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Generator coordinate approach to nuclear reactions. I. Potential scattering of a nucleus and dynamical distortions

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The problem of a mathematically consistent description of reactions involving composite nuclei is reexamined in the case where the individual nuclear states are given in terms of Slater determinants constructed with single-particle orbitals. The relationship between the single projection method of Peierls and Yoccoz and the double projection method of Peierls and Thouless is clarified. The general scattering functions are then constructed, and a set of scattering equations of the Griffin-Hill-Wheeler type is derived, in which the Hamiltonian and the overlap kernels can be evaluated directly in the independent particle coordinate representation. Proper boundary conditions are specified by the procedure of prediagonalization. To simplify the problem to basic essentials, we consider in this paper the motion of a nucleus in an external potential. The specially simple cases in which the Slater determinants factorize into the internal and external parts are considered as an illustration. The distortion of a nucleus during the scattering process is incorporated here by an explicit dependence of the single-particle orbitals of the Slater determinants on the generator coordinate and momentum. The double projection method is found to be naturally adaptable for this generalization.

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

I. INTRODUCTION

The microscopic study of nuclear reactions requires a set of reliable cluster wave functions with the full Pauli exchange effect. Such wave functions are often easily constructed in the form of Slater determinants from independent-particle orbitals. The center-of-mass (c.m.) motion of the clusters is then completely neglected in the description of the clusters, whereas the reaction problem would consist in deriving in detail such a motion from the dynamics. Various generator coordinate methods (GCM) have thus been developed[1] to correct the determinantal wave functions without modifying their single-particle nature. The single-projection method of Griffin-Hill-Wheeler[2] (GHW) and Peierls and Yoccoz[3] (PY) has been widely used in the past when the determinant factorizes into a part which is purely internal and another which depends explicitly on the c.m. variable. When such a factorization is not possible, the double projection method of Peierls and Thouless[4] (PT) should be adopted, although the PT procedure is more difficult to apply in practice.

A rigorous treatment of the nucleus-nucleus scattering problem within the independent-particle, shell-model formalism can be given[5,6] by means of the PT or PY-GHW procedure. This is then a direct extension of the continuum shell model[7,8] (CSM) for the proton-nucleus scattering, which accomodates projectiles other than single nucleons. In fact, the problem of localization of composite projectiles as well as target nuclei was the initial motivation for such a study.[5] More recently, the GHW-PY type approach has been applied[9-13] to several simple systems involving light nuclei, demonstrating the potential usefulness of the GCM in practical situations and also clarifying the connection of the GCM to the usual resonating group method[14,15] (RGM). Only the simple factorizable cases involving harmonic oscillator wave functions have been treated. It is the purpose of this paper to reexamine the GCM carefully so that the nonfactorizable general cases may also be treated. Since many intermediate steps in this development may look intricate, abstract, and often complicated, we limit ourselves here to the simple model of a nucleus scattered by an external potential. This model contains all the technical difficulties of the more general nucleus-nucleus scattering system, and no coordinates in the system are wasted because the c.m. coordinate is, in fact, the scattering variable itself. Thus, for the N independent particle coordinate variables $\vec{x}_i$, $i=1,2,\ldots,N$, with respect to an arbitrary fixed reference frame O_x, we have the c.m. coordinate $\vec{R}$ and momentum $\vec{P}$ defined by (omitting the explicit vector symbols throughout for convenience)

$$R=\sum_{i=1}^{N} x_i/N, \tag{1.1}$$

$$P=\sum_{i=1}^{N} p_i\,, \tag{1.2}$$

where p_i is the momentum conjugate to x_i. The internal coordinates are then defined by $\xi_i \equiv x_i - R$, with the important constraint $\sum_i \xi_i = 0$. The single particle orbitals are generated by the equation

$$h(x_i)\varphi_n(x_i) \equiv [K(x_i)+W(x_i)]\varphi_n(x_i) = e_n\varphi_n(x_i)\,. \tag{1.3}$$

The model Hamiltonian that one uses in the continuum shell model and also in the bound state shell model to describe a nucleus is usually taken to be simply

$$H_M^{(0)}(x)=\sum_{i=1}^{N} h(x_i)\,, \tag{1.4}$$

while the correct internal Hamiltonian, for example, should be

$$\begin{aligned} H_N(\xi) &= \sum_{i=1}^{N} K(\xi_i) + \sum_{i>j=1}^{N} v(\xi_i,\xi_j) \\ &= H_M^{(0)}(x) - P^2/2M \\ &\quad + \left\{ \sum_{i>j=1}^{N} v(\xi_i,\xi_j) - \sum_{i=1}^{N} W(x_i) \right\}. \end{aligned} \tag{1.5}$$

The determinants which are the eigenstates of $H_M^{(0)}$ are then constructed as

$$\Phi_c(x)=\frac{1}{\sqrt{N!}}\det\{\varphi_{c_1}(x_1)\varphi_{c_2}(x_2)\cdots\varphi_{c_N}(x_N)\}\,, \tag{1.6}$$

where $c \equiv (c_1, c_2, \ldots, c_N)$ and $x \equiv (x_1, x_2, \ldots, x_N)$.

Because of the constraints (1.1), (1.2), and $\sum_i \xi_i = 0$, the N-particle system described by (1.5) is more complex and strongly correlated (the c.m. correlation), while (1.4) and (1.6) describe a set of uncorrelated nucleons (except for the Pauli correlations). Therefore, the form (1.6) is very convenient to use in the calculation of matrix elements and perhaps in the solution of a scattering problem if a proper theory can be formulated. It is the main purpose of this paper to construct such a theory in the simple case of the potential scattering of a composite nucleus.

