Variational estimates of exclusive cross sections

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A variational principle, based on microscopic trial wave functions to calculate corrections to the Born amplitude, is described. The case of high multiplicity final channels is considered. It is shown that the transition amplitude for exclusive processes can always be estimated.

[NUCLEAR REACTIONS Variational principle gives microscopic transition amplitudes for heavy ion fragmentation.]

I. INTRODUCTION

Heavy ion collisions at intermediate energies, 10 MeV $\lesssim E/A \lesssim$ 100 MeV, raise a serious challenge to the theory of collisions. Indeed, at lower energies comparable to the Coulomb barrier and not exceeding the binding energy per nucleon, 3 MeV $\lesssim E/A \lesssim$ 10 MeV, it has been found that nuclear viscosity helps in restricting the basic reaction mechanism to two-body situations, even though preequilibrium,[1] fast fission,[2] and evaporation[3] phenomena, among others, may create final channels with more than two bodies in the continuum. This low energy domain has been described by quite a few theories, ranging from DWBA (Ref. 4) to transport[5] equations, all involving the excitation or explicit treatment of a limited number of degrees of freedom. The other extreme domain, corresponding to high energies, $E/A > 100$ MeV, does involve the excitation of all nuclear degrees of freedom, not to mention mesonic degrees. The theories proposed and used in this domain range from multiple scattering[6] for a single nucleon projectile to various statistical and classical limits, such as fire-ball[7] and cascade[8] models. The Pauli principle and the many-body correlations are often considered of limited importance in this limit.

In the transition region, however, the complete nucleon breakup threshold, $E/A \approx 10$ MeV, and the Fermi energy, $\epsilon_F \approx 50$ MeV, just create a situation in which a theory of collisions should allow for a microscopic, antisymmetrized description of all degrees of freedom. As long as the time-dependent Hartree-Fock (TDHF) description of scattering[9] has not evolved into a reliable theory of collisions, the analysis of exclusive or partly exclusive cross sections seems to be beyond reach except through rather phenomenological models. It should be noted, however, that some attempts in this direction are now in progress.[10]

Some performed or planned experiments at heavy ion facilities, however, involve a stimulating degree of exclusive or partly exclusive measurements. The purpose of this paper is to show how a microscopic theory of collisions may give at least some estimates of such exclusive processes. The theory which follows is based on a formally exact variational derivation of the many-body transition amplitude.[11] It is already clear at this stage, however, that a variational principle is only as good as the class of trial functions that are allowed in a practical calculation. The theory will thus provide gross estimates rather than accurate amplitudes for exclusive processes. It is the ratios of these estimates for various final states and various mechanisms which will have to be considered when analyzing experimental evidence.

This paper is organized as follows. Section II contains a brief reminder of the variational principle[11] under study and a short description of the schemes available for practical calculations. An illustrative example is given in Sec. III with a numerical application. It corresponds to the elastic scattering of two heavy ions in the approximation where their internal structure is ignored. This example discusses at length the technicalities considered in making the variational principle a realistic approximation. Section IV shows how the theory can be extended to processes considering the details of internal structure and more than two bodies in a channel. The problem of antisymmetrization is treated in Sec. V. In Sec. VI we discuss the

classes of trial functions which can be implemented for the description of various mechanisms. Section VII is the general discussion and conclusion.

II. THE VARIATIONAL PRINCIPLE

We consider a system of N nucleons, their coordinates $\vec{x}\equiv(\vec{x}_1\cdots\vec{x}_N)$, momenta $\vec{p}\equiv(\vec{p}_1\cdots\vec{p}_N)$, and their Hamiltonian $H=\mathcal{T}+\mathcal{V}$. Here $\mathcal{V}$ is a sum of two-body potentials,

$$\mathcal{V}=\sum_{i<j}\mathcal{V}_{ij}\ ,$$

and the center of mass kinetic energy operator is removed from the total energy; hence

