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Generator coordinate approach to nuclear reactions. II. Nucleus-nucleus scattering with distorted basis functions

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The generator coordinate formulation of the single nucleus scattering by an external potential presented in the preceding paper is generalized here to the nucleus-nucleus scattering, in which the complete antisymmetrization of all nucleons involved is explicitly carried out and the correct internal states are extracted by the double-projection method of Peierls and Thouless. General distortion effects are incorporated, where the single nucleon orbitals may depend on the relative distance and relative momentum generator coordinates of two nuclei. The special case of nuclear molecular orbitals is also considered. The connection between the distorted orbitals and a restricted time-dependent Hartree-Fock procedure is clarified.

[NUCLEAR REACTIONS Generator coordinate methods; nucleus-nucleus scattering; distortion effects.]

I. INTRODUCTION

In a first paper[1] (to be referred to as I in the following), we have given a microscopic formulation of the scattering of a nucleus by a fixed external potential. From a set of determinantal wave functions, mathematically consistent scattering wave functions are constructed using either the single projection method of Peierls and Yoccoz[2] (PY) or the double projection method of Peierls and Thouless[3] (PT). The single-particle nature of the wave function is thus preserved, which makes the evaluation of various matrix elements with these functions rather simple. The scattering problems are then solved in the generator coordinate (GC) variables so that the usual kinematic complications encountered in the resonating group method (RGM) are avoided. The Griffin-Hill-Wheeler[4] type scattering equations are explicitly derived, and a prediagonalization procedure is formulated to provide an improved representation of the internal states in specifying the asymptotic boundary conditions. Extensions of the theory to incorporate both the energy and coordinate-dependent distortion effects are then carried out; it is found that the projection methods can naturally be adapted for this purpose.

We continue the above study by extending the formalism of I to the practically more interesting case of nucleus-nucleus scattering.[5,6] Since we expect the approach of I to be equally applicable to this case, with minor modifications in the kinematics, a brief summary of the result of I relevant to the present paper will be given in Sec. II. The scattering equations and explicit boundary conditions are derived for the nucleus-nucleus scattering in Sec. III. Then Sec. IV contains the extension of these results to incorporate distortions, which naturally leads to the time-dependent Hartree-Fock (TDHF) procedure in the parametrized form.

II. PRELIMINARY DISCUSSION

Since the development of the formalism below will depend heavily on the results obtained in I, we briefly summarize the relevant points of that paper and also define notations.

For a nucleus with N_A nucleons, Slater determinantal functions of the form

$$\Phi_a^A(x)=\frac{1}{\sqrt{N_A!}}\det[\varphi_{a_1}^A(x_1)\varphi_{a_2}^A(x_2)\cdots\varphi_{a_{N_A}}^A(x_{N_A})] \tag{2.1}$$

may be constructed, where the φ's are the single-particle functions and the x_i's are the single nucleon coordinates measured from a fixed point O_x. (We drop the explicit notation describing vectors for simplicity). In a special case, the function $\Phi_a^A(x)$ assumes the factorizable form

$$\Phi_a^A(x)=G_a^A(R_A)\Phi_a^{A\,\mathrm{int}}(\xi^A)\,, \tag{2.2}$$

where

$$x=(x_1^A,x_2^A,\ldots,x_{N_A}^A)\,,$$
$$\xi^A=(\xi_1^A,\xi_2^A,\ldots,\xi_{N_A}^A)\,,$$
$$\xi_i^A=x_i-R_A\,,$$

and

$$R_A=\sum_{i=1}^{N_A}x_i/N_A\,.$$

In this factorizable case (2.2), we have

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$$\Phi^{A\text{-PY}}_{q'a}(x) = \int dR'_A e^{iq'\cdot R'_A}\Phi^A_a(x-R'_A) \xrightarrow[q'\to 0]{} \left[\int dR'_A G_a(R_A-R'_A)\right]\Phi^{A\,\mathrm{int}}_a(\xi^A)\,. \tag{2.3}$$

Of course, this separation (2.2) is not always possible, and the extraction of the internal wave function requires then a special projection procedure. When Φ^A_a does not factorize, we have to adopt the PT procedure in extracting the internal wave function, as

$$\Phi^{A\text{-PT}}_{0a}(\xi^A) \equiv \int dq' \tilde{F}_a(q') e^{-iq'\cdot R_A}\Phi^{A\text{-PY}}_{q'a}(x) = \int dR'_A F_a(R_A-R'_A)\Phi^A_a(x-R'_A)\,, \tag{2.4}$$

where F_a is the Fourier transform of $\tilde{F}_a$ and $\Phi^A_a(x-R'_A)=\Phi^A_a(\xi^A_a+R_A-R'_A)$. As in I, we neglect the $(2\pi)^{-3/2}$ factors throughout for notational simplicity.