Distortion effects during the scattering process are usually incorporated into the theory either by a coupled-channel method (CCM) or by the presence of some optical distortion potentials in the scattering equations. For slow collisions, adiabatically distorted basis sets are also often used. We consider a similar procedure within the GCM, and show that the GCM of the PT type adapts itself very naturally to such generalizations.

In Sec. II, we critically review the GCM, both the single and double projection approaches, and examine their connections to the RGM and the CSM. The general form of the scattering wave function is constructed by a superposition of the projected states. The scattering equations are derived in Sec. III on the basis of such wave functions, and the asymptotic boundary conditions are specified by a prediagonalization procedure similar to that developed for the CSM. The factorizable case is considered at each stage of the above formal development to illustrate the approach. An important extension of the result to incorporate cluster distortions during the scattering is considered in Sec. IV. Both adiabatic and energy-dependent distortions are examined.

The more practical problem of nucleus-nucleus collision will be the subject of a future report. The general formulation follows, however, mainly from the results developed in the present paper.

II. THE SINGLE AND DOUBLE PROJECTIONS AND CONSTRUCTION OF SCATTERING WAVE FUNCTIONS

We first summarize here both the single-projection method of Peierls and Yoccoz[3] and the double-projection method of Peierls and Thouless,[4] which were developed to extract the purely internal cluster wave functions from a Slater determinant constructed with a set of single-particle orbitals. Let $\Phi_c(x)$ be a localized shell model wave function taken as a Slater determinant of the type (1.6), where x denotes collectively all the single nucleon coordinates with respect to a fixed reference frame O_x. Then, following PY, we may first construct a projected wave function[3]

$$\Phi^{\mathrm{PY}}_{q'c}(x)=\int dR' e^{iq'\cdot R'}\Phi_c(x-R')\,, \tag{2.1}$$

where one recognizes a translated shell model function $\Phi_c(x-R')$ obtained with a displacement operator $D_{R'}=\exp(-iR'\cdot\hat{K})$. The total c.m. momentum operator is given by $\hat{K}=\sum_{i=1}^{N}\hat{p}_i/\hbar$ and we set $\hbar=1$ throughout. Thus, $D_{R'}\Phi_c(x)=\Phi_c(x-R')$. In general, the internal motion contained in the state $\Phi^{\mathrm{PY}}_{q'c}(x)$ of (2.1) will be q' dependent. (In the factorizable case, the q'-dependent part can be isolated from the internal part, as will be discussed below.) To obtain a truly internal state which is *independent* of q', we define[4] the zero-momentum internal wave function by mixing the q'-dependent $\Phi^{\mathrm{PY}}_{q'c}$'s,

$$\Phi^{\mathrm{PT}}_{0c}(\xi)=\int dq' \bar{F}_c(q') e^{-iq'\cdot R}\Phi^{\mathrm{PY}}_{q'c}(x)\,, \tag{2.2}$$

where the internal coordinate variables ξ are defined by $\xi \equiv x - R$ and where R is the c.m. coordinate of the nucleus. The weighting function $\bar{F}_c(q')$ in (2.2) is left unspecified, but would be determined dynamically by a prediagonalization procedure; this will be discussed in greater de-

tail in Sec. III.

To see that (2.2) indeed gives an internal wave function, we combine (2.2) and (2.1) to obtain

$$\Phi_{0c}^{PT}(\xi) = \int dq' \tilde{F}_c(q') \int dR' e^{-iq'\cdot(R-R')} \Phi_c(x-R')$$

$$= \int dR' F_c(R-R') \Phi_c(x-R'), \tag{2.3}$$

where F_c is the Fourier transform of $\tilde{F}_c$, $F_c(R-R') \equiv \int dq' \tilde{F}_c(q') e^{-iq'\cdot(R-R')}$, and $\Phi_c(x-R') = \Phi_c(\xi, R-R')$. The fact that only the combination $(R-R')$ appears in (2.3) guarantees that $\Phi_{0c}^{PT}(\xi)$ is an internal function of ξ only. In the following, we neglect the $(2\pi)^{-3/2}$ factors throughout to simplify notations, and all the c-number variables are denoted with primes.

When $\Phi_c(x)$ factorizes, as, for example, when the single particle orbitals in Φ_c are all of the harmonic oscillator type in their lowest energy allowed states, we have

$$\Phi_c(x) = G_c(R) \Phi_c^{int}(\xi), \tag{2.4}$$

and (2.1) reduces to a form

$$\Phi_{q'c}^{PY}(x) = [\tilde{G}_c(-q') e^{iq'\cdot R}] \Phi_c^{int}(\xi), \tag{2.5}$$

where

$$\tilde{G}_c(-q') = \int ds' G_c(s') e^{-iq'\cdot s'}$$

while (2.2) gives

$$\Phi_{0c}^{PT}(\xi) = \left[\int dq' \tilde{F}_c(q') \tilde{G}_c(-q') \right] \Phi_c^{int}(\xi). \tag{2.6}$$

Therefore, Φ_{0c}^{PY} of (2.5) with $q'=0$ and $\Phi_{0c}^{PT}(\xi)$ of (2.6) are equally effective in isolating the internal component of Φ_c. Hence, as is well-known, Eq. (2.1) *without* the additional mixing of the q'-dependent states in (2.2) should be sufficient in isolating the internal part for the factorizable cases. However, when $\Phi_c(x)$ is not factorizable, then the q' mixing in (2.2) may be essential to obtain a dynamically significant internal state. For later applications, a slightly more convenient form of Φ_{0c}^{PT} may be derived from (2.3) by a change of variable $q' = K - K'$ and $dq' = dK'$, which gives[5]

$$\Phi_{Kc}^{PT}(x) = e^{iK\cdot R} \Phi_{0c}^{PT}(\xi) \tag{2.7a}$$

$$= \int dK' \tilde{F}_c(K-K') e^{iK'\cdot R}$$

$$\times \int dR' e^{i(K-K')\cdot R'} \Phi_c(x-R'). \tag{2.7b}$$

The form (2.5) for $\Phi_{Kc}^{PY}(x)$ is recovered from (2.7b) with the choice $\tilde{F}_c(K-K') = \delta(K')$ in the factorizable case.