$$\mathcal{T}=\sum_i \mathcal{T}_i-\mathcal{T}_{\text{c.m.}}\ .$$

The Hamiltonian acts only in the space of $N-1$ vector Jacobi coordinates $\vec{\xi}$, but for obvious technical reasons it is better to perform integrations and write wave functions and operators in the $\vec{x}$ or $\vec{p}$ representation. The precaution to take is to use only wave functions of the form

$$\Phi(\vec{x})=\Phi_{\text{c.m.}}(\vec{R})\Phi_{\text{int}}(\vec{\xi})\ , \tag{2.1}$$

where internal and center-of-mass motions are decoupled. Such a factorization is trivial to implement with plane waves and harmonic oscillators. It has also been extensively studied and reasonably satisfied in the framework of the shell model, the Hartree-Fock, and the generator coordinate theories.

This precaution for center-of-mass elimination will be understood in the following. Hence any physical (internal) operator $A(\vec{x})\equiv A(\vec{\xi})$ will appear in matrix elements

$$\langle\Phi'_{\text{int}}\,|\,A\,|\,\Phi_{\text{int}}\rangle_{\vec{\xi}}=\frac{\langle\Phi'\,|\,A\,|\,\Phi\rangle_{\vec{x}}}{\langle\Phi'_{\text{c.m.}}\,|\,\Phi_{\text{c.m.}}\rangle_{\vec{R}}}\ , \tag{2.2}$$

where the numerator is obtained by an integration over all the single nucleon coordinates (or momenta) and the denominator is the overlap of the relevant center-of-mass wave packets, just an integral over $\vec{R}$ (or $\vec{P}$). In the following, the left-hand side of Eq. (2.2) will henceforth be denoted by $\langle\Phi'\,|\,A\,|\,\Phi\rangle$.

Let $\chi(\vec{x})$ denote the initial channel wave function and V the corresponding channel (prior) interaction. The function χ is defined by the channel momentum $\vec{k}$, the projectile and target internal wave functions $\psi_p(\vec{\xi}_p)$ and $\psi_t(\vec{\xi}_t)$, with the corresponding Jacobi coordinates $\vec{\xi}_p$ and $\vec{\xi}_t$, and a suitable wave packet motion. As usual the prior interaction is

$$V=\sum_{\substack{i\in p\\ j\in t}}\mathcal{V}_{ij}\ . \tag{2.3}$$

In the same way let $\chi'(\vec{x})$ denote the final channel wave function. While χ is a two-body channel, χ' may have any fragmentation. If, for instance, three fragments $f_1f_2f_3$ are involved, one needs to specify two relative momenta k'_{12} and k'_{13}, three internal wave functions $\psi_1(\vec{\xi}_{f_1})$, $\psi_2(\vec{\xi}_{f_2})$, $\psi_3(\vec{\xi}_{f_3})$, and again a center-of-mass motion. The post potential is then trivially

$$V'=\sum_{\substack{i\in f_1\\ j\in f_2}}\mathcal{V}_{ij}+\sum_{\substack{i\in f_2\\ j\in f_3}}\mathcal{V}_{ij}+\sum_{\substack{i\in f_3\\ j\in f_1}}\mathcal{V}_{ij}\ , \tag{2.4}$$

and one is interested in the transition amplitude

$$\begin{aligned}T&\equiv T_{\text{Born}}+\Delta T\\ &\equiv\langle\chi'\,|\,V\,|\,\chi\rangle+\langle\chi'\,|\,V'(E^+-H)^{-1}V\,|\,\chi\rangle\ .\end{aligned} \tag{2.5}$$

The Born term T_{Born} is usually straightforward, even though sometimes tedious to calculate. The correction ΔT is a different matter. In order to estimate it we introduce the functional

$$F\equiv\frac{\langle\Phi'\,|\,V\,|\,\chi\rangle\langle\chi'\,|\,V\,|\,\Phi\rangle}{\langle\Phi'\,|\,(E-H)\,|\,\Phi\rangle}\ , \tag{2.6}$$

which depends upon two arbitrary trial functions Φ, Φ'. It is trivial to check that the stationarity conditions[11] of F with respect to Φ and Φ' read, respectively,

$$\langle\Phi'\,|=\frac{\langle\Phi'\,|\,(E-H)\,|\,\Phi\rangle}{\langle\chi'\,|\,V'\,|\,\Phi\rangle}\langle\chi'\,|\,V'(E-H)^{-1} \tag{2.7a}$$

and

$$|\,\Phi\rangle=\frac{\langle\Phi'\,|\,(E-H)\,|\,\Phi\rangle}{\langle\Phi'\,|\,V\,|\,\chi\rangle}(E-H)^{-1}V\,|\,\chi\rangle\ . \tag{2.7b}$$

