Calculating reactions with use of no-core shell-model states

Victor D. Efros
National Research Centre "Kurchatov Institute," 123182 Moscow, Russia
and National Research Nuclear University MEPhI, 115409 Moscow, Russia

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A scheme to compute reactions is described that uses the Slater determinants constructed of oscillator orbitals. Simple linear equations are suggested for this purpose and shown to be efficient in model examples. A universal method to evaluate the required matrix elements is given.

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I. INTRODUCTION

Since the mid-1990s, much progress has been made in the *ab initio* description of *p*-shell nuclei in the framework of the no-core shell-model (ncsm) method [1]. As already was pointed out [2], a challenging task is to extend this method to describe reactions.

Work in this direction was done in Refs. [3–8]. In Ref. [3] the resonating-group method has been employed. The bound-state wave functions of the heavier of reaction partners were taken in the form of the ncsm expansions over the Slater determinants. The bound-state wave functions of the lighter of reaction partners were treated as an expansion over oscillator functions in the Jacobi coordinates. The coupled set of integrodifferential equations describing relative motion of fragments in a reaction has been obtained. Kernels of the equations were derived in the fashion of Ref. [2] for the cases when the mass numbers of the lighter reaction partner are equal to one [3], two [5], and three [6].

Ncsm pseudostates of fragments were subsequently included in the calculations. This resulted in increase of the number of the integrodifferential equations while convergence with respect to adding pseudostates proved to be too slow in certain cases. In this connection, it was suggested [4] to supplement the resonating group ansatz with a set of states belonging to the ncsm pseudospectrum of the whole system. To realize this, the *R*-matrix approach was used and the Bloch-Schrödinger equation was solved in conjunction with the resonating group description. The required additional matrix elements (ME) were obtained in a way similar to that of Ref. [2]. In the latter paper, at calculating the spectroscopic function of a nucleus the heavier cluster and the lighter one were treated in the same manner as mentioned above and formulas for the ME were obtained separately for the cases of lighter clusters consisting of one, two, three, and four nucleons. In this sequence, the formulas become increasingly complicated, and the same refers to the above-mentioned resonating group ME. The convergence issue was scrutinized in those investigations and stability of the reaction observables, at least at the qualitative level, was established.

Other shell-model approaches to describe reactions such as the no-core Gamow shell model, e.g., Ref. [7], and the *J*-matrix one [8] are also being developed.

Our purpose is to propose a simple and universal extension of ncsm to calculate reactions. The case of two-fragment reactions is considered. In the next section, simple linear equations suitable for this purpose are described. Unlike the resonating-group approach, they do not involve antisymmetrization between nucleons belonging to different reaction partners. They prove to lead to rather precise results in model examples.

In Secs. III–V the issue of calculating the ME entering the equations is addressed. In the difference to the above-mentioned approach [3–6] we employ the ncsm-type Slater determinant expansions for both fragments and we do not use Jacobi coordinates. We provide simple formulas to calculate the required ME. They are universal, i.e., the same for fragments consisting of different numbers of nucleons.

Below the notation like $\Psi_{nlm}(\mathbf{X})$ refers to the eigenfunctions of the oscillator Hamiltonian $-(1/2)\Delta_{\mathbf{X}} + (1/2)X^2$. These eigenfunctions are assumed to be normalized to unity, n denotes the radial quantum number, and l and m denote the angular-momentum quantum numbers. In the nucleon orbital case, $\mathbf{X} = \mathbf{r}/r_0$, where $\mathbf{r}$ is the nucleon position vector and r_0 denotes the nucleon oscillator radius.

II. SCHEME FOR COMPUTING REACTIONS

A. Formulation

Continuum wave functions we shall deal with are the following. Assume that only two-fragment reaction channels are open. Quantities referring to such a reaction channel, say, i, will be supplied with the corresponding subscript. We denote the wave number and the orbital momentum of relative motion of fragments as k_i and l_i. We denote the mass numbers of fragments pertaining to a reaction channel as A_{1i} and A_{2i} and the vector connecting their centers of masses prior to interfragment antisymmetrization as $\boldsymbol{\rho}_i$,

$$\boldsymbol{\rho}_i = (A_{1i})^{-1} \sum_{k=1}^{A_{1i}} \mathbf{r}_k - (A_{2i})^{-1} \sum_{k=A_{1i}+1}^{A_{1i}+A_{2i}} \mathbf{r}_k, \qquad (1)$$

where $\mathbf{r}_k$ are nucleon positions. The following radial functions of relative motion of fragments will be employed,

$$f_i^{(0)}(\rho_i) = \left(\frac{A_{1i}A_{2i}}{k_i}\right)^{1/2} \frac{\tilde{G}_{l_i}(k_i,\rho_i)}{\rho_i},$$
$$f_i^{(1)}(\rho_i) = \left(\frac{A_{1i}A_{2i}}{k_i}\right)^{1/2} \frac{F_{l_i}(k_i,\rho_i)}{\rho_i}, \tag{2}$$

where F_l is the regular Coulomb function and $\tilde{G}_l$ is obtained from the irregular Coulomb function G_l by means of a regularization at small distances. One may set, for example, $\tilde{G}_l(k,\rho) = g_l(\rho)G_l(k,\rho)$ with

$$g_l(\rho) = [1-\exp(-\rho/\rho_{\rm cut})]^{2l+1}, \tag{3}$$

where $\rho_{\rm cut}$ is a parameter.

Define the "surface functions" φ_i,

$$\varphi_i = \left[\left[\phi_1^{I_1}(1,\ldots,A_{1i})\phi_2^{I_2}(A_{1i}+1,\ldots,A_{1i}+A_{2i})\right]_S Y_l(\hat{\boldsymbol{\rho}}_i)\right]_{JM}, \tag{4}$$

where $\phi_1^{I_1M_1}$ and $\phi_2^{I_2M_2}$ are bound-state wave functions of fragments. They contain, respectively, nucleons with the numbers from 1 to A_{1i} and from $A_{1i}+1$ to $A_{1i}+A_{2i}=A$, where A is the total number of nucleons in a system. These are internal wave functions depending on Jacobi vectors and possessing given total momenta and their projections. The latter quantities are denoted as I_1, M_1 and I_2, M_2. These wave functions possess also given parities and isospins and they are the eigenfunctions of corresponding internal Hamiltonians. The brackets $[\ldots]$ represent couplings to the spin S of the two fragments and to the total spin J and its projection M.

We shall deal with the channel functions of two types denoted as $\psi_i^{(0)}$ and $\psi_i^{(1)}$. They are of the form

$$\psi_i^{(0),(1)} = \mathcal{A}_i\varphi_i f_i^{(0),(1)}(\rho_i)\Psi_{000}(\bar{\mathbf{R}}_{\rm c.m.}), \tag{5}$$

where the functions $f_i^{(0),(1)}$ are defined in Eq. (2). Here $\mathcal{A}_i$ is the interfragment antisymmetrizer,

$$\mathcal{A}_i = \nu_i^{-1/2}\sum_P (-1)^{\pi(P)}P, \tag{6}$$

where ν_i is the number of channels in the configuration space which are associated with a given reaction channel i. These channels in the configuration space correspond to different distributions of nucleons over the fragments so that

$$\nu_i = \frac{A!}{A_{1i}!A_{2i}!\upsilon}, \tag{7}$$

where $\upsilon = 2$ if the fragments are identical and $\upsilon = 1$ otherwise. The number of terms in the sum is ν_i and the permutations P are such that with their help one obtains all the channels in the configuration space from one of them. The quantity $\pi(P)$ is either zero or one depending on the parity of a permutation. As mentioned above, in Eq. (5) Ψ_{000} is the ground-state harmonic oscillator function and $\bar{\mathbf{R}}_{\rm c.m.} = \mathbf{R}_{\rm c.m.}\sqrt{A}/r_0$, where $\mathbf{R}_{\rm c.m.}$ is the center-of-mass vector of the whole system.

Define approximate (or trial, or truncated) continuum wave functions

$$\Psi_j = \psi_j^{(0)} + \sum_{i=1}^{n} a_i^j\psi_i^{(1)} + \sum_{k=1}^{N-n} b_k^j\chi_k, \tag{8}$$

$1 \leqslant j \leqslant n$. The functions $\psi_m^{(0),(1)}$ are defined in Eq. (5) and they correspond to open reaction channels whose number is denoted as n.[1] The functions χ_k are short ranged. They are linear combinations of the Slater determinants constructed of the oscillator orbitals. Their choice is discussed below.

