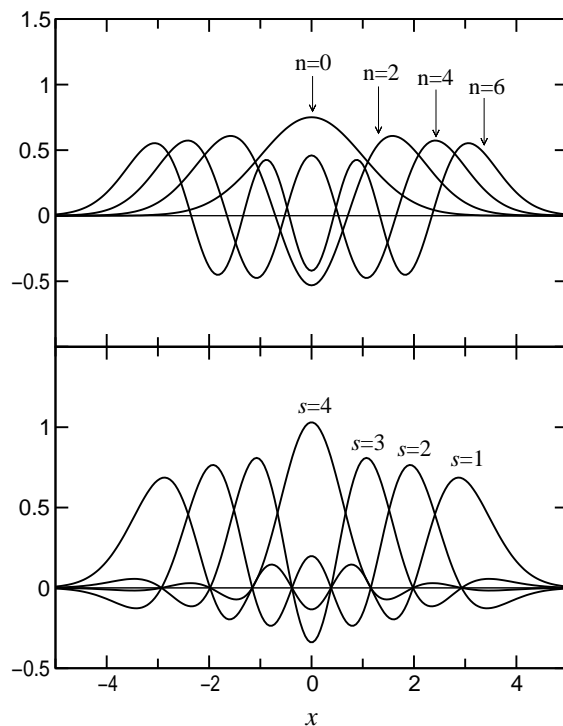
FIG. 9: Harmonic oscillator wave functions corresponding to $n = 0, 2, 4$ and 6 (upper figure) and associated Symmetric Localized States, labeled with the index s.

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