The scattering functions are constructed from (2.3) and (2.4) by a linear superposition, as

$$\Psi^{A\text{-PY}}_a \equiv \int dq' \tilde{f}^{A\text{-PY}}_a(-q')\Phi^{A\text{-PY}}_{q'a}(x) = \int dR'_A f^{A\text{-PY}}_a(R'_A)\Phi^A_a(x-R'_A) \tag{2.5}$$

and

$$\Psi^{A\text{-PT}}_a \equiv \int dK'_A \tilde{f}^{A\text{-PT}}_a(-K'_A)e^{iK'_A\cdot R_A}\Phi^{A\text{-PT}}_{0a}(\xi^A) \equiv u^A_a(R_A)\Phi^{A\text{-PT}}_{0a}(\xi^A)\,, \tag{2.6}$$

respectively.

A form equivalent to (2.6) which is found to be useful in I is given by

$$\Psi^{A\text{-PT}}_a(x) = \int dK'_A \int dR'_A \mathcal{F}_a(K'_A,R'_A) \times e^{iK'_A\cdot(R_A-R'_A)}\Phi^A_a(x-R'_A) \tag{2.7}$$

with

$$\mathcal{F}_a(K'_A,R'_A) = \int dK''_A \tilde{F}_a(K''_A-K'_A)\tilde{f}^{A\text{-PT}}_a(-K''_A)e^{iK''_A\cdot R'_A}\,. \tag{2.8}$$

Equation (2.7) results immediately by the change of variable $q'=K'_A-K''_A$ in (2.6).

For notational convenience, we introduce the boost and displacement operators by

$$D_{R'_A} \equiv \exp(-iR'_A\cdot\hat{K}_A)\,, \qquad B_{K'_A} \equiv \exp(iK'_A\cdot\hat{R}_A)\,, \tag{2.9}$$

where $\hat{K}_A$ and $\hat{R}_A$ are operators, while the primed quantities are generator coordinates. In terms of these operators, we have

$$\Psi^{A\text{-PT}}_a(x) = \int dK'_A \int dR'_A \mathcal{F}_a(K'_A,R'_A) D_{R'_A}B_{K'_A}\Phi^A_a(x)\,. \tag{2.10}$$

The connection between the PY and PT forms of the wave functions can be derived by choosing the weighting function $\tilde{F}_a(K''-K') \to \delta(K')\,\tilde{G}^{-1}_a(K'')$, where $\tilde{G}_a(K'')$ is the relevant, momentum dependent normalization.

The scattering equation is obtained from a variational principle,

$$\delta[I]/\delta\,\mathcal{F}^*_{a''}(Z''_A) = 0\,, \tag{2.11}$$

where the variational functional $[I]$ is defined by

$$[I] = \lambda_t + \langle\Psi_t,[H-E]\Psi_t\rangle_x\,, \tag{2.12}$$

and

$$\Psi_t = \sum_a \Psi^{A\text{-PT}}_a(x)\,.$$

In (2.12), $\langle\ \rangle_x$ denotes the integrations over all the x_i variables and λ_t is an asymptotic amplitude parameter in Ψ_t. Equation (2.11) then gives

$$\sum_{a'}\int dZ'_A[H_{a''a'}(Z''_A,Z'_A) - EN_{a''a'}(Z''_A,Z'_A)] \times\mathcal{F}_{a'}(Z'_A) = 0\,, \tag{2.13}$$

where $Z'_A \equiv (K'_A,R'_A)$.

An improved description of the nuclear internal states and mathematically consistent boundary conditions for the amplitudes $\mathcal{F}_{a'}$ which satisfy (2.13) can be derived by the prediagonalization procedure formulated in I. A slightly intricate argument can be given to show that such a prediagonalization of (2.13) involving the nuclear internal Hamiltonian H_A is in fact equivalent to the diagonalization using (2.4). Thus, we finally obtain

$$\Psi \approx \sum_d \Psi^{PTD}_d \tag{2.14}$$

with

$$\Psi^{PTD}_d = \sum_{a'}\int dK'_A \int dR'_A \mathcal{F}^d_{a'}(K'_A,R'_A) \times e^{iK'_A\cdot(R_A-R'_A)}\Phi_{a'}(x-R'_A)\,, \tag{2.15}$$

and the boundary conditions

$$\mathcal{F}^d_{a'}(K'_A,R'_A) = \tilde{F}^d_{a'}(K'_A-K_d)a_d e^{iK_d\cdot R'_A} + \sum_{d'}\int dK''_A \frac{T_{dd'}(K''_A,K_d)a_d}{K^2_d-K''^2_A+i\epsilon} \times\tilde{F}^{d'}_{a'}(K''_A-K'_A)e^{iK''_A\cdot R'_A}\,. \tag{2.16}$$

Several generalizations of the above formalism to incorporate various forms of distortion effects were made in I.