We now turn to the construction of scattering wave functions. As preliminary to the scattering problem to be discussed in Sec. III, we consider here only the general form that the scattering wave functions should assume. Thus in the factorizable case, a simple superposition of the PY type functions gives

$$\Psi = \sum_c \Psi_c^{PY},$$

where

$$\Psi_c^{PY} \equiv \int dq' \tilde{f}_c(-q') \Phi_{q'c}^{PY}(x)$$

$$= \int dR' f_c(R') \Phi_c(x-R'). \tag{2.8}$$

More explicitly, (2.5) immediately reduces (2.8) to an RGM wave function

$$\Psi_c^{PY} = u_c^{PY}(R) \Phi_c^{int}(\xi) \tag{2.9}$$

with

$$u_c^{PY}(R) = \int dq' \tilde{f}_c(-q') \tilde{G}_c(-q') e^{iq'\cdot R}$$

$$= \int dR' f_c(R') G_c(R-R'). \tag{2.10}$$

The form (2.8) has been used extensively[9-13] in the analyses of nuclear reactions with elementary Gaussian models for nuclei, and shown to be more convenient than the RGM form (2.9). Instead of solving a set of equations for $u_c^{PY}(R)$, the amplitudes $f_c(R')$ in (2.8) are determined directly from the GHW equations. The label c here could correspond to the actual physical channels if $\Phi_c^{int}(\xi)$ are reasonably close to the eigenstates of the internal Hamiltonian $H_N(\xi)$. Otherwise, one has to go through the prediagonalization procedure[5,7] to improve the channel functions. We will discuss this problem in Sec. III and relabel the improved channels by d.

For the nonfactorizable case, a similar construction of scattering wave functions using the $\Phi_{0c}^{PT}(\xi)$ can be carried out. From the definition of $\Phi_{Kc}^{PT}(x)$, (2.7a), we have then

$$\Psi = \sum_c \Psi_c^{PT}(x),$$

where

$$\Psi_c^{PT}(x) \equiv \int dK \tilde{f}_c(-K) e^{iK\cdot R} \Phi_{0c}^{PT}(\xi)$$

$$\equiv u_c(R) \Phi_{0c}^{PT}(\xi). \tag{2.11}$$

The form (2.11) is nothing but the usual wave functions in the RGM. However, the use of the Φ_{0c}^{PT} in the construction of a coupled set of scattering equations for the u_c is already an improvement

over the RGM, because we can now evaluate in the x variables directly the integrals which are needed in the construction of the scattering equations. It should be stressed here also that, when the asymptotic cluster functions are not available in an exact form, as is usually the case, the explicit construction of $\Phi_{0c}^{PT}(\xi)$ and possible additional linear combinations of various $\Phi_{0c}^{PT}(\xi)$ to improve the channel functions are essential both in the RGM and GCM.

A slightly more convenient form of $\Psi_c^{PT}(x)$ can be obtained[5] from (2.7b) [by the change of variable $q' = K - K'$ in (2.3)],

$$\Psi_c^{PT}(x) = \int dK \tilde{f}_c(-K)\Phi_{Kc}^{PT}(x)$$

$$= \int dK' \int dR' \mathcal{F}_c(K',R') e^{iK'\cdot(R-R')}\Phi_c(x-R'), \tag{2.12}$$

where

$$\mathcal{F}_c(K',R') \equiv \int dK \tilde{F}_c(K-K')\tilde{f}_c(-K)e^{iK\cdot R'}. \tag{2.13}$$

This is the main result of this section. Since (2.12) with (2.13) will be the basis of our discussion of the scattering formulation in the next section, we briefly examine their structure a little further. First of all, when $\tilde{F}_c(K-K') = \delta(K')$ for the factorizable case, (2.12) immediately reduces to (2.8). Secondly, we can define Ψ_c^{PT} in a compact form using the displacement and boost operators

$$D_{R'} = \exp(-iR'\cdot\hat{K}) \text{ and } B_{K'} = \exp(iK'\cdot\hat{R}). \tag{2.14}$$

Thus (6.8) can be written as

$$\Psi_c^{PT}(x) = \int dK' \int dR' \mathcal{F}_c(K',R') D_{R'} B_{K'} \Phi_c(x) \tag{2.15a}$$

$$= \int dK' \int dR' \mathcal{F}_c'(K',R') B_{K'} D_{R'} \Phi_c(x), \tag{2.15b}$$

where

$$\mathcal{F}_c'(K',R') \equiv \mathcal{F}_c(K',R') e^{-iK'\cdot R'}. \tag{2.16}$$

Finally, note that the amplitude function $\mathcal{F}_c(K',R')$ is, in general, not an arbitrary function of two variables, but specifically dependent on the cluster structure factor $\tilde{F}_c$ through (2.13). This is an important point because boundary conditions on $\mathcal{F}_c$ can be explicitly derived using (2.13), as will be discussed in Sec. III.