Hence the stationary value of F is

$$F_{\text{stat}}=\frac{\langle\chi'\,|\,V'(E-H)^{-1}V\,|\,\chi\rangle^2}{\langle\chi'\,|\,V'(E-H)^{-1}(E-H)(E-H)^{-1}V\,|\,\chi\rangle}=\Delta T\ . \tag{2.8}$$

It will be noticed that F does not depend upon the normalization of Φ and Φ'. The normalization coefficients in Eqs. (2.7) actually turn out to be equal to 1 in the exact case and can be taken as 1 in any restricted variational space. In order to avoid difficulties in the validity of the relation

$$(E-H)(E-H)^{-1}=1$$

used in Eq. (2.8) it is advisable to give to E a noninfinitesimal imaginary part. Hence the resolvent $(E-H)^{-1}$ becomes a *bona fide* bounded operator.

Alternatively one may consider the functional[11]

$$G\equiv\langle\Phi'\,|\,V\,|\,\chi\rangle+\langle\chi'\,|\,V'\,|\,\Phi\rangle-\langle\Phi'\,|\,(E-H)\,|\,\Phi\rangle\,, \tag{2.9}$$

which depends upon the normalizations of Φ and Φ', but yields the same stationarity conditions and stationary value as F.

As will be seen in more detail below, it is also proper, for practical calculations, to take square integrable functions as simulations of channel wave functions χ and χ'. This amounts to considering the averages of transition amplitudes around the central value $\vec{k}$ of initial momenta and $\vec{k}\,'$ of final momenta. The imaginary part of E can obviously be made compatible with the width of such averages.

As a consequence of the choice of a complex E and square integrable χ and χ' it is obvious from Eqs. (2.7) that Φ and Φ' can be restricted to a class of square integrable trial functions. This is also of some advantage for practical calculations.

III. AN ILLUSTRATIVE EXAMPLE

A. General description

We consider the scattering of two heavy ions of equal mass by an S-wave separable potential acting between their centers of mass. The example studied here is merely to study the feasibility of the variational method discussed in Sec. II to yield reasonable estimates of the correction to the lowest order Born amplitude. Thus, the internal structures of the heavy ions are suppressed and the problem is treated in the framework of the collision of two wave packets.

The Hamiltonian of the system is

$$H=\mathscr{T}+\mathscr{V}\,, \tag{3.1}$$

where $\mathscr{T}$ is the kinetic energy operator of the relative motion of the centers of mass of the colliding heavy ions (since the total center-of-mass kinetic energy has been subtracted out) and $\mathscr{V}$ is a separable nonlocal potential of rank 1. In momentum space, the representation of $\mathscr{V}$ is defined by

$$\langle\vec{q}\,|\,\mathscr{V}\,|\,\vec{q}\,'\rangle=-\lambda\gamma(\vec{q})\gamma(\vec{q}\,')\,, \tag{3.2}$$

$$\gamma(\vec{q})=\exp[-\nu^2q^2]\,, \tag{3.3}$$

where λ is the strength of the potential in units of MeV fm^3 and $\vec{q}$ is the relative momentum of the colliding nuclei.