The expansion coefficients a_i^j and b_k^j are to be found. One has $a_i^j = -K_{ij}$, where K_{ij} is the K matrix. The S matrix sought for is

$$S = (iK+I)(iK-I)^{-1}. \tag{9}$$

For brevity we rewrite the ansatz (8) as

$$\Psi_j = \zeta_0^j + \sum_{i=1}^{N} c_i\zeta_i, \qquad 1 \leqslant j \leqslant n, \tag{10}$$

where $\zeta_0^j = \psi_j^{(0)}$, and at $1 \leqslant i \leqslant n$ one has $\zeta_i = \psi_i^{(1)}$. At $i = n+k$ one has $\zeta_i = \chi_k$. To find the coefficients of the expansions of the type of Eq. (8) simple equations of the form

$$\sum_{i=1}^{N} A_{ki}c_i = B_k^{(j)}, \qquad k = 1,\ldots,N, \tag{11}$$

will be employed.

In the case of small systems, the Hulthén-Kohn variational method, see, e.g., Ref. [9], is traditionally applied. It leads to the equations of the form of Eqs. (11) with $A_{ki} = (\zeta_k, [H-E]\zeta_i)$ and $B_k^{(j)} = -(\zeta_k, [H-E]\zeta_0^j)$. Here H is an internal Hamiltonian and E is the energy of the whole system. The disadvantage of such equations in our case is that they thus include the "free-free" ME like $(\psi_k^{(1)}, [H-E]\psi_l^{(0),(1)})$ which represent a class of ME additional to bound-bound and bound-free ME and which are more involved than the latter ones.

In view of this, in Ref. [10] (subsection 5 of Sec. 1 in that reference) another set of equations has been suggested. Formulating them, let us take into account that the quantities like $[H-E]\psi_i^{(0),(1)}$ are localized. This is seen when one interchanges $H-E$ with the $\mathcal{A}_i$ operator entering Eq. (5) and then writes, as usual,

$$H-E = (H_1-\epsilon_1) + (H_2-\epsilon_2) + \left[T_{\rm rel} + \bar{V}_{\rm ext}^{\rm coul}(\rho_i) - E_{\rm rel}\right] + \left[V_{\rm ext}^{\rm nucl} + V_{\rm ext}^{\rm coul} - \bar{V}_{\rm ext}^{\rm coul}(\rho_i)\right], \tag{12}$$

where H_1 and H_2 are internal Hamiltonians of the fragments, ϵ_1 and ϵ_2 are fragment eigenenergies, $T_{\rm rel}$ is the operator of kinetic energy of the fragment relative motion, $E_{\rm rel}$ is the energy of this relative motion, $\bar{V}_{\rm ext}^{\rm coul} = Z_1Z_1e^2/\rho_i$ is a subsidiary potential that reproduces the large-distance Coulomb

[1] Terms of the same structure as $\psi_k^{(0),(1)}$ but describing closed channels may be included in the expansion (8) to speed up the convergence at energies lying below the corresponding thresholds close to them.

interfragment interaction, and $V_{\rm ext}^{\rm nucl}$ and $V_{\rm ext}^{\rm coul}$ are nuclear and Coulomb interfragment interactions.

The third term in Eq. (12) acts on the relative motion functions $f_i^{(0),(1)}(\rho_i)Y_{lm}(\hat{\boldsymbol{\rho}}_i)$ and the corresponding contribution decreases exponentially as ρ_i increases. The contribution of the nuclear interaction $V_{\rm ext}^{\rm nucl}$ entering the last term also decreases exponentially as ρ_i increases while the difference $V_{\rm ext}^{\rm coul} - \bar{V}_{\rm ext}^{\rm coul}$ of the Coulomb interactions there decreases as ρ_i^{-2}.

Since in the class of trial Ψ_j of Eq. (10) the state $[H - E]\Psi_j$ is thus localized, to select the best of the Ψ_j it is natural to require [10] that $[H - E]\Psi_j$ is orthogonal to N lowest localized states χ_k that are of the type of the $N - n$ states χ_k entering Eq. (8). That is, we set $(\chi_k, [H - E]\Psi_j) = 0$ with $1 \leqslant k \leqslant N$. These are the equations that have the form of Eq. (11) with

$$A_{ki} = (\chi_k, [H - E]\zeta_i), \quad B_k^{(j)} = -\big(\chi_k, [H - E]\zeta_0^j\big). \quad (13)$$

These equations include bound-bound and bound-free ME only. As pointed out in Ref. [10] one more advantage of such equations is that in ME entering them antisymmetrization with respect to nucleons belonging to different fragments may be omitted. These equations were not studied numerically in Ref. [10] and, to our knowledge, they were not employed in the literature in practical scattering calculations. The corresponding comments in Ref. [10] were general ones and were not specially intended for applications of the type of the present paper. However, these equations are very suitable for our present purpose of extending ncsm to describe reactions. In the subsequent sections the calculation of bound-free ME entering them is addressed.

In an independent paper [11] the least-squares type equations have been suggested to solve the problem. It was pointed out there that the equations of the form of (11) and (13) are the limiting case of the least-squares method. In our case, when the matrix of the $H - E$ operator in the Slater determinant basis is large and sparce, this general least-squares method seems to be less efficient than these equations.

The above trial wave functions include regularization parameters like $\rho_{\rm cut}$ in Eq. (3). Let us discuss their choice. One may suggest that in the case of a sufficiently accurate calculation there should exist ranges of these parameters such that reaction amplitudes are nearly independent of their choice within these ranges. If so, the optimal values of these parameters are those which belong to these ranges, see the examples below. This prescription corresponds to the fact that the convergent values of reaction amplitudes are independent of such parameters.

Let us discuss the choice of the short-range basis states χ_k entering Eqs. (8), (10), and (13). In our case, they are many-body oscillator states. In the case of projection equations such as Eqs. (13), the results of a calculation are completely determined by a linear space the χ_k states span. If the problem is considered in the space of all the corresponding oscillator states with the numbers of many-body oscillator quanta up to some value, then it may occur that the convergence is not reached unless the space is very large. But the existing experience on solving large systems of linear equations, see, e.g., Ref. [12], suggests that it may be sufficient to solve the problem only in a modest size Krylov subspace of that large space. This subspace is spanned by the states $\phi, PH\phi, \ldots, (PH)^{N_0}\phi$, where P is the projector onto the mentioned space of oscillator states and ϕ is a pivot state belonging to this space. The N_0 value is expected [12] not to exceed several hundreds to reach convergence.

The set of $(PH)^n\phi$ states is "ill posed." An equivalent basis set in the above Krylov subspace which is convenient for performing calculations is the Lanczos basis set that starts from the ϕ state; that is, the χ_k states are the corresponding Lanczos states at such a choice.

In our case, it is convenient to have the pivot ϕ state in the form of a superposition of the Slater determinants. When N_0 is sufficiently high, the results of such calculations [12] are often not sensitive to the choice of the ϕ state. In the literature in a number of cases this state is chosen to be an approximate solution, if known in advance, of the set of linear equations to be solved. In other cases it is chosen to be the right-hand side of linear equations to be solved.

The latter choice may be realized approximately in our problem as follows. One first constructs directly a complete subset, with not-too-high maximal number of many-body oscillator quanta, of basis oscillator functions having the center of mass of the whole system in the lowest oscillator state and having given total angular-momentum quantum numbers. Then, expanding the right-hand side term $(H - E)\psi_j^{(0)} \equiv (H - E)\zeta_0^j$ over this subset with the help of the method described below, one gets a sought-for ϕ state.

The choice of an approximate solution of our problem as the ϕ state may also be realized at use of the mentioned subset of basis oscillator functions. Then the whole problem is to be solved directly with the corresponding limited number of these basis functions. The linear combination $\sum_{k=1}^{N-n} b_k^j \chi_k$ from Eq. (8) obtained in the framework of this approximation may then be employed as the ϕ state in subsequent more extensive calculations. [At constructing such a pivot state it is natural to take all the corresponding states with the total number of oscillator quanta up to some value as the $N - n$ states χ_k entering Eq. (8). Then the question arises how to choose n extra χ_k states on which the projecting in Eqs. (13) is to be done. See the model example below in this connection.]

It is desirable to deal with the χ_k states for which the center of mass of the whole system is in the lowest oscillator state and the total angular momentum and its projection have given values. Most calculations of the ME below refer to this case. The M-scheme approach is adopted below so that the projection of the total angular momentum is given anyway. As to the two other mentioned properties, the discussed pivot ϕ state has these properties and hence the same is valid for all the other χ_k states if the exact arithmetic is assumed.

However, in certain cases these properties along with the nice properties of the Lanczos basis may be destroyed because of round-off errors even in computations with the quadrupole precision. Despite this, the χ_k states provided by the above procedures still may be employed as basis states. Of course, this is to be done without relying on the mentioned properties. The angular momentum and the center-of-mass

quantum numbers then will be recovered in the total wave function once convergence of a calculation is reached. In this version, ME more general than those mentioned above are required. We want to note that the evaluation of these ME is discussed in short at the end of Sec. V while the rate of convergence in this regime is to be investigated.