The projection procedures considered in this paper are especially simple, because the c.m. variable R is, in fact, the scattering variable. The situation becomes more complicated when more than one nuclei are involved in a collision. Then the total c.m. variable has to be projected out altogether, as the physical H does not depend on it. The complete antisymmetrization of all of the nucleons involved also complicates the problem. These problems can be handled more conveniently in the GCM approach and will be carefully discussed in a second paper. The next section of the present paper rather deals with the scattering of one nucleus by an external potential, which is simpler but still of physical interest.

III. POTENTIAL SCATTERING OF A NUCLEUS

In this section, we formulate the complete scattering and structure problem by means of the wave function, Eq. (2.12). A set of coupled equations of the GHW type is derived, which depends explicitly on the generator coordinates K' and R'. The boundary conditions on the scattering amplitude functions $\mathcal{F}_c(K',R')$ are determined by the prediagonalization procedure.

The Hamiltonian of the system is given by

$$H = K(R) + H_N(\xi) + V(R,\xi) \equiv H^{(0)} + V, \tag{3.1}$$

where $K(R)$ is the c.m. kinetic energy operator for the moving nucleus, $H_N(\xi)$ is the internal Hamiltonian for the nucleus, and $V(R,\xi)$ is the interaction potential. The scattering equations for $\mathcal{F}_c$ are obtained from the variational principle

$$\delta[I]/\delta\mathcal{F}_{c''}(Z'') = 0, \tag{3.2}$$

where $Z'' \equiv (K'',R'')$ denoted collectively and the variational functional $[I]$ is defined by

$$[I] = \lambda_t + \langle\Psi_t, [H-E]\Psi_t\rangle_x. \tag{3.3}$$

Here, the bracket indexed by x means integration with respect to all the single-nucleon variables x_i, the Ψ_t is a trial function given by a finite sum of Ψ_c^{PT},

$$\Psi_t = \sum_c \Psi_c^{PT}(x), \tag{3.4}$$

and λ_t is an asymptotic amplitude parameter in Ψ_t. [The expression (3.3) should be evaluated carefully, with possible regularization factors if necessary. But this does not affect the final equations we derive below.] Thus, (3.2) gives

$$\sum_{c'} \int dZ' [H_{c''c'}(Z'',Z') - EN_{c''c'}(Z'',Z')]\mathcal{F}_{c'}(Z') = 0, \tag{3.5}$$

where

$$H_{c''c'}(Z'',Z') = \langle\Phi_{c''}^{K''}(x-R'')|H|\Phi_{c'}^{K'}(x-R')\rangle_x,$$

$$N_{c''c'}(Z'',Z') = \langle\Phi_{c''}^{K''}(x-R'')|\Phi_{c'}^{K'}(x-R')\rangle_x, \tag{3.6}$$

with

$$\Phi^{K'}_{c'}(x-R') \equiv e^{iK'\cdot(R-R')}\Phi_{c'}(x-R') \tag{3.7}$$

and

$$\int dZ' \equiv \int dK' \int dR' .$$

The $\exp(-iK'\cdot R')$ factor in (3.7) may easily be absorbed in the $\mathcal{F}_{c'}(Z')$, as in $\mathcal{F}'_{c'}(Z')$, which results in slightly simpler boundary conditions for $\mathcal{F}'_{c'}(Z')$, but we stay with the form (3.5) for $\mathcal{F}_{c'}(Z')$ here. Although the scattering Eqs. (3.5) are quite similar in form to the GHW equations one obtains with (2.9) and used in Refs. 9–13, the presence of K' and K'' in addition to R' and R'' in (3.5) greatly complicates the task of solving them for $\mathcal{F}_{c'}$. Such complications are, however, intrinsic to the problem when the cluster functions Φ_c are not factorizable. Even the asymptotic boundary conditions are not easily obtainable; although they are an essential part in completely defining the scattering problem itself.

In order to derive the complete boundary conditions for the functions $\mathcal{F}_{c'}(Z')$, we first have to determine the cluster amplitudes $\tilde{F}_{c'}(K')$ in $\Phi^{\mathrm{PT}}_{\mathcal{E}}$. Equation (2.13), combined with the form for $f_{c'}(K)$, will then provide an explicit form that $\mathcal{F}_{c'}$ should assume. Thus, using (2.3), we construct another functional for the prediagonalization purpose

$$[\mathcal{S}] = \sum_{c'c''} \langle \Phi^{\mathrm{PT}}_{0c''}(\xi) | H_N(\xi) - E^d_t | \Phi^{\mathrm{PT}}_{0c'}(\xi)\rangle_\xi , \tag{3.8}$$

where

$$\Phi^{\mathrm{PT}}_{0c'}(\xi) = \int dq' \tilde{F}_{c'}(q')\tilde{\Phi}_{c'}(\xi,q') , \tag{3.9}$$

with

$$\tilde{\Phi}_{c'}(\xi,q') \equiv \int dR' e^{-iq'\cdot(R-R')}\Phi_{c'}(x-R') . \tag{3.10}$$

The variations in $\tilde{F}_{c''}(q'')$,

$$\delta[\mathcal{S}]/\delta\tilde{F}_{c''} = 0 ,$$

give

$$\sum_{c'} \int dq' \langle \tilde{\Phi}_{c''}(\xi,q'') | H_N(\xi) - E^d_t | \tilde{\Phi}_{c'}(\xi,q')\rangle_\xi \tilde{F}^d_{c'}(q') = 0 . \tag{3.11}$$

The solution of this diagonalization problem provides a set of eigenstates labeled d. We stress that this label is now that of a *physical* channel. Although (3.11) is fairly complicated to solve, it is a *prerequisite* in treating any scattering problem. Since the correct asymptotic boundary conditions are not available in general, the internal parts of $\Phi_{c'}$ have to be first isolated and then suitably combined to provide such information. In the case of factorizable $\Phi_{c'}$, the q' mixing in (2.2) is not available. This means that $\tilde{F}^d_{c'}(q')$ become constants in (3.11).