(a) For adiabatic distortions in which the basis functions $\Phi_a^{ad}(x)$ are explicitly dependent on the generator coordinate R'_A, with the asymptotic property that

$$\Phi_a^{ad}(x;R'_A) \xrightarrow[R'_A\to\infty]{} \Phi_a(x), \tag{2.17}$$

the ansatz (2.4) gives

$$\Phi_{0a}^{A\text{-PT}} = \int dt'_A F_a(t'_A)\Phi_a^{ad}(\xi^A, t'_A; R_A - t'_A), \tag{2.18}$$

where $t'_A \equiv R_A - R'_A$. Evidently, Φ_{0a}^{ad} will be an explicit function of both ξ^A and R_A. However, for large R_A, $\Phi_{0a}^{A\text{-PT}}(\xi^A;R_A) \to \Phi_{0a}^{A\text{-PT}}(\xi^A)$, as a consequence of (2.17) and the fact that Φ_a^{ad} is peaked around the value $t'_A = 0$.

The scattering functions are defined just as in the first line of (2.6), and the scattering equations are the same as before, (2.13) without change. It is assumed that center-of-mass spuriosity will not contaminate asymptotic regions. In the factorizable case, the form (2.5) should be sufficient, i.e.,

$$\Psi_a^{A\text{-PY}} = \int dR'_A f_a^A(R'_A) G_a^A(R_A - R'_A; R'_A)\Phi_a^{A\,int}(\xi^A; R'_A), \tag{2.19}$$

again as long as the additional R'_A dependence disappears when $R'_A \to \infty$.

(b) For momentum-dependent distortions, the optical potential description of scattering phenomena suggests, in general, that the effective interactions should be momentum-dependent as well as coordinate-dependent. Such a feature can be incorporated in the construction of the basis sets, as

$$\Phi_a(x) \to \Phi_a(x;K'_A). \tag{2.20}$$

The double projection method can again be used to construct the scattering wave functions Ψ_a, as in (2.6) or (2.7). Note here that the generator coordinate K'_A in (2.20) is that variable in (2.7), and not the q' variable in (2.5), so that one is to consider (2.13) from the outset. In the factorizable case, the single projection should be sufficient, as evident from a slightly different form of (2.5) given by

$$\Phi_a^{A\text{-PY}} = \int dq' \tilde{f}_a^A(-q')\tilde{G}_a(-q';q')e^{iq'\cdot R_A}\Phi_a^{A\,int}(\xi^A;q'). \tag{2.21}$$

Here, we have taken the q' variable in $\Phi_a^{A\,int}$, contrary to (2.20). The q' dependence of $\Phi_a^{A\,int}$ should induce no polarization when $R_A \to \infty$.

(c) For coordinate and momentum-dependent distortions, we combine the extensions (a) and (b) above, and construct a general basis function of the form

$$\Phi_a^A(x) \to \Phi_a^A(x;K'_A,R'_A), \tag{2.22}$$

where K'_A here is again the generator coordinate which appears in (2.7). Thus,

$$\Psi_a^{PT}(x) = \int dK'_A \int dR'_A \mathfrak{F}_a(K'_A,R'_A)e^{iK'_A\cdot(R_A-R'_A)} \times \Phi_a^A(x-R'_A;K'_A,R'_A). \tag{2.23}$$

In the factorizable case, however, the simpler form (2.5) is not possible and we have instead

$$\Psi_a^{A\text{-PY}} = \int dq' \int dR'_A \tilde{f}_a(-q')e^{iq'\cdot R'_A}G_a(R_A - R'_A;q',R'_A) \times \Phi_a^{A\,int}(\xi^A;q',R'_A), \tag{2.24}$$

which still requires the double integrations.

III. NUCLEUS-NUCLEUS SCATTERING

We now generalize the result of I as summarized in Sec. II above to nucleus-nucleus scattering. Although the kinematics involved is more complicated, the formalism should be straightforward to construct. The cluster wave functions for the nuclei A and B, with N_A and N_B nucleons, are given by single-particle Slater determinants $\Phi_a^A(x)$ and $\Phi_b^B(x)$. The coordinates $x = (x_i,\ i = 1,\ldots,N)$, with $N = N_A + N_B$, are measured from an arbitrary external reference point O_x, so that the Φ's are obviously not translation invariant. The total Hamiltonian H_{tot} is given by