The channel wave functions χ and χ' are chosen as a product of two wave packets for the two ions, i.e.,

$$\chi(\vec{q}_1,\vec{q}_2;\vec{k})=\left[\frac{\beta^2}{\pi}\right]^3\exp\left[-\frac{\beta^2}{2}(\vec{q}_1-\vec{k})^2\right]\times\exp\left[-\frac{\beta^2}{2}(\vec{q}_2+\vec{k})^2\right]\,, \tag{3.4}$$

where the wave packets are centered around the real momenta $+\vec{k}$ and $-\vec{k}$, respectively. An identical form is taken for χ', with $\vec{k}$ replaced by another real momentum $\vec{k}\,'$.

The Gaussian form of the wave packets has the property that the total center-of-mass motion is decoupled from the relative motion, i.e.,

$$\chi(\vec{q}_1,\vec{q}_2;\vec{k})=\varphi_{\text{c.m.}}(\vec{P})\left[\frac{\beta^2}{\pi}\right]^{3/2}\times\exp[-\beta^2(\vec{q}-\vec{k})^2]\,, \tag{3.5}$$

where the center-of-mass wave function is

$$\varphi_{\text{c.m.}}(\vec{P})=\left[\frac{\beta^2}{\pi}\right]^{3/2}\exp\left[-\frac{\beta^2}{4}P^2\right] \tag{3.6}$$

and is not normalized, whereas the wave function of relative motion is a wave packet which tends to a delta function $\delta(\vec{k}-\vec{q})$ in the limit of large β. [The normalization of the wave packet is chosen such that its integral over $\vec{q}$ is unity just as the integral of the delta function $\delta(\vec{k}-\vec{q})$ is unity.] In view of the fact that all the matrix elements are defined by dividing the c.m. overlap, we shall not refer to the total c.m. in the future.

For the trial wave functions, we choose wave functions of the form

$$\langle\vec{q}\,|\,\Phi\rangle=\exp[-\nu^2(\vec{q}-\vec{K})^2]\,, \tag{3.7}$$

$$\langle\Phi'\,|\,\vec{q}\,\rangle=\exp[-\nu^2(\vec{q}-\vec{K}')^2]\,, \tag{3.8}$$

where $\vec{K}$ and $\vec{K}'$ are to be treated as variational parameters and can, in general, be complex.

The variational functional, Eq. (2.5), is

$$F(\Phi',\Phi)\equiv F(\vec{K}',\vec{K}) = \frac{\langle\Phi'|\mathscr{V}|\chi\rangle\langle\chi'|\mathscr{V}|\Phi\rangle}{\langle\Phi'|E-H|\Phi\rangle} . \tag{3.9}$$

Explicitly,

$$F(\vec{K}',\vec{K})=\frac{\langle\chi'|\mathscr{V}|\chi\rangle}{[\langle\Phi'|(E-\mathscr{T})|\Phi\rangle/\langle\Phi'|\mathscr{V}|\Phi\rangle]-1} , \tag{3.10}$$

where the particular form of factorization is due to the separable nature of the potential. With the numerator

$$\langle\chi'|\mathscr{V}|\chi\rangle=-\lambda\left[\frac{\beta^2}{\beta^2+\nu^2}\right]^3 \times\exp\left[-\frac{\beta^2\nu^2(k^2+k'^2)}{\beta^2+\nu^2}\right] , \tag{3.11}$$

the variational parameters occur only in the denominator and thus one can investigate the properties of the function

$$J(\vec{K}',\vec{K})=\langle\Phi'|(E-\mathscr{T})|\Phi\rangle/\langle\Phi'|\mathscr{V}|\Phi\rangle . \tag{3.12}$$

The variation of $J(\vec{K}',\vec{K})$ with respect to changes in $\vec{K}$ and $\vec{K}'$ yields two stationary points

$$\vec{K}=\vec{K}'=0 , \tag{3.13a}$$

and

$$\vec{K}=\vec{K}'; \quad |\vec{K}|^2=\frac{2\mu}{\hbar^2}\left[E-\frac{7\hbar^2}{8\mu\nu^2}\right] , \tag{3.13b}$$

where μ is the reduced mass of the two heavy ions. The corresponding stationary values of $F(\vec{K}',\vec{K})$ are