The main complication in evaluating the kernels in (3.11) is of course the use of the internal variable ξ. After all, the principal reason for using the GCM over the RGM is to avoid such direct use of ξ and R as much as possible during the actual calculation. It is therefore desirable to rewrite (3.11) in a form which contains the dx integrations directly. In fact, Eq. (3.11) is not exactly the form one encounters in solving the scattering Eq. (3.5); however, we show below that Eq. (3.11) is completely equivalent to the prediagonalization of (3.5) defined by

$$\sum_{c'} \int dZ' \langle \Phi^{K''}_{c''}(x-R'') \times | H_N(\xi) - E^d | \Phi^{K'}_{c'}(x-R')\rangle_x \mathcal{F}^d_{c'}(Z') = 0 . \tag{3.12}$$

Here, the integration inside the bracket is over all the x_i variables, i.e., $dx = \Pi_{i=1}^N dx_i \equiv d\xi dR$. As a result, (3.12) contains four integrations over $dK'dR'dR\,d\xi$. On the other hand, (3.11) with (3.10) contains four integrals over the slightly different set of variables $dq'dR'dR''d\xi$. Therefore, to prove that (3.11) is equivalent to (3.12), it is necessary to connect these two sets of integrations and to show that $\tilde{F}^d_{c'}(K') \rightarrow \mathcal{F}^d_{c'}(K',R')$. The integrands are then the same in both expressions, under the exchange of $(-q')$ for K' and $(-q'')$ for K''.

First of all, the $d\xi$ integration is common to both cases. Also dK' in (3.12) and dq' in (3.11) play exactly the same role. Noting that the kernel of (3.12) depends only on the difference $(R'-R'')$, we *can* replace $\mathcal{F}^d_{c'}(K',R')$ by $\tilde{F}^d_{c'}(-K')$, followed by $K' \rightarrow (-K')$. Then, the dR' integration in (3.12) can be carried out explicitly as in (3.11); the R dependence appears then only in $\Phi^{K''}_{c''}$ through the combination $R-R''$, so that the dR'' and dR integrations are equivalent. Thus, (3.12) and (3.11) are exactly the same, and the prediagonalization with either form will give the same $\tilde{F}^d_{c'}(K')$ and E^d. Consequently, the new scattering function with more physical channel functions (labeled d) is given by

$$\Psi = \sum_d \Psi^{\mathrm{PTD}}_d , \tag{3.13}$$

where

$$\Psi^{\mathrm{PTD}}_d = \sum_{c'} \int dK' \int dR' \mathcal{F}^d_{c'}(K',R') e^{iK'\cdot(R-R')}\Phi_{c'}(x-R') \tag{3.14}$$

and

$$\mathfrak{F}^d_{c'}(K',R') = \int dK \tilde{\mathfrak{F}}^d_{c'}(K-K')\tilde{f}_d(-K)e^{iK\cdot R'}\,, \qquad (3.15)$$

$$\mathfrak{F}_{c'} = \sum_d \mathfrak{F}^d_{c'}\,.$$

Equation (3.14) is equivalent to the RGM function

$$\Psi^{PTD}_d = u_d(R)\Phi^{PTD}_d(\xi)\,, \qquad (3.16)$$

where

$$\Phi^{PTD}_d(\xi) = \sum_{c'} \int dq' \tilde{F}^d_{c'}(q')e^{-iq'\cdot R} \times \int dR' e^{iq'\cdot R'}\Phi_{c'}(x-R')\,. \qquad (3.17)$$

Now the boundary conditions on $\mathfrak{F}_{c'}(K',R')$ can be derived. From (3.16) and (2.11), we expect that the momentum space wave functions $\tilde{f}_d(-K)$ in channel d assume the form

$$\tilde{f}_d(-K) = a_d\delta(K-K_d) + \sum_{d'} \frac{T_{dd'}(K,K_d)a_{d'}}{K_d^2 - K^2 + i\epsilon}\,, \qquad (3.18)$$

with $a_d = 0$, except for the initial channel, and the $T_{dd'}$ are half-off-shell T matrices. Thus, from (3.15) and (3.18), we finally have

$$\mathfrak{F}^d_{c'}(K',R') = \tilde{F}^d_{c'}(K'-K_d)a_d e^{iK_d\cdot R'} + \sum_{d'} \int dK'' \frac{T_{dd'}(K'',K_d)a_{d'}}{K_d^2 - K''^2 + i\epsilon} \tilde{F}^{d'}_{c'}(K''-K') \times e^{iK''\cdot R'}\,, \qquad (3.19)$$

hence $\mathfrak{F}_{c'} = \sum_d \mathfrak{F}^d_{c'}$, where of course the $\tilde{F}^{d'}_{c'}$ are already available from the prediagonalization of (3.11) and (3.12). With the definition (2.15b), we will have a slightly simpler boundary condition for $\mathfrak{F}'_{c'}(K',R')$ than (3.19), without the $\exp(iK_d\cdot R')$ factor, for example.