$$H_{tot} = \sum_{i=1}^{N} T(x_i) + \sum_{i<j}^{N} v(x_i,x_j), \tag{3.1}$$

while the physical Hamiltonian H is given by $H = H_{tot} - T_{c.m.}$, where $T_{c.m.}$ is the total center-of-mass kinetic energy with respect to the fixed point O_x. The single particle orbitals φ^A are defined in terms of a localized shell-model potential $U^A(x_i)$ by

$$h^A(x_i)\varphi_n^A(x_i) = e_n^A\varphi_n^A(x_i), \tag{3.2}$$

where

$$h^A(x_i) = T(x_i) + U^A(x_i). \tag{3.3}$$

The determinantal functions $\Phi_a^A(x^A)$, $x^A = (x_i,\ i = 1,\ldots,N_A)$, are then constructed with (φ_n^A) as

$$\Phi_a^A(x^A) = \frac{1}{\sqrt{N_A!}}\det[\varphi_1^A(x_1)\varphi_2^A(x_2)\cdots\varphi_{N_A}^A(x_{N_A})], \tag{3.4}$$

and similarly for the cluster B.

Basic antisymmetrized functions for the total system $A+B$ are given by

$$\Phi_c(x) = \mathcal{A}_{A-B}\{\Phi_a^A(x^A)\Phi_b^B(x^B)\}, \tag{3.5}$$

where $c=(a,b)$ and $\mathcal{A}_{A-B}$ is the antisymmetrization operator, exchanging the nucleons in A with nucleons in B.

The corresponding kinematics which are needed in the construction of internal wave functions from Φ_c using the projection methods are given as follows (Fig. 1):

$$R_A = \sum_{i=1}^{N_A} x_i/N_A\,, \quad R_B = \sum_{j=N_A+1}^{N=N_A+N_B} x_j/N_B\,,$$

$$R = \sum_{i=1}^{N} x_i/N = (R_A N_A + R_B N_B)/N\,, \tag{3.6a}$$

$$K_A = \sum_{i=1}^{N_A} K_i\,, \quad K_B = \sum_{j=N_A+1}^{N} K_j\,, \quad K = K_A + K_B$$

and

$$r = R_A - R_B\,, \quad k = (N_B K_A - N_A K_B)/N\,,$$
$$r_A = N_B r/N \equiv \beta r\,, \quad r_B = -N_A r/N = -\alpha r\,. \tag{3.6b}$$

The K_i's are the single-particle momenta conjugate to x_i's.

Using the result of Sec. II, we have from (2.3) and (2.4), for example,

$$\Phi_c^{\mathrm{PT}}(\xi) \equiv \Phi_a^{A\text{-PT}}(\xi^A)\Phi_b^{A\text{-PT}}(\xi^B)$$
$$= \int dq'_A \tilde{F}_a(q'_A) e^{-iq'_A\cdot R_A} \Phi^{A\text{-PY}}_{q'_A a}(x^A)$$
$$\times \int dq'_B \tilde{F}_b(q'_B) e^{-iq'_B\cdot R_B} \Phi^{B\text{-PY}}_{q'_B b}(x^B) \tag{3.7}$$

and the scattering function is then given by

$$\Psi_t = \sum_c \Psi_c^{\mathrm{PT}} \equiv \sum_c \int \tilde{f}_c^{\mathrm{PT}}(-k')\, \mathcal{A}_{A-B} e^{ik'\cdot r} \Phi_c^{\mathrm{PT}}(\xi) dk'. \tag{3.8}$$

Changing the variables

$$q'_A = k - k'_A\,, \quad q'_B = -k' - k'_B\,,$$

we have, with $Z'_A = (K'_A, R'_A)$ and similarly for Z'_B,

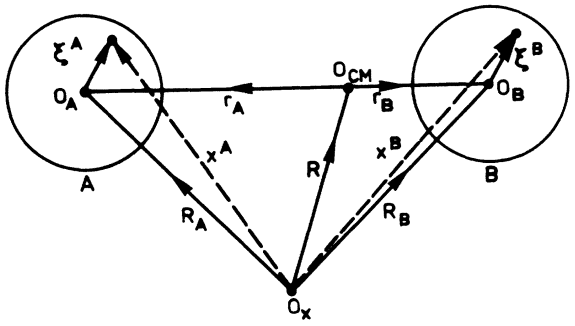

FIG. 1. Coordinates and momenta. $x=\{x_1\cdots x_{N_A}\}$ $\{x_{N_A+1}\cdots x_N\}$ = coordinates of nucleons in the nuclei A and B with respect to a fixed reference frame O_x; R_A and R_B = center of mass coordinates of A and B with respect to O_x; K_A and K_B = momenta conjugate to R_A and R_B; r_A, r_B, and r = center of mass coordinates of A and B and the relative coordinate with respect to the total center of mass $O_{\mathrm{c.m.}}$; k_A, k_B, and k = momenta conjugate to r_A, r_B, and r.