Another way to diminish the influence of round-off errors discussed in the literature, e.g., Ref. [13], is the following. At calculating spectra, the $\beta[H_{\rm c.m.} - (3/2)\hbar\omega]$ operator, $H_{\rm c.m.}$ being the oscillator center-of-mass Hamiltonian, with a large β constant is added to the internal Hamiltonian. This shifts above the spurious center-of-mass excitations [14]. If one imagines the influence of round-off errors as an action of a perturbation added to the Hamiltonian, then it may be concluded that the added operator, indeed, diminishes coupling due to round-off errors between center-of-mass excited and unexcited states. If this picture is valid, then it may be reasonable to diagonalize the Hamiltonian in the Lanczos basis, i.e., to get a number of the standard ncsm solutions for the whole A-nucleon system, and to use these solutions as χ_k, cf. Ref. [4]. The corresponding Lanczos, or Krylov, subspace is, however, different from such subspaces discussed above and, unlike those subspases, it is not related to the inhomogenous equations to be solved.

In fact, in general no reasons are known for convergence to be faster in the case of the Hulthén-Kohn type equations than in the case of Eqs. (11) with the coefficients (13). Below a good convergence is demonstrated in the case of the latter equations in model examples.

Reaction parameters obtained from various dynamics equations are sometimes considered to be the first approximation and presumably improved values of these parameters are then obtained taking the stationary values of the corresponding Hulthén-Kohn functionals to be final results. However, in reality these functionals do not exist in the literal sense in the case when bound-state wave functions of reaction participants are not exact. The derivations of the Hulthén-Kohn variational principle for this case we know in the literature [15,16] are inconclusive. In view of this, only in cases when the accuracy of a calculated reaction wave function is considerably lower than the accuracy of fragment wave functions entering it one could hope that the values of reaction parameters thus obtained are more accurate than the original ones. Besides, the Hulthén-Kohn functionals include undesirable free-free ME. For these reasons, we refrain from this improvement procedure.

The calculation can also be performed in the incoming and outgoing wave representation. In such a case the following radial functions of the relative motion of fragments are employed instead of functions (2),

$$f_i^{\pm}(\rho_i) = \left(\frac{A_{1i}A_{2i}}{k_i}\right)^{1/2} \frac{\tilde{H}_{l_i}^{(\pm)}(k_i, \rho_i)}{\rho_i}, \tag{14}$$

where

$$\tilde{H}_l^{(\pm)}(k, \rho) = \tilde{G}_l(k, \rho) \pm iF_l(k, \rho).$$

Correspondingly, the following channel functions are used instead of functions (5),

$$\psi_i^{\pm} = \mathcal{A}_i\varphi_i f_i^{\pm}(\rho_i)\Psi_{000}(\bar{\mathbf{R}}_{\rm c.m.}). \tag{15}$$

The representation of the form

$$\Psi_j = \psi_j^- + \sum_{i=1}^{n} a_i^j \psi_i^+ + \sum_{k=1}^{N-n} b_k^j \chi_k, \tag{16}$$

$1 \leqslant j \leqslant n$, similarly to Eq. (8) is used to obtain the approximate continuum wave functions. The χ_k terms are the same as in Eq. (8). One has $a_i^j = -S_{ij}$, where S_{ij} is the S matrix. Let us rewrite the ansatz of Eq. (16) in the form of Eq. (10), where now $\zeta_0^j = \psi_j^-$, and at $1 \leqslant i \leqslant n$ one has $\zeta_i = \psi_i^+$. As above, $\zeta_i = \chi_k$ at $i = n + k$. With this notation, the equations of the same form as (11) and (13) are applicable in the present case.

In Secs. IV and V bound-free ME entering Eqs. (13) are calculated. Let us use the notation

$$Z^{nl}_{I_1I_2SJM} = \big[\big[\phi_1^{I_1}(1, \ldots, A_1)\phi_2^{I_2}(A_1 + 1, \ldots, A_1 + A_2)\big]_S \Psi_{nl}(\bar{\boldsymbol{\rho}})\big]_{JM} \Psi_{000}(\bar{\mathbf{R}}_{\rm c.m.}). \tag{17}$$

These quantities are obtained from those of Eqs. (4) and (5), or (4) and (15), via disregarding antisymmetrization and replacing the function of relative motion of fragments with an oscillator function. The quantity $\bar{\boldsymbol{\rho}}$ here equals $[A_1A_2/(A_1 + A_2)]^{1/2}\boldsymbol{\rho}/r_0$, where $\boldsymbol{\rho}$ is the interfragment distance of the type of Eq. (1). The ME we deal with below are of the form

$$\big(\chi_k, \hat{O}Z^{nl}_{I_1I_2SJM}\big), \tag{18}$$

where χ_k are as above and $\hat{O}$ is a scalar operator.

B. Examples

To verify the convergence of the method of calculating scattering at use of Eqs. (13) consider first the model problem of the s-wave scattering of a particle by the potential $-V_0\exp(-r/R)$, $V_0 > 0$. It was employed in the literature [11,17] to study the Hulthén-Kohn and least-squares methods. The problem allows an analytic solution, see, e.g., Ref. [18].

The precise values of the phase shift δ can be obtained as follows. Let us use the notation k for the wave number and denote $\hbar^2/(\mu R^2)$, μ being the particle mass, as E_0. Define

$$F = \sum_{n=0}^{\infty} a_n, \quad a_n = \frac{-2V_0/E_0}{n(n + 2ikR)} a_{n-1}, \tag{19}$$

with $a_0 = 1$. Then $\tan\delta = {\rm Im}F/{\rm Re}F$.

We want to find out whether Eqs. (11) and (13) lead to the exact solution of the problem.[2] Let us take, for example,

[2]In Ref. [11] solutions to the equations of the type of Eqs. (11) and (13) for the present problem were obtained in some cases with a modest accuracy in the context of the least-squares method. This was done for the cases when the set of localized states onto which the Schrödinger equation was projected differed from the set of localized states entering the expansion of the solution. In our case these two sets are the same which would be required in the ncsm-type calculations for technical reasons.

TABLE I. Dependence of $\tan\delta$ on the number of the short-range functions retained in Eq. (20).

$N-1$	$\tan\delta$
$d/R=0.4$	
2	−0.9803861
4	−0.9810342
6	−0.9807419
8	−0.9800367
10	−0.9798684
20	−0.9798734
22	−0.9798735
$d/R=1.0$	
2	−0.7998181
8	−0.9783943
20	−0.9802085
30	−0.9798741
48	−0.9798735

TABLE II. Dependence of $\tan\delta$ on the choice of $\chi_{m_{\rm last}}$, see the text.

$m_{\rm last}$	$\tan\delta$
$N=11$	
11	−0.9798684
12	−0.9798479
13	−0.9798180
14	−0.9797937
15	−0.9797773
16	−0.9797675
17	−0.9797620
$N=21$	
21	−0.9798734
22	−0.9798734
23	−0.9798734
24	−0.9798734
25	−0.9798734
26	−0.9798735
27	−0.9798735

$V_0=E_0$ and $kR=0.1$. The number of bound states in the system is determined solely by a V_0/E_0 value. At the above condition, there exists one bound state and its binding energy E_b is small compared to V_0. One has $E_b/E_0\simeq 0.013$. Once V_0/E_0 and kR values are given the phase shift δ is independent of R and thus it refers to a family of potentials. Let R be, say, 1.5 f. If, in addition, μ is chosen to be the reduced mass of the two-nucleon system, then at the chosen V_0/E_0 and kR values the potential has the depth V_0 about 37 MeV and the center-of-mass scattering energy is about 0.2 MeV. At the chosen V_0/E_0 and kR values the value of $\tan\delta$ equals -0.9798735 that is exact in all the listed digits.[3]

In the present case the expansion (8) reads as

$$\psi(r)=\frac{\sin kr}{kr}+\tan\delta\left[\left(1-e^{-r/R_{\rm cut}}\right)\frac{\cos kr}{kr}\right]+\sum_{m=1}^{N-1}b_m\chi_m(r), \tag{20}$$

where $R_{\rm cut}$ is a parameter similar to $\rho_{\rm cut}$ in (3). We choose the localized functions $\chi_m(r)$ to be the following:

$$\chi_m(r)=d^{-3/2}[m(m+1)]^{-1/2}L^2_{m-1}(r/d)e^{-r/(2d)}, \tag{21}$$

where $L^2_n(x)$ are the Laguerre polynomials. The basis set is orthonormalized. It is equivalent to the $r^{m-1}\exp[-r/(2d)]$ set but provides a higher stability at solving the equations. The ME required in the problem are calculated analytically in Appendix A.