Equation (3.5), with (3.19) and (3.12), forms a dynamical system one can solve for the potential scattering of a nucleus. Construction of a set of basis functions Φ^{PTD}_d is already a significant improvement over the initial Φ_c, because the internal states are isolated by the projection method and the channel description after the prediagonalization procedure should be more realistic.

The development of the theory presented above is rather abstract, and we illustrate the structure of the theory in the simple factorizable case for Φ_c. With (2.4), we have for (3.11), after some algebra,

$$\sum_{c'} \tilde{G}^*_{c''}(-q'')\{e_{c''c'} - n_{c''c'}\tilde{e}^D\} \times \int dq' \tilde{G}_{c'}(-q')\tilde{F}_{c'}(q') = 0\,, \qquad (3.20)$$

where

$$e_{c''c'} = \int d\xi\, \Phi^{int*}_{c''}(\xi)H_N(\xi)\Phi^{int}_{c'}(\xi)\,,$$

$$n_{c''c'} = \int d\xi\, \Phi^{int*}_{c''}(\xi)\Phi^{int}_{c'}(\xi)\,.$$

As expected from (2.5) and (2.6), the q' dependence of $\tilde{F}_{c'}(q')$ is not necessary in this case, so that we may set $\tilde{F}_{c'}(q') = \tilde{F}_{c'} = \text{constant}$. These constants are, of course, determined by the diagonalization of the matrix $e_{c''c'} - \tilde{e}^D n_{c''c'}$ (with proper allowance for the known factors $\tilde{G}_{c''}$ and $\tilde{G}_{c'}$).

On the other hand, the problem posed by Eq. (3.12) requires a prediagonalization process based on the equation

$$\sum_{c'} (e_{c''c'} - n_{c''c'}e^d) \int dK' \int dR' \int dq' \mathfrak{F}^d_{c'}(K',R')e^{-i(K'-q')\cdot(R'-R'')}\tilde{G}_{c'}(q')\tilde{G}^*_{c''}(K''-K'+q') = 0\,. \qquad (3.21)$$

Equation (3.21) depends only on $(R'-R'')$, except for the $\mathfrak{F}^d_{c'}(K',R')$, which suggests immediately that $\mathfrak{F}^d_{c'}(R',K')$ are in fact functions of K' *only*. Thus we replace $\mathfrak{F}^d_{c'}(K',R')$ by $\tilde{F}^d_{c'}(-K')$. The dR' integration can then be carried out in the variable $(R'-R'')$, which results in a factor $\delta(K'-q')$. Finally then,

$$\sum_{c'} \tilde{G}^*_{c''}(K'')\{e_{c''c'} - n_{c''c'}e^d\} \int dK' \tilde{F}^d_{c'}(-K')\tilde{G}_{c'}(K') = 0\,, \qquad (3.22)$$

which is exactly the form (3.20). Thus we have shown explicitly again in the factorizable case that the diagonalization using (3.11) is completely equivalent to the prediagonalization required in (3.12).

Evidently, the $(R'-R'')$ dependence in (3.21) is a consequence of the commutativity of $H_N(\xi)$ and $\hat{K}$, and not a result of the factorizability of $\Phi_{c'}$. On the other hand, the simple result of (3.20) with $\tilde{F}^d_{c'}(q') = \text{constants}$, is a direct consequence of the factorizability of $\Phi_{c'}$. When we generalize $\Phi_{c'}$ in the next section to incorporate distortions, some of these properties will be lost in the interaction region. However, asymptotically they are retained in order to be able to specify the asymptotic boundary conditions.

IV. DISTORTION EFFECTS—COORDINATE AND MOMENTUM-DEPENDENT BASIS FUNCTIONS

Distortion of the nucleus during the nuclear collision is often taken into account in a reaction theory by including in Eq. (3.13) several channels which are strongly coupled to each other. As is well known, such a procedure has its limitations. Firstly, as the number of important channels to be included grows, the computation for the solution will become prohibitively complicated very quickly. Secondly, there is always the lingering question of the effect of other channels which are being neglected. Thirdly, even if we can take into account a sufficient number of them, the separation of internal parts from Φ_c becomes difficult even in the factorizable cases.[9] Of course, there are known procedures to approximately overcome some of these difficulties, for example, introducing a set of pseudostates or by constructing effective optical potentials for the various channels.

In this section, we show that the formalism developed in Secs. II and III can be naturally extended to incorporate such distortions. To minimize the number of explicit channels in (3.5), a set of distorted cluster states are introduced; the distorted Slater determinants are dependent on the generator coordinate variables, R' or K', or both, so that the nonlocality and energy-dependence of the actual scattering process are adequately reproduced. Precise choice for the single-particle potential $W(x_i)$ in (1.3) depends, of course, on the dynamics. A rough estimate of W may be obtained by examining the optical potential corresponding to channel d, with the channel cluster function $\Phi_d^{PTD}(\xi) \equiv |d\rangle$. Then we have[16]

$$U_d = \langle d|V|d\rangle_\xi + \left\langle d\left| V \frac{1}{Q_d(E+i\epsilon-H)Q_d} V \right| d \right\rangle, \quad (4.1)$$

where $Q_d = I_\xi - |d\rangle_\xi\langle d|$. Because of the Green's function $[Q_d(E+i\epsilon-H)Q_d]^{-1}$, U_d is nonlocal in R, and is also energy dependent. Thus, if we are to describe the elastic scattering in the d channel with a single determinantal function Φ_d^{dis}, then the W potential for the single-nucleon states φ^{dis} should reflect the similar nonlocal and energy-dependent properties of (4.1). Therefore, Φ_d^{dis} and W^{dis} can, in general, depend on the R and K variables for the c.m. motion of the nucleus, as

$$\Phi_d^{dis}(\xi;R,K) \text{ and } W^{dis}(x_i;R,K). \quad (4.2)$$

Since we are going to apply the projection procedures of Sec. II to the determinantal functions Φ_c, the explicit dependence of Φ_d^{dis} on R and K may be incorporated in these Φ_c through their dependence on the generator coordinates R' and K'. This is, of course, not the most general procedure, but probably the simplest. In the following, we consider in sequence R' distortions, K' distortions, and (R',K') distortions.