$$\Psi_c^{\mathrm{PT}} = \int dZ'_A \int dZ'_B\, \tilde{\mathcal{F}}_c(Z'_A, Z'_B)\mathcal{A}_{A-B}$$
$$\times\{[D_{R'_A B_{K'_A}}\Phi_a^A(x^A)]\,[D_{R'_B B_{K'_B}}\Phi_b^B(x^B)]\}, \tag{3.9}$$

where

$$\tilde{\mathcal{F}}_c(Z'_A, Z'_B) = \int dk' \tilde{f}_c^{\mathrm{PT}}(-k')\tilde{F}_a(k' - K'_A)\tilde{F}_b(-k' - K'_B)e^{ik'\cdot r}, \tag{3.10}$$

(3.9) is the direct analog of (2.10).

Using the relations inverse to those in (3.6),

$$R_A = R + \beta r\,, \quad R_B = R - \alpha r$$
$$K_A = k + \alpha K\,, \quad K_B = -k + \beta K\,, \tag{3.11}$$

we have

$$K_A R_A + K_B R_B = K\cdot R + k\cdot r\,.$$

Thus (3.9) becomes

$$\Psi_c^{\mathrm{PT}} = \int dk' \int dr' \int dK' \int dR' \mathcal{A}_{A-B}\{e^{ik'\cdot(r-r')}e^{iK'\cdot(R-R')}\mathcal{F}_c(K',R';k',r')\Phi_a^A[\xi^A + (R-R') + \beta(r-r')]$$
$$\times \Phi_b^B[\xi^B + (R-R') - \alpha(r-r')]\}, \tag{3.12}$$

where

$$\mathcal{F}_c(K',R';k',r') = \int dk'' e^{ik''\cdot r'} \tilde{F}_a(k'' - k' - \alpha K')$$
$$\times \tilde{F}_b(-k'' + k' - \beta K') \tilde{f}_c^{\mathrm{PT}}(-k''). \tag{3.13}$$

Noticing that $\mathcal{F}_c$ of (3.13) is independent of R', we can carry out the dR' integration of (3.12). In addition, since the entire formalism should be independent of K', we may set

$$\mathcal{F}_c(K';k',r') \to \mathcal{F}_c(k',r')\delta(K'). \tag{3.14}$$

This may not be the most general situation, but greatly simplifies the discussion below. Consequences of (3.14) should require further analysis. Thus, with (3.14), we have

$$\Psi_c^{\mathrm{PT}} = \int dk' \int dr' \mathfrak{F}_c(k', r') \mathcal{A}_{A-B}\{e^{ik'\cdot(r-r')}\Phi_c(\xi, r-r')\}, \tag{3.15}$$

where

$$\Phi_c(\xi, r-r') = \int dR' \Phi_a^A[\xi^A + (R-R') + \beta(r-r')] \times \Phi_b^B[\xi^B + (R-R') - \alpha(r-r')], \tag{3.16a}$$

$$\mathfrak{F}_c(k', r') = \int dk'' e^{ik''\cdot r'} \bar{F}_a(k''-k') \bar{F}_b(k'-k'') \times \bar{f}_c^{\mathrm{PT}}(-k''). \tag{3.16b}$$

Evidently, (3.15) is exactly the form of (2.7), except for the operator $\mathcal{A}_{A-B}$ and the physical interpretation of the variables k and r. Indeed, with $z' \equiv (k', r')$, the equations that $\mathfrak{F}_{c'}(k', r')$ satisfy are derived by the variational principle and given by

$$\sum_{c'} \int dz' [H_{c''c'}(z'', z') - E N_{c''c'}(z'', z')] \mathfrak{F}_{c'}(z') = 0, \tag{3.17}$$

where

$$H_{c''c'}(z'', z') = \langle \psi_{c''}(z'') | H | \psi_{c'}(z') \rangle_x, \quad N_{c''c'}(z'', z') = \langle \psi_{c''}(z'') | \psi_{c'}(z') \rangle_x, \tag{3.18}$$

and

$$\psi_{c'}(z') = \mathcal{A}_{A-B}\{e^{ik'\cdot(r-r')}\Phi_c(\xi, r-r')\}. \tag{3.19}$$

Defining further that $\bar{F}_c(k'-k'') \equiv \bar{F}_a(k''-k')\bar{F}_b(k'-k'')$, the prediagonalization procedure will provide $\bar{F}_c(-k')$.