$$F_1(\vec{k}',\vec{k})=\frac{\langle\chi'|\mathscr{V}|\chi\rangle}{-\frac{1}{\lambda}\left[\frac{2\nu^2}{\pi}\right]^{3/2}\left[E-\frac{3\hbar^2}{8\mu\nu^2}\right]-1} \quad \text{for } \vec{K}'=\vec{K}=0 , \tag{3.14a}$$

and

$$F_2(\vec{k}',\vec{k})=\frac{\langle\chi'|\mathscr{V}|\chi\rangle}{-\frac{1}{\lambda}\left[\frac{2\nu^2}{\pi}\right]^{3/2}\exp\left[\frac{2\mu E\nu^2}{\hbar^2}-\frac{7}{4}\right]-1} \quad \text{for } \vec{K}'=\vec{K}; \quad |\vec{K}|^2=\frac{2\mu}{\hbar^2}\left[E-\frac{7\hbar^2}{8\mu\nu^2}\right] . \tag{3.14b}$$

The quantity $F_i(\vec{k}',\vec{k})$ represents the correction to the Born amplitude. The total "off-shell" T matrix for the scattering between wave packets, as defined by

$$T(\vec{k}',\vec{k};E)=\langle\chi'|\hat{T}(E)|\chi\rangle , \tag{3.15}$$

where $\hat{T}$ is here the operator

$$\hat{T}\equiv\mathscr{V}+\mathscr{V}(E-H)^{-1}\mathscr{V} ,$$

is the sum of the Born amplitude and the correction term. Our approximation yields two estimates

$$T_i(\vec{k}',\vec{k};E)=\langle\chi'|\mathscr{V}|\chi\rangle+F_i(\vec{k}',\vec{k}) \quad i=1,2 . \tag{3.16}$$

Thus, in the two cases, we find

$$T_i(\vec{k}',\vec{k};E)=\langle\chi'|\mathscr{V}|\chi\rangle\left[1+\frac{1}{J_i(\vec{k}',\vec{k})-1}\right] =\langle\chi'|\mathscr{V}|\chi\rangle\left[\frac{J_i(\vec{k}',\vec{k})}{J_i(\vec{k}',\vec{k})-1}\right] =\frac{\langle\chi'|\mathscr{V}|\chi\rangle}{1-\frac{1}{J_i(\vec{k}',\vec{k})}} . \tag{3.17}$$

Thus,

$$T_1(\vec{k}',\vec{k};E)=\frac{\langle\chi'|\mathscr{V}|\chi\rangle}{1+\lambda\left[\frac{\pi}{2\nu^2}\right]^{3/2}\left[E-\frac{3\hbar^2}{8\mu\nu^2}\right]^{-1}} \quad \text{for } \vec{K}=\vec{K}'=0 , \tag{3.18a}$$

and

$$T_2(\vec{k}',\vec{k};E)=\frac{\langle\chi'|\mathscr{V}|\chi\rangle}{1+\lambda\left[\frac{\pi}{2\nu^2}\right]^{3/2}\left[\frac{2\mu\nu^2}{\hbar^2}\right]\exp\left[-\left[\frac{2\mu E\nu^2}{\hbar^2}-\frac{7}{4}\right]\right]} . \tag{3.18b}$$

The expressions Eqs. (3.18) have to be compared with the exact expression

$$T^{\text{exact}}(\vec{k}',\vec{k};E)=\frac{\langle\chi'|\mathscr{V}|\chi\rangle}{1+\left[\frac{2\mu}{\hbar^2}\right]\Delta(E)}, \tag{3.19a}$$

where

$$\Delta(E)=\int d\vec{q}\,\frac{e^{-2\nu^2q^2}}{k_0{}^2-q^2}, \tag{3.19b}$$

and where

$$k_0{}^2=\frac{2\mu E}{\hbar^2}. \tag{3.19c}$$

The on-shell T matrix is related to the phase shift through the relation

$$e^{i\delta(E)}\sin\delta(E)=-\frac{4\pi^2\mu}{\hbar^2}k_0T(k_0), \tag{3.20}$$

where

$$T(k_0)=T\left[\vec{k}_0,\vec{k}_0;E=\frac{\hbar^2k_0{}^2}{2\mu}\right]. \tag{3.21}$$