The calculation involves two nonlinear parameters, $R_{\rm cut}/R$ and d/R. The $R_{\rm cut}/R$ quantity is taken to be 1.0 in all the cases and the results are insensitive to its choice within a wide range around this value. Equations (11) and (13) correspond to projecting the Schrödinger equation onto the first N basis functions from the set (21).

In Table I the values of $\tan\delta$ obtained are listed for various numbers $N-1$ of the basis functions (21) retained in Eq. (20). The results are shown for the choice $d/R=0.4$ and for a less-favorabale choice $d/R=1.0$. It is seen that in the former case rather accurate results emerge already at small N values. The convergence patterns are rather similar in the whole energy region of interest.

The following feature has been observed in our calculations. In Eqs. (11) and (13) the last of the functions (21) corresponded to $m=m_{\rm last}=N$. In place of it, now let us use functions $\chi_{m_{\rm last}}$ of the form of Eq. (21) with $m_{\rm last}=N+1$, or $N+2$, etc. It occurs that the results thus obtained are quite insensitive to the choice of the $m_{\rm last}$ value. This is illustrated in Table II at the $d/R=0.4$ choice.

This means that, at a sufficiently large number of basis functions retained in Eq. (20), the emerging scattering phase is in general insensitive to the space onto which the Schrödinger equation is projected. At the same time, the projecting onto higher basis states would be helpful if unphysical zero eigenvalues of the A_{ki} matrix (13) occur in an energy region of interest.

The choice of both the above potential and the basis (20) aimed to verify with a high confidence convergence of the method in general. Now let us clarify features of the corresponding calculations in the case when the oscillator basis is used and the number of retained basis functions is moderate. For this purpose, the model of Ref. [19], see also Ref. [20], is convenient. In this model, the dipole photodisintegration of the bound state of three particles interacting via a hypercentral potential is considered. Up to an energy-independent constant, the model is equivalent to a one-body problem in which the hypercentral potential is represented as a central one and nucleon with the "orbital momentum" 3/2 bound in this potential passes to the continuum state with the "orbital momentum" 5/2. The potential is a Gauss one, $V(r)=$

[3]This value is not small in magnitude while kR is small. This is because the scattering length a is large compared to R due to the presence of the shallow level. At our choice of V_0/E_0 one gets, see Ref. [18], $a/R\simeq 8.7$. Thus the ka quantity that is relevant here is not small.

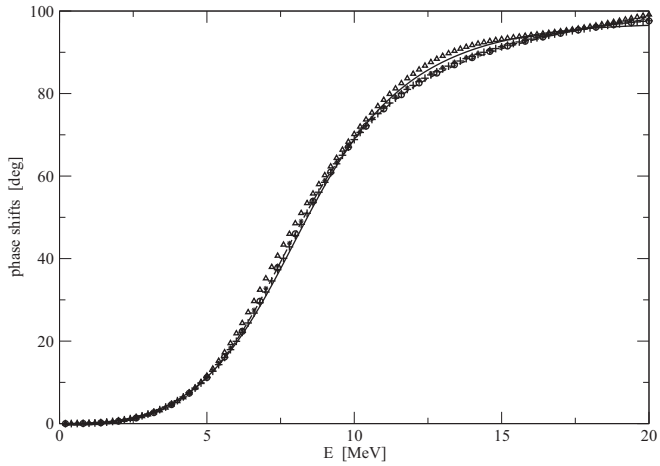

FIG. 1. Comparison of the exact phase shift (full line) with those calculated with use of the oscillator basis. Pluses, circles, dotted line, stars, and triangles correspond to Eq. (22) with $N = 7$ and with $R_{\rm cut} = 2.5$ f, 3 f, 4 f, 5 f, and 6 f respectively.

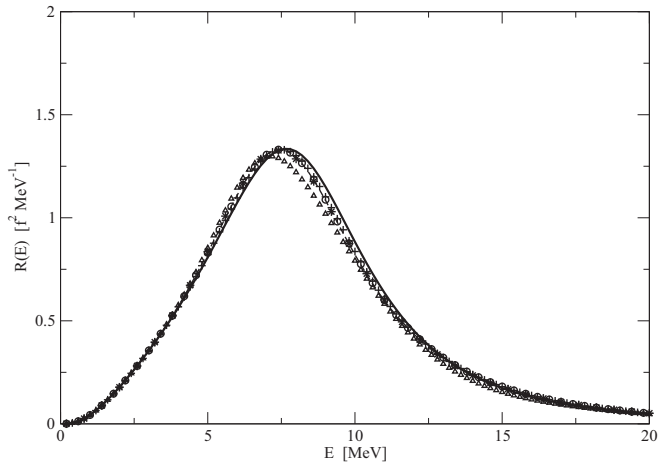

FIG. 2. Comparison of the exact response function (full line) with those calculated with use of the oscillator basis. Notation is as in Fig. 1.

$-V_0 \exp[-(r/R_0)^2]$, with $V_0 = 75$ MeV and $R_0 = 2.5$ f. The initial state binding energy is about 3.5 MeV.

We seek for the final-state continuum wave function in the form

$$\psi_E(r) = \frac{J_{l+1/2}(kr)}{(kr)^{1/2}} - \tan\delta\{1 - \exp[-(r/R_{\rm cut})^2]\}^{l+1/2} \times \frac{N_{l+1/2}(kr)}{(kr)^{1/2}} + \sum_{n=1}^{N} c_n R_{nl}(r), \tag{22}$$

where $l = 5/2$, $R_{\rm cut}$ is a parameter, and R_{nl} are the radial oscillator functions. All the terms here behave as r^l at $r \to 0$. The oscillator radius has been chosen to roughly optimize the calculation of the inital state binding energy and it equaled 2 f. We retain the seven lowest oscillator functions in the calculation, $N = 7$ in Eq. (22). Equations of the same form as in the preceding example are used to determine the $\tan\delta$ and c_n coefficients. Exact results to compare with may be obtained, in particular, within the same approach using sufficiently large N values in Eq. (22).

In Fig. 1 the phase shifts obtained are plotted along with the exact phase shift. The calculations were done with the values of the $R_{\rm cut}$ parameter in Eq. (22) of 2.5 f, 3 f, 4 f, 5 f, and 6 f. It is seen that the results pertaining to all the $R_{\rm cut}$ values except for 6 f are nearly indistinguishable and are close to the exact phase shift. This agrees with the above guess that stability of calculated reaction observables with respect to such type parameters indicates a sufficient accuracy of a calculation. The results at $R_{\rm cut} = 6$ f are a little less accurate. At $R_{\rm cut} = 2$ f the phase shift exhibits a nonphysical oscillation in the low energy region. At somewhat higher numbers of the retained oscillator functions this feature disappears and the phase shift becomes close to the exact one at any energy also with this $R_{\rm cut}$ value.

In Fig. 2 the dipole photodisintegration response function defined as

$$R(E) = \left[\int_0^\infty r^2 dr\, \bar{\psi}_E(r) r \psi_0(r)\right]^2 \tag{23}$$

is plotted. Here $\bar{\psi}_E = \psi_E \cdot (mk/\hbar^2)^{1/2} \cos\delta$, where ψ_E is given by Eq. (22), and ψ_0 is the wave function of the initial bound state normalized to unity and represented by 30 oscillator functions. The same comments as above apply to this case. Thus it is sufficient to retain seven basis oscillator functions to represent the final continuum state.

The above results suggest that the maximum number of many-body oscillator quanta required in a many-body calculation to reach convergence may be moderate.

The Coulomb interaction was disregarded in the above calculations but its inclusion could not change the picture. ME of the Coulomb potential itself would not enter a calculation due to the presence of the Coulomb wave functions in the corresponding ansatz of Eq. (20) or (22) type. The Coulomb wave functions in the internal region only are involved and the difference between their behavior in this region and the behavior of the spherical Bessel functions is of no importance.

III. SHELL-MODEL WAVE FUNCTIONS OF FRAGMENTS EXCITED WITH RESPECT TO CENTER OF MASS

The wave functions of fragments entering Eq. (4) are supposed to be taken from ncsm calculations. In fact, such calculations give products of these wave functions and the lowest oscillator functions of the fragment centers of mass. These products are provided in the form of expansions over the Slater determinants. Let us denote such products as $X^{000}_{I_1M_1}$ and $X^{000}_{I_2M_2}$,

$$X^{000}_{I_1M_1}(1,\ldots,A_1) = \phi_1^{I_1M_1}(1,\ldots,A_1)\Psi_{000}\big(\bar{\mathbf{r}}^{(1)}_{\rm c.m.}\big),$$
$$X^{000}_{I_2M_2}(A_1+1,\ldots,A_1+A_2) = \phi_2^{I_2M_2}(A_1+1,\ldots,A_1+A_2)\Psi_{000}\big(\bar{\mathbf{r}}^{(2)}_{\rm c.m.}\big), \tag{24}$$

where as in Eq. (4) $\phi_1^{I_1M_1}$ and $\phi_2^{I_2M_2}$ represent the eigenfunctions of internal Hamiltonians having the angular momenta $I_{1,2}$ and their projections $M_{1,2}$. The notation $\bar{\mathbf{r}}_{\rm c.m.}^{(1),(2)}$ denotes $\mathbf{r}_{\rm c.m.}^{(1),(2)}\sqrt{A_{1,2}}/r_0$, where $\mathbf{r}_{\rm c.m.}^{(1),(2)}$ are the center-of-mass vectors of the fragments.