The prediagonalization of (3.17) is carried out by first examining the matrix elements $H_{c''c'}$ and $N_{c''c'}$; we set[5]

$$H_{c''c'} = H^D_{c''c'} + H^I_{c''c'},$$

where $H^D_{c''c'}$ contains matrix elements with states which correspond to particles in the cluster A *or* cluster B, but not between A and B. Because of the antisymmetrization operator $\mathcal{A}_{AB}$, it is not possible to isolate the A-B interaction from H; $H^D_{c''c'}$ has to be selected from the matrix element $H_{c''c'}$ directly in order to contain cluster self-energies only.

Following the argument given in I, we have $H^D_{c''c'}$ to be independent of the r' and r'' variables, so that

$$\sum_{c'} \int dk' [H^D_{c''c'}(k'', k') - E^d N_{c''c'}(k'', k')] F^d_{c'}(k') = 0. \tag{3.20}$$

Thus, only the $H^I_{c''c'}$ part affects the scattering of A by B, and this is treated by solving for $f_d(k')$ or $\mathfrak{F}_d(k', r')$ the following set of equations

$$\sum_{d'} \int dz' [H_{d\,d'}(z'', z') - E N_{d''d'}(z'', z')] \mathfrak{F}_{d'}(z') = 0, \tag{3.21}$$

with the boundary conditions $[\bar{F}_{d'}(k') \equiv \sum_{c'} \bar{F}^{d'}_{c'}]$

$$\mathfrak{F}_{d'}(k', r') = \bar{F}_{d'}(k' - k_d) a_d e^{ik_d\cdot r'} + \sum_{d'} \int dk'' \frac{T_{dd'}(k'', k_d) a_{d'}}{k_d^2 - k''^2 + i\epsilon} \times \bar{F}_{d'}(k''-k') e^{ik''\cdot r'}. \tag{3.22}$$

Equation (3.21), with the boundary conditions (3.22), forms the dynamical system one can solve to describe the nucleus-nucleus scattering. It involves the evaluation of $H_{c''c'}$ and $N_{c''c'}$ which require integrations over the single-particle variables $x = (x_1 \cdots x_N)$. This greatly simplifies the computation. On the other hand, the scattering amplitudes $\bar{f}_d$ or $\mathfrak{F}_d(z')$ depend on the generator coordinates $z' = (k', r')$, which are much simpler to deal with. Furthermore, distortion effects can be included into the above formalism when the basis functions Φ's become dependent on z', as will be discussed in the next section.

In the factorizable case, we have, from (3.16)

$$\Phi_c(\xi, r-r') = \int dR' G_a^A[R - R' + \beta(r-r')] G_b^B[R - R' - \alpha(r-r')] [\Phi_a^{A\,\mathrm{int}}(\xi^A)\Phi_b^{B\,\mathrm{int}}(\xi^B)] \equiv G_c(r-r')\Phi_c^{\mathrm{int}}(\xi), \tag{3.23}$$

and with

$$F_c(k'-k'') \to \delta(k')\bar{G}_c^{-1}(k'') \tag{3.24}$$

we have

$$\Psi_c^{\mathrm{PY}} = \int dr' f_c^{\mathrm{PY}}(r') \mathcal{A}_{A-B}\{\Phi_c(\xi, r-r')\} = \mathcal{A}_{A-B}\left\{\int dr' f_c^{\mathrm{PY}}(r') G_c(r-r')\Phi_c^{\mathrm{int}}(\xi)\right\}. \tag{3.25}$$

IV. DISTORTION EFFECTS AND TDHF

During the collision between two nuclei A and B, various inelastic channels can be coupled to the elastic channels through excitations of the clusters. These distortion effects may be incorporated by explicitly including some of the strongly coupled states in the sum for Ψ_t of (3.8). However, this is generally difficult to do in practice not only because the number of coupled equations in (3.21) will increase, but also because the separation (2.2) may be difficult[7] even in the simple case of harmonic oscillator wave functions. Therefore, it is of interest to generalize the single-particle orbitals $\{\varphi_n\}$ in (2.1) to take into account some of the effect of distortions, as discussed in Sec. II for the case of potential scattering.

A. Adiabatic distortions

We begin the discussion with the r-dependent distortions, which are especially important when the collision velocity is small compared with the average orbital velocity of nucleons inside the nuclei. Since we are trying to incorporate the distortion effect in the basis set $\{\Phi_c\}$, of (3.16), it is more advantageous to introduce the generator coordinate r' *directly*, rather than the R'_A and R'_B coordinates. Thus, $\Phi_c(\xi, r-r')$ of (3.16) is modified to a form

$$\Phi_c(\xi, r-r';r') = \int dR' \Phi_a^A[\xi^A + R - R' + \beta(r-r');r'] \times \Phi_b^B[\xi^B + R - R' - \alpha(r-r');r'] \xrightarrow[r'\to\infty]{} \Phi_c(\xi, r-r'), \tag{4.1}$$

and thus

$$\Psi_c^{PT} = \int dk' \times \int dr' \mathfrak{F}_c(k', r') \mathcal{A}_{A-B}\{e^{ik'\cdot(r-r')}\Phi_c(\xi, r-r';r')\}. \tag{4.2}$$

As in the potential scattering case summarized in Sec. II, the prediagonalization procedure will be complicated somewhat because of the explicit r' dependence of Φ_c, but the scattering equations that $\mathfrak{F}_c$ satisfy would be identical to (3.20). The boundary conditions (3.22) are unchanged in the asymptotic region $r' \to \infty$.