The two possible solutions $\vec{K}=\vec{K}'=0$ and

$$\vec{K}=\vec{K}';\quad K^2=\left[\frac{2\mu}{\hbar^2}E-\frac{7}{4\nu^2}\right]$$

yield the best possible solutions for the Gaussian type of trial functions we have used. One can obtain a better approximation by considering a linear superposition of the two, i.e.,

$$\langle\vec{q}\,|\,\Phi\rangle=\alpha_1\langle\vec{q}\,|\,\Phi_1\rangle+\alpha_2\langle\vec{q}\,|\,\Phi_2\rangle, \tag{3.22a}$$

$$\langle\Phi'\,|\,\vec{q}\,\rangle=\alpha_1'\langle\Phi_1'\,|\,\vec{q}\,\rangle+\alpha_2'\langle\Phi_2'\,|\,\vec{q}\,\rangle, \tag{3.22b}$$

where $|\Phi_1\rangle,\langle\Phi_1'|$ and $|\Phi_2\rangle,\langle\Phi_2'|$ are the two solutions just obtained. The variational parameters α_1, α_2, α_1', α_2' are then provided from the functional G, Eq. (2.9), by the two independent linear systems

$$\begin{aligned}
&\langle\Phi_1'|(E-H)|\Phi_1\rangle\alpha_1+\langle\Phi_1'|(E-H)|\Phi_2\rangle\alpha_2=\langle\Phi_1'|\mathscr{V}|\chi\rangle,\\
&\langle\Phi_2'|(E-H)|\Phi_1\rangle\alpha_1+\langle\Phi_2'|(E-H)|\Phi_2\rangle\alpha_2=\langle\Phi_2'|\mathscr{V}|\chi\rangle,
\end{aligned} \tag{3.23}$$

$$\begin{aligned}
&\alpha_1'\langle\Phi_1'|(E-H)|\Phi_1\rangle+\alpha_2'\langle\Phi_2'|(E-H)|\Phi_1\rangle=\langle\chi'|\mathscr{V}'|\Phi_1\rangle,\\
&\alpha_1'\langle\Phi_1'|(E-H)|\Phi_2\rangle+\alpha_2'\langle\Phi_2'|(E-H)|\Phi_2\rangle=\langle\chi'|\mathscr{V}|\Phi_2\rangle.
\end{aligned} \tag{3.24}$$

It turns out in this special case that the two systems are identical, as $\langle\Phi_1'|\vec{q}\,\rangle=\langle\vec{q}\,|\Phi_1\rangle$ and $\langle\Phi_2'|\vec{q}\,\rangle=\langle\vec{q}\,|\Phi_2\rangle$. The generalization of this linear procedure to a more general basis of functions $|\Phi_i\rangle,\langle\Phi_j'|$ is trivial. The resulting expression for the correction to the Born amplitude in this approximation yields

$$F_3=\langle\chi'|\mathscr{V}|\chi\rangle\frac{[\mathscr{O}_{11}\mathscr{V}_{22}-2\mathscr{O}_{12}\mathscr{V}_{12}+\mathscr{O}_{22}\mathscr{V}_{11}]}{(\mathscr{O}_{11}\mathscr{O}_{22}-\mathscr{O}_{12}{}^2)}, \tag{3.25}$$

where we have defined

$$\mathscr{O}_{ij}=\langle\Phi_i'|(E-H)|\Phi_j\rangle \tag{3.26a}$$

and

$$\mathscr{V}_{ij}=\langle\Phi_i'|\mathscr{V}|\Phi_j\rangle. \tag{3.26b}$$

Alternatively we find $F_3=S'^{\dagger}O^{-1}S$, where S is the column vector whose components are $S_i\equiv\langle\Phi_i'|\mathscr{V}|\chi\rangle$ and, in the same way, the components of the column vector S' are $S_i'=\langle\Phi_i|\mathscr{V}'|\chi'\rangle$.