We shall need also products of the internal wave function of a fragment and the wave function of its center of mass in a given excited state.[4] Let us denote these products as $X_{I_1M_1}^{nlm}$,

$$X_{I_1M_1}^{nlm}(1,\ldots,A_1)=\phi_1^{I_1M_1}(1,\ldots,A_1)\Psi_{nlm}\big(\bar{\mathbf{r}}_{\rm c.m.}^{(1)}\big) \qquad (25)$$

($A_1>1$). We shall obtain them in the form of linear combinations of the Slater determinants as well. Use of these products in this form is a key element of the present approach.

They are to be obtained in some $\mathcal{N}$ range, $2n+l\leqslant\mathcal{N}$, of numbers of the center of mass oscillator quanta. If the states (24) include components with the numbers of total many-body oscillator quanta up to some $N_{\rm tot}$, then the states (25) will include the Slater determinants with total many-body oscillator quanta up to $N_{\rm tot}+\mathcal{N}$. For heavier fragments and at higher $2n+l$ values the amount of these determinants may be too large. However, the states (25) with large $2n+l$ will play only a role of small corrections in what follows. Therefore, in the expansion of the states (25) over the Slater determinants it may be acceptable to retain only the determinants with total many-body oscillator quanta up to some $N_{\rm tot}+\mathcal{N}_0$ value with $\mathcal{N}_0<\mathcal{N}$. Then at $2n+l\leqslant\mathcal{N}_0$ the procedure is exact while at $2n+l>\mathcal{N}_0$ the components of the states (24) only with total many-body oscillator quanta up to $N'_{\rm tot}$, such that $N'_{\rm tot}+2n+l=N_{\rm tot}+\mathcal{N}_0$, will contribute to the result.

This truncation does not violate the separation of the internal and center-of-mass motions. Indeed, from the fact of the separation of these motions in Eqs. (24) it follows that the same separation, of course, takes place for separate components of the states (24) having given numbers of total many-body oscillator quanta. The procedure then merely either allows or forbids contributions of these components to a resulting center-of-mass excited state. [Obviously, $\mathcal{N}_0$ should be such that at least the minimal configuration of a state like (24) is not forbidden. This reads as $N_{\rm tot}+\mathcal{N}_0\geqslant N_{\rm min}+\mathcal{N}$, where $N_{\rm min}$ is the number of many-body oscillator quanta in the minimal configuration.]

Let us denote the internal Hamiltonian of a fragment as h, the oscillator Hamiltonian of its center of mass as $h_{\rm c.m.}$, and the operators of the center-of-mass orbital momentum and its projection as $l^2_{\rm c.m.}$ and $(l_z)_{\rm c.m.}$. The function $X_{I_1M_1}^{nlm}$ may be obtained as an eigenfunction of the operator $\lambda_1 h+\lambda_2 h_{\rm c.m.}+\lambda_3 l^2_{\rm c.m.}+\lambda_4(l_z)_{\rm c.m.}$, where λ_i constants are not equal to zero and arbitrary otherwise. At the diagonalization of this operator in the subspace of the Slater determinants with the number of quanta up to $N_{\rm tot}+\mathcal{N}_0$ the eigenvalue pertaining to this eigenfunction is $\lambda_1\epsilon_0+\lambda_2(2n+l+3/2)+\lambda_3 l(l+1)+\lambda_4 m$, where ϵ_0 is an approximate bound-state energy of the fragment.

It seems simpler to compute the $X_{I_1M_1}^{nlm}$ states in another way. Let us write Ψ_{nlm} in terms of Ψ_{000}, see, e.g., Ref. [22],

$$\Psi_{nlm}\big(\bar{\mathbf{r}}_{\rm c.m.}^{(1)}\big)=\alpha_{nl}\sqrt{4\pi}(\boldsymbol{\eta}\cdot\boldsymbol{\eta})^n\mathcal{Y}_{lm}(\boldsymbol{\eta})\Psi_{000}\big(\bar{\mathbf{r}}_{\rm c.m.}^{(1)}\big), \qquad (26)$$

where $\alpha_{nl}=(-1)^n[(2n+2l+1)!!(2n)!!]^{-1/2}$, $\boldsymbol{\eta}$ are the oscillator creation operators,

$$\boldsymbol{\eta}=\frac{1}{\sqrt{2}}\left[\bar{\mathbf{r}}_{\rm c.m.}^{(1)}-\frac{d}{d\bar{\mathbf{r}}_{\rm c.m.}^{(1)}}\right], \qquad (27)$$

and $\mathcal{Y}_{lm}$ are the solid harmonics. The $X_{I_1M_1}^{nlm}$ states are expressed in terms of the $X_{I_1M_1}^{000}$ states in the same way as in Eq. (26). Then, using Eq. (26), one may obtain $X_{I_1M_1}^{nlm}$ from $X_{I_1M_1}^{000}$ via recurrence relations. First, one may employ the relation following from Eq. (26)

$$X_{I_1M_1}^{0l+1,l+1}=(l+1)^{-1/2}\eta_+X_{I_1M_1}^{0ll}. \qquad (28)$$

Here spherical components of vectors like $\eta_\pm=\mp2^{-1/2}(\eta_x\pm i\eta_y)$ and $\eta_0=\eta_z$ are used. Once $X_{I_1M_1}^{0ll}$ is constructed in the form of a linear combination of the Slater determinants, Eq. (28) makes possible to construct in this form also $X_{I_1M_1}^{0l+1,l+1}$ using the relation

$$\boldsymbol{\eta}=\frac{1}{\sqrt{A_1}}\sum_{i=1}^{A_1}\boldsymbol{\eta}_i, \qquad (29)$$

where $\boldsymbol{\eta}_i$ are the oscillator creation operators for separate nucleons,

$$\boldsymbol{\eta}_i=\frac{1}{\sqrt{2}}\left(\bar{\mathbf{r}}_i-\frac{d}{d\bar{\mathbf{r}}_i}\right), \qquad \bar{\mathbf{r}}_i=\mathbf{r}_i/r_0. \qquad (30)$$

In what follows only the states (25) with l values of the same parity will be required. In this connection, the relation, similar to Eq. (28),

$$X_{I_1M_1}^{0l+2,l+2}=[(l+1)(l+2)]^{-1/2}\eta_+^2X_{I_1M_1}^{0ll} \qquad (31)$$

may also be useful in conjunction with Eq. (29). One- and two-body matrix elements are then to be calculated.

Next, one obtains the $X_{I_1M_1}^{nll}$ states with $n\neq0$ as a combination of the Slater determinants applying the relation following from Eq. (26),

$$X_{I_1M_1}^{n+1,ll}=-[(2n+2l+3)(2n+2)]^{-1/2}\boldsymbol{\eta}\cdot\boldsymbol{\eta}X_{I_1M_1}^{nll}. \qquad (32)$$

One needs to calculate one- and two-body matrix elements also in this case.

If the above discussed approximation is adopted and the $N_{\rm tot}+\mathcal{N}_0$ maximal number of the total many-body oscillator quanta is reached, then at performing each further step of the procedure the Slater determinants that have this maximal number of quanta are to be dropped in the right-hand sides of the corresponding recursion relations, Eqs. (32), (28), or (31).