A. Adiabatic distortions (R')

We first consider a set of adiabatically distorted single-particle states localized near the origin O_x which are now explicitly dependent on the generator coordinate R'. Such states are convenient in describing a slow collision of a nucleus which can easily be distorted. Thus, instead of (1.3), we consider[5] a new single-particle potential $W^{ad}(x_i;R')$, which is centered near O_x and generates a set of orbitals

$$\begin{aligned} &h^{ad}(x_i;R')\varphi_n^{ad}(x_i;R') = e_n^{ad}(R')\varphi_n^{ad}(x_i;R'), \\ &h^{ad}(x_i;R') = K(x_i) + W^{ad}(x_i;R'), \end{aligned} \quad (4.3)$$

with the important constraint that, as $R' \to \infty$, we return to the undistorted case of Sec. I, as

$$\begin{aligned} &e_n^{ad}(R') \to e_n, \\ &W^{ad}(x_i;R') \to W(x_i), \\ &\varphi_n^{ad}(x_i;R') \to \varphi_n(x_i). \end{aligned} \quad (4.4)$$

They are completely equivalent to the usual "molecular orbital" states, and much simpler to deal with, since the model here does not allow nucleon exchanges. As in Sec. I, Slater determinants $\Phi_c^{ad}(x,R')$ can be constructed as

$$\Phi_c^{ad}(x;R') = \frac{1}{\sqrt{N!}} \det[\varphi_{c_1}^{ad}(x_1;R')\varphi_{c_2}^{ad}(x_2;R')\cdots\varphi_{c_N}^{ad}(x_N;R')] \quad (4.5)$$

with the obvious property that again, as $R' \to \infty$,

$$\Phi_c^{ad}(x;R') \to \Phi_c(x). \quad (4.6)$$

The projection procedure (2.1) or (2.2) for the construction of internal wave functions is no longer valid with $\Phi_c^{ad}(x;R')$. We have

$$D_{R'}\Phi_c^{ad}(x;R') = \Phi_c^{ad}(x-R';R') = \Phi_c^{ad}(\xi,R-R';R'), \quad (4.7)$$

so that (2.3) becomes

$$\begin{aligned} \Phi_{0c}^{ad} &= \int dq' \bar{F}_c(q') \int dR' e^{-iq'\cdot(R-R')} \Phi_c^{ad}(\xi,R-R';R') \\ &= \int dt' F_c(t') \Phi_c^{ad}(\xi,t';R-t'), \end{aligned} \quad (4.8)$$

where $t' \equiv R - R'$. Evidently, from (4.8), the resulting Φ_{0c}^{PT} will be an explicit function of *both* ξ and R. With the asymptotic property (4.6) for large R', however, we expect that $\Phi_{0c}^{ad}(\xi;R)$

$\to \Phi_{0c}^{PT}(\xi)$ as $R \to \infty$. This is a consequence of the fact that $\Phi_c^{ad}(\xi, t'; R - t')$ is peaked around the value $t' = 0$, so that its dependences on R and R' are similar. Thus Φ_{0c}^{ad} defined by (4.8) becomes purely internal in the limit of large R.

The scattering functions can be constructed either with (2.8) in the factorizable case or with (2.12) in the more general cases (with a slight change in the R'-dependent Slater determinants) as, for example,

$$\Psi_c^{ad}(x) = \int dK' \int dR' \mathcal{F}_c(K', R') e^{iK' \cdot (R - R')} \Phi_c(x - R'; R'). \tag{4.9}$$

The scattering equations that $\mathcal{F}_c(K', R')$ satisfy are exactly the same as (3.5). This is the very point mentioned earlier that the forms (2.12) and (3.5) already contain the GCM R' and K', so that (4.9) is perfectly a natural extension, with the potentially powerful means to improve the theory. The prediagonalization program defined by (3.12) will be slightly more complicated because the kernels are no longer functions of $R' - R''$. [Previously, this property allowed us to connect Eq. (3.12) to Eq. (3.11), and to drop the R' dependence in $\mathcal{F}_{c'}^{d}(Z')$.] However, there are no more complications of principles, and the resulting $\mathcal{F}_{c'}^{d}$ and E^d can be used to specify the necessary boundary conditions similar to (3.19). In all these manipulations it is clear that one introduces some c.m. spuriosity, but this disadvantage should be compensated by the advantage brought about by the introduction of the polarization effects controlled by R'.

Instead of using only the nuclear internal Hamiltonian $H_N(\xi)$ in (3.12) for the prediagonalization, we may also include the interaction term $V(\xi, R)$ during the prediagonalization. Then, the resulting E^d will be explicitly R dependent, as expected from the general consideration of an adiabatic picture.