We can rewrite the total amplitude in this approximation as

$$T_3(\vec{k}',\vec{k};E)=\langle\chi'|\mathscr{V}|\chi\rangle+F_3. \tag{3.27}$$

B. Numerical

To illustrate the method, we consider a specific example of two nuclei of mass 16, i.e., $\mu=8$. The strength of the separable potential was chosen to be $\lambda=1000$ MeV fm^3. The values of β and ν were chosen to be

$$\beta=4\text{ fm},$$

$$\nu=0.1\text{ fm}.$$

The exact phase shift was calculated for a series of energies in the range $250\le E\le1000$ in units of MeV. Since the width Δk induced by β is of order $\Delta k=0.25$ fm^{-1}, the imaginary part of E is taken to be $\text{Im}E=2k^{-1}\Delta k\,\text{Re}E=0.5k^{-1}\text{Re}E$.

In Fig. 1, we compare the results of the variational calculation with the exact one. The full line curve shows the squared modulus of the exact transition amplitude, Eqs. (3.19). The dashed line represents the approximate results (squared modulus again) for $\vec{K}=\vec{K}'=0$; the dashed-dotted

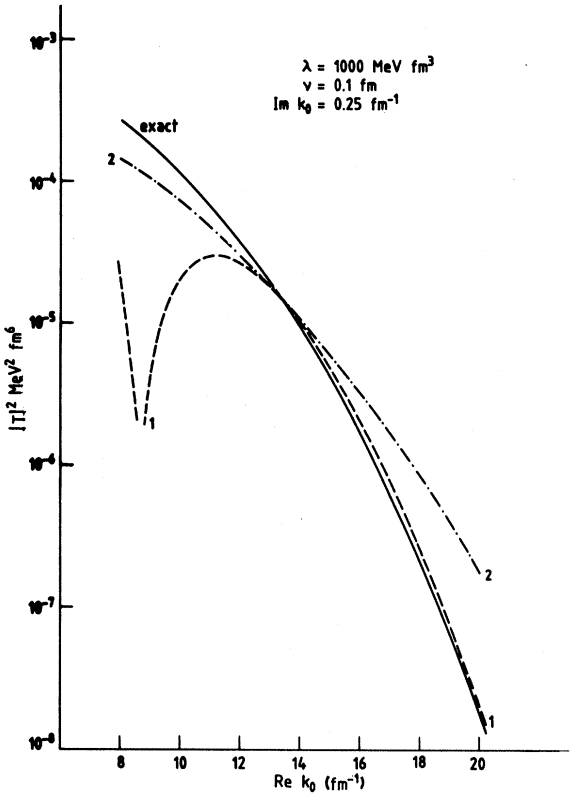

FIG. 1. Comparison of the exact, squared, off-shell transition amplitude, with the first two approximations provided by the variational principle, as functions of the energy.

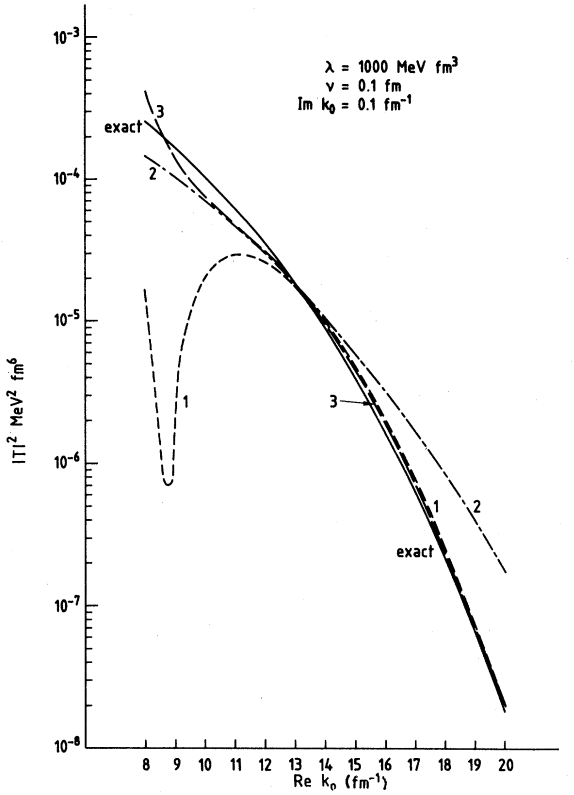

FIG. 2. Same comparison for a situation closer to the on-shell amplitude. The third approximation provided by the variational principle is also shown.