In a certain case below the $X_{I_1M_1}^{nlm}$ states with $m<l$ are also required. They can be constructed with the help of the

[4] After the present manuscript was submitted I learned about Ref. [21], where the states of Eq. (25) form were constructed numerically using the center-of-mass creation and annihilation operators. In the present paper this is done analytically proceeding from Eq. (26) below. The oscillator cluster model (with no explicit antisymmetrization) in the frame of which these states are used in Ref. [21] is quite different from the present scheme to calculate reactions.

lowering operators. Writing $\mathbf{l} = -i\boldsymbol{\eta} \times \boldsymbol{\eta}^+$, where

$$\boldsymbol{\eta}^+ = \frac{1}{\sqrt{2}}\left[\bar{\mathbf{r}}^{(1)}_{\text{c.m.}} + \frac{d}{d\bar{\mathbf{r}}^{(1)}_{\text{c.m.}}}\right],$$

one gets

$$X^{nl,m-1}_{I_1M_1} = 2^{1/2}[(l+m)(l-m+1)]^{-1/2} \times (\eta_-\eta_0^+ - \eta_0\eta_-^+)X^{nlm}_{I_1M_1}. \quad (33)$$

Along with Eq. (29) one uses the relations

$$\boldsymbol{\eta}^+ = \frac{1}{\sqrt{A_1}}\sum_{i=1}^{A_1}\boldsymbol{\eta}_i^+, \quad \boldsymbol{\eta}_i^+ = \frac{1}{\sqrt{2}}\left(\bar{\mathbf{r}}_i + \frac{d}{d\bar{\mathbf{r}}_i}\right) \quad (34)$$

to calculate these states in the required form. One-body contributions to the operator from Eq. (33) are the single-particle orbital momenta $l^{(i)}_-$.

IV. RELATION BETWEEN CLUSTER AND SHELL-MODEL ME

In this section we address the ME (18) for the case when the χ_k functions discussed in Sec. II possess given J values and correspond to the center of mass in the lowest oscillator state. To signify these properties, these functions will be denoted as $\chi_k^{JM,0}$ in such a case. The corresponding ME (18) do not depend on M. We want to express them in terms of the ME,

$$\left[\chi_k^{JM,0}, \hat{O}X^{nlm}_{I_1M_1}(1,\ldots,A_1)X^{000}_{I_2M_2}(A_1+1,\ldots,A_1+A_2)\right] \equiv \mathcal{M}(I_1M_1I_2M_2, nlm, J), \quad (35)$$

where $M_1 + M_2 + m = M$. The states $X^{nlm}_{I_1M_1}$ and $X^{000}_{I_2M_2}$ are of the form of Eqs. (24) and (25) of the preceding section. The $X^{000}_{I_2M_2}$ state is directly provided by a bound-state ncsm calculation. At $A_1 > 1$ the $X^{nlm}_{I_1M_1}$ states are obtained from a ncsm bound state by means of the center-of-mass excitation as described in the preceding section. Both $X^{nlm}_{I_1M_1}$ and $X^{000}_{I_2M_2}$ are sums of the Slater determinants as well as $\chi_k^{JM,0}$.

At $A_1 = 1$, i.e., in the case when the first fragment is a nucleon, the function $\phi_1^{I_1M_1}$ in Eqs. (24) and (25) is to be replaced with the corresponding spin-isospin function of the nucleon. The $X^{nlm}_{I_1M_1}$ wave function is then merely the product of this spin-isospin function ($I_1 = 1/2$) and $\Psi_{nlm}(\bar{\mathbf{r}}^{(1)}_{\text{c.m.}})$.

Consider the quantities

$$\sum_{M_1+M_2=M-m} C^{S,M-m}_{I_1M_1I_2M_2}\mathcal{M}(I_1M_1I_2M_2, nlm, J). \quad (36)$$

Since in the ME (35) $\chi_k^{JM,0}$ is a state with a given total momentum and its projection, it is clear that these quantities are proportional to the corresponding ME in which $X^{nlm}_{I_1M_1}$ and $X^{000}_{I_2M_2}$ are coupled to the total momentum according to the $((I_1I_2)Sl)J$ scheme and the proportionality coefficient is the Clebsh-Gordan coefficient $C^{JM}_{S,M-m,lm}$. Furthermore, in Eq. (35) the wave function pertaining to $X^{nlm}_{I_1M_1}$ includes $\Psi_{nlm}(\bar{\mathbf{r}}^{(1)}_{\text{c.m.}})$ as a factor and that pertaining to $X^{000}_{I_2M_2}$ includes $\Psi_{000}(\bar{\mathbf{r}}^{(2)}_{\text{c.m.}})$ as a factor. One may write

$$\Psi_{nlm}\left(\bar{\mathbf{r}}^{(1)}_{\text{c.m.}}\right)\Psi_{000}\left(\bar{\mathbf{r}}^{(2)}_{\text{c.m.}}\right) = \sum_{n'l'NL}\langle n'l'NL|nl00\rangle_l^{\varphi} \times [\Psi_{n'l'}(\bar{\boldsymbol{\rho}})\Psi_{NL}(\bar{\mathbf{R}}_{\text{c.m.}})]_{lm}, \quad (37)$$

where $\langle n'lNL|nl00\rangle_l^{\varphi}$ are the oscillator brackets corresponding to the orthogonal transformation

$$\bar{\mathbf{r}}^{(1)}_{\text{c.m.}} = \bar{\boldsymbol{\rho}}\cos\varphi + \bar{\mathbf{R}}_{\text{c.m.}}\sin\varphi,$$
$$\bar{\mathbf{r}}^{(2)}_{\text{c.m.}} = -\bar{\boldsymbol{\rho}}\sin\varphi + \bar{\mathbf{R}}_{\text{c.m.}}\cos\varphi \quad (38)$$

with $\cos\varphi = (A_2/A)^{1/2}$ and $\sin\varphi = (A_1/A)^{1/2}$. Since in the ME (35) the $\chi_k^{JM,0}$ wave function is proportional to $\Psi_{000}(\bar{\mathbf{R}}_{\text{c.m.}})$, only the term from the sum in the right-hand side with $N = L = 0$ and hence with $l' = l$ and $n' = n$ contributes to the result. Therefore, one has the relation

$$\sum_{M_1+M_2=M-m} C^{S,M-m}_{I_1M_1I_2M_2}\mathcal{M}(I_1M_1I_2M_2, nlm, J) = C^{JM}_{S,M-m,lm}\langle nl00|nl00\rangle_l^{\varphi}\left(\chi_k^{JM,0}, \hat{O}Z^{nl}_{I_1I_2SJM}\right). \quad (39)$$

The m and $M - m$ values here are arbitrary. This relation expresses the ME (18) that contain cluster type wave functions in terms of the ME (35) that involve only oscillator orbitals. Similar relations have been derived, e.g., in Refs. [2,23–25], their differences with Eq. (39) refer to dealing with angular momenta. A more general relation is given in Ref. [26]. [One has $\langle nl00|nl00\rangle_l = (A_2/A)^{(2n+l)/2}$ in Eq. (39). This known relation follows, e.g., from Eq. (53).]

One may choose $m = l$ in Eq. (39). With this choice, the Clebsh-Gordan coefficient in the right-hand side of Eq. (39) is different from zero at least when $M = J$ is chosen. Indeed [27],

$$C^{JJ}_{S,J-l,ll} = (-1)^{l+S-J}\left[\frac{(2l)!(2J+1)!}{(l+S+J+1)!(l-S+J)!}\right]^{1/2}. \quad (40)$$

Thus the ME sought for may be computed, e.g., from the relation

$$\left(\chi_k^{JM,0}, \hat{O}Z^{nl}_{I_1I_2SJM}\right) = \left[C^{JJ}_{S,J-l,ll}\langle nl00|nl00\rangle_l^{\varphi}\right]^{-1} \times \sum_{M_1+M_2=J-l} C^{S,J-l}_{I_1M_1I_2M_2}\mathcal{M}(I_1M_1I_2M_2, nll, J). \quad (41)$$

It is clear that in the above relations it is expedient to choose the lighter of the two fragments to be the fragment number one in the notation we use. A similar type relation can be written also in the case when the χ_k states do not possess given momentum J but still correspond to the center of mass of the whole system in the ground state.