When Φ_c "factorizes" as

$$\Phi_c(\xi, r-r';r') = G_c(r-r';r')\Phi_c^{int}(\xi;r') \xrightarrow[r'\to\infty]{} G_c(r-r')\Phi_c^{int}(\xi), \tag{4.3}$$

the single integration form (3.25) can still be applied, because the dk' integration induced by (3.24) for $f_c^{PY}(r')$ is unaffected by the additional r'-dependence of Φ_c.

Instead of introducing the separate distorted functions Φ_a^A and Φ_b^B in (4.1), it is often more convenient to generate a set of "molecular" orbital basis functions $\{\varphi_n^M(x_i)\}$; the single-particle Hamiltonian is given by

$$h^M(x_i, r') \equiv T(x_i) + U(x_i, r') \tag{4.4}$$

with

$$U(x_i, r') \xrightarrow[r'\to\infty]{} U^A(x_i) + U^B(x_i). \tag{4.5}$$

Then,

$$h^M(x_i, r')\varphi_n^M(x_i, r') = e_n^M(r')\varphi_n^M(x_i, r') \tag{4.5'}$$

with the asymptotic property that as $r' \to \infty$

$$e_n^M(r') \to e_n^A \text{ or } e_n^B$$
$$\varphi_n^M(x_i, r') \to \varphi_n^A(x_i) \text{ or } \varphi_n^B(x_i). \tag{4.6}$$

The antisymmetrized function in (3.15) can be constructed as

$$\mathcal{A}_{A-B}\{e^{ik'\cdot(r-r')}\Phi_c(\xi, r-r';r')\} \to \Phi_{ck'}^M(\xi, r-r';r') \equiv \frac{1}{\sqrt{N!}} \int dR' \det\{\tilde{\varphi}_{c_1}^M[\xi_1^A + R - R' + \beta(r-r');r']\tilde{\varphi}_{c_2}^M[\xi_2^A + R - R' + \beta(r-r');r'] \cdots \tilde{\varphi}_{cN_A}^M[\xi_{N_A}^A + R - R' + \beta(r-r');r']\tilde{\varphi}_{cN_A+1}^M[\xi_{N_A+1}^B + R - R' - \alpha(r-r');r'] \cdots \tilde{\varphi}_{cN}^M[\xi_N^B + R - R' - \alpha(r-r');r']\}, \tag{4.7}$$

where

$$\tilde{\varphi}_{c_i}^M = \varphi_{c_i}^M e^{ik'\cdot(x_i/N_A - r')}, \quad 1 \le i \le N_A$$
$$\tilde{\varphi}_{c_j}^M = \varphi_{c_j}^M e^{ik'\cdot(-x_j/N_B - r')}, \quad N_A + 1 \le j \le N. \tag{4.8}$$

The "traveling-wave" factors in $\tilde{\varphi}^M$ are introduced to construct the proper phase $\exp[ik'\cdot(r-r')]$ in (4.7) with correct exchange symmetry. Thus

$$\Psi_c^{PT} = \int dk' \int dr' \mathfrak{F}_c(k', r') \Phi^M_{ck'}(\xi, r - r'; r') . \tag{4.9}$$

It can be noticed that the orthogonality among the functions φ_n^M for each fixed r' is lost when $\bar{\varphi}^M$ are constructed in (4.8), but this is only a technical, minor complication.

B. Momentum-dependent distortions

From the general property of the optical potential for the two interacting composite nuclei, we expect that the single-nucleon state should be momentum-dependent, as much as it is coordinate-dependent. Thus we may consider explicitly for the functions in (3.16a)

$$\Phi_c(\xi, r - r') \to \Phi_c(\xi, r - r'; k') . \tag{4.10}$$

Here again we want the k' dependence to induce no polarization when $r \to \infty$. Note that we have used in (4.10) the k' generator coordinate variable, rather than the q'_A and q'_B in (3.7). This is physically more reasonable and also greatly simplifies the formulation. In fact, (3.15) and (3.16) are essentially unchanged, as the dk'' integration in (3.16b) can still be carried out without having the Φ_c's mixed in. Thus, just as with the potential scattering discussed in I, the momentum dependence of the basis set does not complicate the formalism when the PT projection is used and the proper generator coordinates are chosen.