A simple example of an R'-dependent distortion effect may be found in the harmonic oscillator model for the dineutron scattering by a fixed potential. The determinantal function is given by

$$\Phi_0(x - R') = G_0(R - R') \Phi_0^{int}(\xi), \tag{4.10}$$

where

$$\Phi_0^{int}(\xi) = \pi^{-3/4} (a\sqrt{2})^{-3/2} \exp(-\xi^2/4a^2),$$

$$G_0(R - R') = \pi^{-3/4} (a/\sqrt{2})^{-3/2} \exp[-(R - R')^2/a^2],$$

$$\xi \equiv r_1 - r_2.$$

The strength constant a may then be replaced by, e.g.,

$$a \to a(R') = a_0[1 - e^{-b_0 R'}].$$

By replacing R' by $R - t'$, with $t' = R - R'$, it is explicitly seen that the R and R' dependences of $\Phi_0(x - R')$ at large R and R' are indeed similar.

B. Momentum-dependent distortion (K')

When $\Phi_c(x)$ depends explicitly on the GCM variable K', as

$$\Phi_c(x) \to \Phi_c(x; K'), \tag{4.11}$$

the entire formalism of Secs. II and III should be applicable without change since, as discussed after Eq. (2.1), internal structures are already momentum dependent. Thus, the resulting formula should be much simpler than that described in Sec. IV A for the R'-dependent distortion. Such a possibility of including some distortions without additional complications should be useful in practice, especially in high energy collisions, because a proper adjustment of the basis set as a function of the scattering energy is difficult to make in the RGM. In fact, this additional K' dependence mixes in Φ_c's, which are basically different sets of functions for each K'.

An example of such a parametrized state is given by the model of (4.10), with $a_0 \to a(K')$.

C. Coordinate and momentum-dependent distortions (K' and R')

We now let the basis functions Φ_c depend on the both GCM variables R' and K', as

$$\Phi_c(x) \to \Phi_c^{dis}(x; K', R'). \tag{4.12}$$

The formalism here naturally follows along the line of Sec. IV A with very minor changes in notation. Thus, (4.12) provides the most general approach within the limited framework in which we require the distortion variables to be identical to the GCM, R', and K'. Otherwise, additional averaging procedures have to be introduced. The model (4.10) provides a simple example in which $a_0 \to a(R', K')$.

V. DISCUSSION AND SUMMARY

Description of a many-nucleon bound system by one or more Slater determinants is most convenient but, by the very nature of such a composite function of single particle orbitals, it becomes difficult to separate out the c.m. variables which are needed in treating the scattering problem. We have carefully studied in this paper such a theory in the case of potential scattering of a nucleus. Our main result is the scattering Eq. (3.5) with the boundary conditions indicated by (3.19), where the cluster mixing functions $\bar{F}_{c'}^{d}(q')$ are to be obtained by the prediagonalization (3.12). Such a formalism should be useful in describing the scat-

tering of light nuclei by a heavy closed-shell nucleus which provides an effective scattering potential V.

From a practical computational point of view, the factorizable case would be most interesting. As noted earlier, the formalism then simplifies a great deal and we have indicated in this paper how the general formalism reduces in such cases. The important problem of incorporating the cluster distortions in the basis determinants has been considered, without increasing the number of coupled channels. The general nucleus-nucleus scattering will be treated later using the basic result of this paper.

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[1]For complete reference to earlier works, see, for example, C. W. Wong, Phys. Rep. 15, 283 (1975); J. Le Tourneux, Lecture Notes at Institut de Physique Nucléaire, Univ. de Lyon, Lyon, France, edited by E. Elbaz, 1976 (unpublished).

[2]D. L. Hill and J. A. Wheeler, Phys. Rev. 89, 1102 (1953); J. J. Griffin and J. A. Wheeler, *ibid.* 108, 311 (1951).

[3]R. E. Peierls and J. Yoccoz, Proc. Phys. Soc. A10, 381 (1951).

[4]R. E. Peierls and D. J. Thouless, Nucl. Phys. 38, 154 (1962).

[5]Y. Hahn, Phys. Rev. 174, 1168 (1968).

[6]C. W. Wong, Nucl. Phys. A191, 193 (1972).

[7]C. Bloch and V. Gillet, Phys. Lett. 16, 62 (1965); 18, 58 (1965).

[8]C. Mahaux and H. A. Weidenmüller, *Shell Model Approach to Nuclear Reactions* (North-Holland, Amsterdam, 1969).

[9]B. Giraud, J. C. Hocquenghem, and A. Lumbroso, Phys. Rev. C 1, 2214 (1973); B. Giraud and J. LeTourneux, Nucl. Phys. A191, 410 (1972); Phys. Rev. Lett. 31, 399 (1973).

[10]H. Horiuchi, Prog. Theor. Phys. 43, 315 (1970).

[11]N. de Takacsy, Phys. Rev. C 5, 1883 (1972).

[12]T. Yukawa, Phys. Lett. B38, 1 (1972); Nucl. Phys. A186, 121 (1972).

[13]T. Fliessbach, Nucl. Phys. A194, 625 (1972).

[14]K. Wildermuth and W. McClure, *Cluster Representation of Nuclei*, Springer Tracts in Modern Physics, (Springer, Berlin, 1966), Vol. 41.

[15]D. Brink, in *Many-Body Description of Nuclear Structure and Reactions*, Proceedings of the International School of Physics, "Enrico Fermi," Course 36, edited by C. Bloch (Academic, N.Y., 1966).

[16]Y. Hahn, Phys. Rev. A 12, 2402 (1975).