V. MATRIX ELEMENTS INVOLVING CHANNEL FUNCTIONS

The coefficients of the dynamic equations of Sec. II are the bound-bound ME and the bound-free ME, i.e., those which include the localized ncsm functions and nonlocalized channel functions of Eqs. (5) and (15). Thus, finally, we need to calculate the bound-free ME using the considerations

above. These ME are of the form

$$(\chi_k, [H-E]\mathcal{A}_i\varphi_i f_i(\rho_i)\Psi_{000}(\bar{\mathbf{R}}_{\text{c.m.}})), \tag{42}$$

where $\mathcal{A}_i$ is the antisymmetrizer (6), φ_i is the surface function (4), f_i one of the functions $f_i^{(0),(1)}$ from Eq. (2) or functions $f_i^{\pm}$ from Eq. (14), and the notation χ_k is as above. Using the fact that χ_k are antisymmetric with respect to permutations, one may rewrite the expression (42) as

$$\begin{aligned}&(\mathcal{A}_i^{\dagger}\chi_k, [H-E]\varphi_i f_i(\rho_i)\Psi_{000}(\bar{\mathbf{R}}_{\text{c.m.}}))\\ &\quad = \nu_i^{1/2}(\chi_k, [H-E]\varphi_i f_i(\rho_i)\Psi_{000}(\bar{\mathbf{R}}_{\text{c.m.}})).\end{aligned} \tag{43}$$

Thus the task of antisymmetrization of the channel functions is removed. The ME in the right-hand side of Eq. (43) is of the structure

$$\begin{aligned}&\big(\chi_k, [H-E]\big[\big[\phi_1^{I_1}(1,\ldots,A_1)\phi_2^{I_2}(A_1+1,\ldots,A_1\\ &+A_2)\big]_S Y_l(\hat{\boldsymbol{\rho}})\big]_{JM} f(\rho)\Psi_{000}(\bar{\mathbf{R}}_{\text{c.m.}})\big).\end{aligned} \tag{44}$$

The channel subscript i is omitted here and below. An efficient way to calculate it is as follows. One uses the $H-E$ operator in the form of (12) and one treats the fragment wave functions as being exact. Then the expression (44) becomes

$$\begin{aligned}&\big(\chi_k, \big[\big[\phi_1^{I_1}\phi_2^{I_2}\big]_S Y_l(\hat{\boldsymbol{\rho}})\big]_{JM}\tilde{f}(\rho)\Psi_{000}(\bar{\mathbf{R}}_{\text{c.m.}})\big)\\ &+\big(\chi_k^{JM,0}, \big[V_{\text{ext}}^{\text{nucl}}+V_{\text{ext}}^{\text{coul}}-\bar{V}_{\text{ext}}^{\text{coul}}(\rho)\big]\big[\big[\phi_1^{I_1}\phi_2^{I_2}\big]_S Y_l(\hat{\boldsymbol{\rho}})\big]_{JM}\\ &\times f(\rho)\Psi_{000}(\bar{\mathbf{R}}_{\text{c.m.}})\big),\end{aligned} \tag{45}$$

where

$$\begin{aligned}\tilde{f}(\rho) = \Big\{ &-\frac{\hbar^2}{2\mu}\Big[\frac{d^2}{d\rho^2}+\frac{2}{\rho}\frac{d}{d\rho}-\frac{l(l+1)}{\rho^2}\Big]\\ &+\bar{V}_{\text{ext}}^{\text{coul}}(\rho)-E_{\text{rel}}\Big\}f(\rho).\end{aligned} \tag{46}$$

The function $\tilde{f}(\rho)$ is localized. Let us approximate it by its truncated expansion over the oscillator functions. Then the first of the ME in Eq. (45) turns to a sum of the ME

$$\big(\chi_k, Z_{I_1I_2SJM}^{nl}\big) \tag{47}$$

of the type of Eq. (18). If $f = f^{(1)}$, then one has $\tilde{f} = 0$ and this contribution is absent.

In the second of the ME in Eq. (45) only values of $f(\rho)$ in a limited ρ range contribute to the result. Therefore, for computation of this ME one may use an approximation of $Y_{lm}f$ by a sum of oscillator functions. For this purpose, $f(\rho)$ is approximated with a linear combination $\sum_{n=0}^{n_{\max}} c_n R_{nl}$ of the radial parts $R_{nl}(\rho)$ of the oscillator functions $\Psi_{nlm}(\bar{\boldsymbol{\rho}})$ used above. This can be done via minimization of the quantity

$$\int_0^{\infty} d\rho\,\omega(\rho)\Big|f(\rho)-\sum_{n=0}^{n_{\max}} c_n R_{nl}(\rho)\Big|^2 \tag{48}$$

with respect to the c_n coeficients, $\omega(\rho)$ being a localized positive weight function. As a result, the contribution of the $V_{\text{ext}}^n + V_{\text{ext}}^c$ term to the ME turns to a sum of the ME

$$\big(\chi_k, \big[V_{\text{ext}}^{\text{nucl}}+V_{\text{ext}}^{\text{coul}}\big]Z_{I_1I_2SJM}^{nl}\big), \tag{49}$$

again of the type of Eq. (18). To calculate the contribution of the $\bar{V}_{\text{ext}}^{\text{coul}}(\rho)$ term, one may represent the arising product $\bar{V}_{\text{ext}}^{\text{coul}}(\rho)\sum_{n=0}^{n_{\max}} c_n R_{nl}(\rho)$ as a sum of the functions $R_{nl}(\rho)$ minimizing the quantity similar to (48) at the same $\omega(\rho)$. As a result, this contribution takes the above form of a sum of Eq. (47) type ME. (Thus, besides the total number of basis functions, the parameters of a calculation with respect to which its stability is to be checked are the $n_{\max}$ type numbers and possibly the above-defined $\mathcal{N}_0$ numbers.)

In what follows, let us first consider the case when the χ_k states possess given J values and correspond to the center of mass of the whole system in the ground state, i.e., $\chi_k^{JM,0}$ states in the above notation. Then applying the relation (39) or (41) one reduces the ME (47) and (49) to a sum of the quantities of Eq. (35) type with $\hat{O} = I$ or $\hat{O} = V_{\text{ext}}^{\text{nucl}} + V_{\text{ext}}^{\text{coul}}$. Each of these quantities is the sum of ME that contain the products of three Slater determinants entering, respectively, the $\chi_k^{JM,0}$ basis function and the $X_{I_1M_1}^{nlm}$ and $X_{I_2M_2}^{000}$ fragment wave functions.

In the $\hat{O} = I$ case, consider such an ME in which the first of the mentioned determinants is constructed of the oscillator orbitals $\psi_l(i)$ with $1 \leqslant i \leqslant A_1 + A_2$ and $l = \{l_1, \ldots, l_{A_1+A_2}\}$, the second determinant is constructed of the oscillator orbitals $\psi_m(j)$ with $1 \leqslant j \leqslant A_1$ and $m = \{m_1, \ldots, m_{A_1}\}$, and the third one is constructed of the oscillator orbitals $\psi_n(k)$ with $A_1 + 1 \leqslant k \leqslant A_1 + A_2$ and $n = \{n_1, \ldots, n_{A_2}\}$. The oscillator orbitals are assumed to be orthonormalized. The ME is calculated performing the Laplace expansion of the first of the mentioned determinants over the minors pertaining to the $\psi_l(i)$ orbitals with $1 \leqslant i \leqslant A_1$. The ME is different from zero only if the $\{l\}$ set of orbitals coincides with the $\{\{m\}, \{n\}\}$ set. (This is only possible if all the orbitals belonging to the $\{m\}$ set differ from those belonging to the $\{n\}$ set.) In this case it is equal to $\pm A_1!A_2!$ and the sign is governed by the simple rule.

In the $\hat{O} = V_{\text{ext}}^{\text{nucl}} + V_{\text{ext}}^{\text{coul}}$ case suppose that $V_{\text{ext}}^{\text{nucl}} + V_{\text{ext}}^{\text{coul}}$ is the sum of two-nucleon interactions $V(ij)$. This sum may be replaced with $A_1A_2V(ij)$, where $V(ij)$ is the interaction between a nucleon belonging to one of the fragments and a nucleon belonging to the other fragment. Then, applying the relation (39) or (41), the contribution (49) is reduced to a sum of ME between a Slater determinant pertaining to $\chi_k^{JM,0}$ and a product of Slater determinants pertaining to $X_{I_1M_1}^{nlm}$ and $X_{I_2M_2}^{000}$. These ME are calculated with the help of the same Laplace expansion as above. They are of the form

$$\begin{aligned}&(\det[\psi_{l'_1}(1),\ldots,\psi_{l'_{A_1}}(A_1)]\\ &\quad\times\det[\psi_{l'_{A_1+1}}(A_1+1),\ldots,\psi_{l'_{A_1+A_2}}(A_1+A_2)],\\ &V(ij)\det[\psi_{m_1}(1),\ldots,\psi_{m_{A_1}}(A_1)]\\ &\quad\times\det[\psi_{n_{A_1+1}}(A_1+1),\ldots,\psi_{n_{A_1+A_2}}(A_1+A_2)]),\end{aligned} \tag{50}$$

where $1 \leqslant i \leqslant A_1$ and $A_1 + 1 \leqslant j \leqslant A_1 + A_2$ and the sets $\{l'_1, \ldots, l'_{A_1}\}$ and $\{l'_{A_1+1}, \ldots, l'_{A_1+A_2}\}$ are subsets of the $\{l_1, \ldots, l_{A_1+A_2}\}$ set. These ME may not vanish only if the latter subsets differ, respectively, from the $\{m\}$ set and the $\{n\}$ set by not more than one orbital. In such cases the set of the $\{\{m\}, \{n\}\}$ orbitals differs from the $\{l\}$ set by not more than two orbitals and these two orbitals cannot belong to the same $\{m\}$ or $\{n\}$ set. (This is only possible if in the $\{m\}$ set not more than two orbitals are the same as in the $\{n\}$ set.) The ME (50) is of the structure similar to that of one-body operators. Therefore,

it is reduced in the usual way (depending on whether the corresponding orbitals are the same or not) to the standard two-body ME like

$$\big(\psi_l(i)\psi_{l'}(j), V(ij)\psi_m(i)\psi_n(j)\big).$$

ME of three-nucleon interactions that contribute to $V_{\rm ext}^{\rm nucl}$ are calculated in a similar way.