In the factorizable case, the dk' integration induced by (3.24) can not be carried out without including the Φ_c's, so that the scattering equation will still have *both* dk' and dr' integrations explicitly.

C. Coordinate and momentum-dependent distortions

The most general distortions within the complexity of the present formulation (of double projections) are represented by the r' and k' dependent basis functions, as

$$\Phi_c(\xi, r - r') \to \Phi_c(\xi, r - r'; k', r') . \tag{4.11}$$

Obviously, (4.2) with (4.1) or (4.10) can be generalized trivially to the present case, as

$$\Psi_c^{PT} = \int dk' \int dr' \mathfrak{F}_c(k', r') \mathfrak{A}_{A-B} \times \{ e^{ik' \cdot (r - r')} \Phi_c(\xi, r - r'; k', r') \} , \tag{4.12}$$

with the scattering equations for $\mathfrak{F}_c(k', r')$ given by (3.17) and the boundary conditions specified by (3.22), as long as the self-energy kernels remain r' and r'' independent at large distance.

As noted above, the factorizable case does not simplify as much because of the k' dependence of the basis functions; both dr' and dk' integrations appear in (3.17).

D. TDHF

Finally, it is of some interest to study the connection between the formalism generated with the scattering functions of the form (4.12) and the time-dependent Hartree-Fock (TDHF) procedure employed in recent years in the nucleus-nucleus collisions. The TDHF equations are generated by the projections

$$\langle \delta\phi \, | i\dot{\phi} \rangle = \langle \delta\phi \, | H \, | \phi \rangle , \tag{4.13}$$

where ϕ is the TDHF solution, then $i\dot{\phi} = h(\phi)\, \phi$ with $h(\phi)$ the Hartree-Fock Hamiltonian, and $\delta\phi$ is a set of particle-hole states. We do not show here the explicit dependence of ϕ on the variables ξ, r and R. In a restricted TDHF, however, the $|ph\rangle$ set is replaced by the parameter-dependence of ϕ, as $\phi(\alpha, \beta, \gamma \cdots)$. Then, (4.13) becomes instead

$$\left\langle \frac{\partial\phi}{\partial\alpha} \middle| i\left(\frac{\partial\phi}{\partial\alpha}\dot{\alpha} + \frac{\partial\phi}{\partial\beta}\dot{\beta} + \cdots \right) \right\rangle = \left\langle \frac{\partial\phi}{\partial\alpha} \middle| H \middle| \phi \right\rangle ,$$
$$\left\langle \frac{\partial\phi}{\partial\beta} \middle| i\left(\frac{\partial\phi}{\partial\alpha}\dot{\alpha} + \frac{\partial\phi}{\partial\beta}\dot{\beta} + \cdots \right) \right\rangle = \left\langle \frac{\partial\phi}{\partial\beta} \middle| H \middle| \phi \right\rangle , \tag{4.14}$$

etc., also for the other parameters, resulting in a set of linear coupled equations in $\dot{\alpha}, \dot{\beta}, \cdots$ (but nonlinear in $\alpha, \beta \cdots$). We denote the solutions by $\bar{\alpha}(t), \bar{\beta}(t), \cdots$. Then, instead of (3.17), we have for example

$$k' \equiv \bar{\alpha}(t) \text{ and } r' \equiv \bar{\beta}(t) \tag{4.15}$$

so that one may use time as a generator coordinate,

$$\Psi_c = \int dt \, f_c(t) \phi_c[\bar{\alpha}(t), \bar{\beta}(t)] . \tag{4.16}$$

V. DISCUSSION

A description of colliding nuclei in terms of Slater determinants is very convenient from the practical computational point of view and also in satisfying the Pauli principle among *all* the nucleons. However, the center of mass motion of these nuclei is more difficult to treat, especially when the numbers of nucleons N_A and N_B are not large. In addition to the usual kinematic corrections, mixing of the independent particle coordinates can often introduce spurious states which can seriously affect the very scattering process one has to analyze.

In I and the present article, we have presented a systematic theoretical construction, with the improved boundary conditions obtained by the prediagonalization procedure. Inclusion of the coordi-

nate- and momentum-dependent distortions should be especially useful in reducing the number of coupled channels, and still capable of representing the physical situations with reasonable accuracy. By its very nature, the formalism in its general form is fairly complicated. But, in the case of factorizable orbitals, with some distortions, actual calculations are probably within the present computational capability.

Several practical applications and possible corrections to the usual TDHF procedure are under investigation.

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