If χ_k is a combination of Slater determinants which does not possess definite quantum numbers of the center of mass of the whole system, then the simplification of the preceding section is not applicable anymore. But then, just as above, the ME (42) still can be written as the sum of quantities of the form of Eq. (18), where $\hat{O}$ is either a unit operator or an operator of two- or three-body interfragment interaction. While above these quantities were expressed in terms of the contributions (35), now they may be represented as the sums of the contributions of the form

$$\big[\chi_k, \hat{O}X_{I_1M_1}^{n_1l_1m_1}(1,\dots,A_1)X_{I_2M_2}^{n_2l_2m_2}(A_1+1,\dots,A_1+A_2)\big], \tag{51}$$

where $X_{I_1M_1}^{n_1l_1m_1}$ and $X_{I_2M_2}^{n_2l_2m_2}$ are obtained via the center-of-mass excitation applied to ncsm wave functions of the fragments as in Sec. III. (In the $X_{I_2M_2}^{n_2l_2m_2}$ case one proceeds in the same way as described in Sec. III as to $X_{I_1M_1}^{n_1l_1m_1}$.) To this aim, let us directly transform the cluster $Z_{l_1l_2SJM}^{nl}$ state to the form of the sum of products of $X_{I_1M_1}^{n_1l_1m_1}$ and $X_{I_2M_2}^{n_2l_2m_2}$. This is achieved via the transformation

$$\Psi_{nlm}(\bar{\boldsymbol{\rho}})\Psi_{000}(\bar{\mathbf{R}}_{\rm c.m.}) = \sum_{n_1l_1n_2l_2} \langle n_1l_1n_2l_2|nl00\rangle_l^{\varphi'} \times \big[\Psi_{n_1l_1}(\bar{\mathbf{r}}_{\rm c.m.}^{(1)})\Psi_{n_2l_2}(\bar{\mathbf{r}}_{\rm c.m.}^{(2)})\big]_{lm}, \tag{52}$$

which corresponds to the coordinate transformation reverse to Eq. (38) so that φ' equals $-\varphi$ from there. [The brackets $\langle n_1l_1n_2l_2|nl00\rangle_l^{\varphi'}$ are as follows:

$$\langle n_1l_1n_2l_2|nl00\rangle_l^{\varphi'} = \cos^{2n_1+l_1}\varphi' \sin^{2n_2+l_2}\varphi' \times(-1)^l[(2l_1+1)(2l_2+1)]^{1/2}\begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0\end{pmatrix}\frac{\alpha_{n_1l_1}\alpha_{n_2l_2}}{\alpha_{nl}}, \tag{53}$$

where the α coefficients are defined in Eq. (26). This relation is obtained in Appendix B.]

It is clear that the quantities (51) are calculated in the same way as the quantities (35) above. In the case we consider now, computations are more lengthy.

In conclusion, reaction observables can be computed from simple linear equations with use of the Slater determinants. The equations do not include free-free matrix elements. Antisymmetrization between nucleons belonging to different fragments is not required. In model examples, the equations lead to rather precise results. The required bound-free ME are calculated in a universal way. Their computation somewhat resembles that of the ncsm bound-state ME. One may expect that the convergence rates of reaction observables in the present scheme should in general be at the level of the convergence rates of typical bound-state observables in ncsm. A method applicable for reactions at higher energy, when channels with three or more fragments are open, may be developed relying on the considerations of the present work in conjunction with the integral transform approach, see Refs. [28–30] and references therein.

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APPENDIX A: MATRIX ELEMENTS INVOLVING THE LAGUERRE-TYPE BASIS

The ME of the $H-E$ operator between the functions entering Eq. (20) are listed below. Subscripts like m refer to the functions (21). The ME of the radial kinetic energy between the functions (21) for a state with an orbital momentum l are as follows:

$$T_{mm'} = \frac{\hbar^2}{2\mu d^2}\left[\frac{(m_<+1)(m_<+2)}{(m_>+1)(m_>+2)}\right]^{1/2}\left[\frac{1}{2} - \frac{\delta_{mm'}}{4} + \frac{m_<}{3} + \frac{l(l+1)(3m_> - m_< + 3)}{6}\right], \tag{A1}$$

where $m_> = \max(m-1, m'-1)$ and $m_< = \min(m-1, m'-1)$. The ME of the exponential potential between the functions (21) are calculated as finite sums with the help of the known relation [31], Eq. 7.414 (4).

To calculate the ME of the $H-E$ operator between the functions χ_m (21) and the two scattering functions entering Eq. (20), the following scheme is convenient. All these ME are readily obtained from the integrals of the form

$$\int_0^\infty dt e^{-zt} t L_{m-1}^2(t), \tag{A2}$$

with $z = a + ib$, $a > 0$, and $b = \mp ikd$. These integrals can be calculated with the help of the following simple relation:

$$\int_0^\infty dt e^{-zt} L_n^1(t) = 1 - \left(\frac{z-1}{z}\right)^{n+1}. \tag{A3}$$

We derived it from an expression [31], Eq. 7.414 (5), involving the general Laguerre polynomial $L_n^\alpha(t)$. The integrals (A2) are obtained from Eq. (A3) via the recurrence relation $tL_{m-1}^2(t) = mL_{m-1}^1(t) - (m+1)L_m^1(t)$.

APPENDIX B: THE OSCILLATOR BRACKET $\langle n_1l_1n_2l_2|nl00\rangle_l^\varphi$.

The definition of the oscillator brackets adopted in the paper is as follows. Suppose that, as in Eq. (38),

$$\mathbf{x} = \mathbf{x}'\cos\varphi + \mathbf{y}'\sin\varphi, \qquad \mathbf{y} = -\mathbf{x}'\sin\varphi + \mathbf{y}'\cos\varphi. \tag{B1}$$

Then one has

$$[\Psi_{n_1l_1}(\mathbf{x})\Psi_{n_2l_2}(\mathbf{y})]_{lm} = \sum_{n_1'l_1'n_2'l_2'} \langle n_1'l_1'n_2'l_2'|n_1l_1n_2l_2\rangle_l^\varphi \big[\Psi_{n_1'l_1'}(\mathbf{x}')\Psi_{n_2'l_2'}(\mathbf{y}')\big]_{lm}. \tag{B2}$$

To get the $\langle n_1l_1n_2l_2|nl00\rangle_l^\varphi$ bracket we shall use the symmetry relation $\langle n_1l_1n_2l_2|nl00\rangle_l^\varphi = \langle nl00|n_1l_1n_2l_2\rangle_l^{-\varphi}$ and calculate the bracket in its right-hand side.

Equation (B2) is a relation between the polynomials of six variables. It leads to relations between their components of a given power. Writing at $\varphi \to -\varphi$ the relation for the highest power polynomials one gets

$$\alpha_{n_1 l_1}\alpha_{n_2 l_2} x^{2n_1} y^{2n_2} [\mathcal{Y}_{l_1}(\mathbf{x})\mathcal{Y}_{l_2}(\mathbf{y})]_{lm} = \sum_{n_1' l_1' n_2' l_2'} \langle n_1' l_1' n_2' l_2' | n_1 l_1 n_2 l_2 \rangle_l^{-\varphi}\, \alpha_{n_1' l_1'}\alpha_{n_2' l_2'} (x')^{2n_1'} (y')^{2n_2'} \times [\mathcal{Y}_{l_1'}(\mathbf{x}')\mathcal{Y}_{l_2'}(\mathbf{y}')]_{lm}, \tag{B3}$$

where in Eqs. (B1) the replacement $\varphi \to -\varphi$ is implied. Let us write $\mathbf{x}$ and $\mathbf{y}$ here in terms of $\mathbf{x}'$ and $\mathbf{y}'$ and then take the $y' \to 0$ limit. This gives $\mathbf{x} = \mathbf{x}' \cos\varphi$ and $\mathbf{y} = \mathbf{x}' \sin\varphi$. In Eq. (B3) only the term with $n_2' = l_2' = 0$ and hence $l_1' = l$ and $n_1' = n$ survives in this limit, n being defined via the relation $2n_1 + l_1 + 2n_2 + l_2 = 2n + l$. Comparing the left- and right-hand sides of the arising equality (which is convenient to do at the $\mathbf{x}'$ vector directed along the z axis) one comes to Eq. (53).

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Correction: A minor typographical error in Eq. (53) has been fixed.