line is for

$$\vec{K}=\vec{K}';\quad K^2=\left[\frac{2\mu}{\hbar^2}E-\frac{7}{4\nu^2}\right],$$

and a long-dashed line would correspond to taking a mixture of the above two solutions if it were distinguishable from the exact results. As a matter of fact, the mixed solution, Eqs. (3.27), is indeed better than the first two approximate solutions, as could be expected. But we may stress that the first two approximate solutions are already remarkably accurate when compared to the bare Born approximation. Indeed it was found systematically in the present case that the Born estimate is about 10^3 to 10^4 too large when compared with the exact amplitude. It is remarkable that the variational principle provides at once, whether one uses Eq. (3.18a) or (3.18b), a significant reduction of this excess and thus the correct order of magnitude.

In regard to the phases of the transition amplitude, our numerical results are less satisfactory, for only a qualitative agreement (within about 20° for a phase of order 200°) is reached. We can notice nonetheless that the Born amplitude is real and provides no phase shift, just a cross section. The variational principle provides a phase shift of a reasonable order of magnitude.

For the sake of curiosity the situation where $\mathrm{Im}E=0.2k^{-1}\mathrm{Re}E$ was also investigated, although the corresponding width $\Delta k=0.1$ fm^{-1} is narrower than that induced by $\beta=4$ fm. The results are displayed in Fig. 2 and are surprisingly satisfactory. In the same way as for Fig. 1 one finds approximation 1 to be good at high energy, approximation 2 to be preferable at low energy, and approximation 3 to be the best compromise.

In Fig. 3 we return to $\Delta k=0.25$ fm^{-1} and consider $\lambda=100$ MeV fm^3, $\nu=0.15$ fm. Approximation 1 dominates, although approximation 2 has a small domain validity at low energy.

A comparison of the moduli of the various wave functions involved in the theory is provided in Fig. 4. The wave functions are artificially normalized to unity at the origin $q=0$ for the comparison. The parameters are those of Fig. 1 and the energy is defined by $\mathrm{Re}k_0=10$ fm^{-1}. The exact solution $\Phi(q)$,

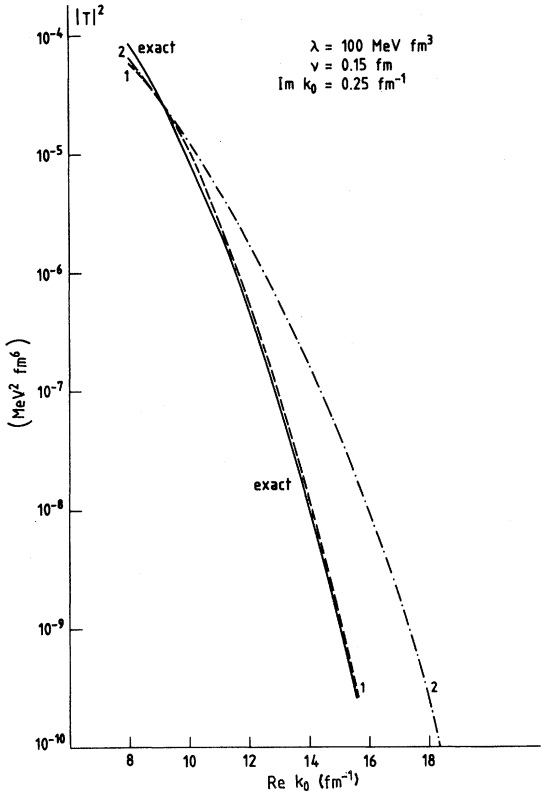

FIG. 3. Same comparison for a different set of interaction parameters.

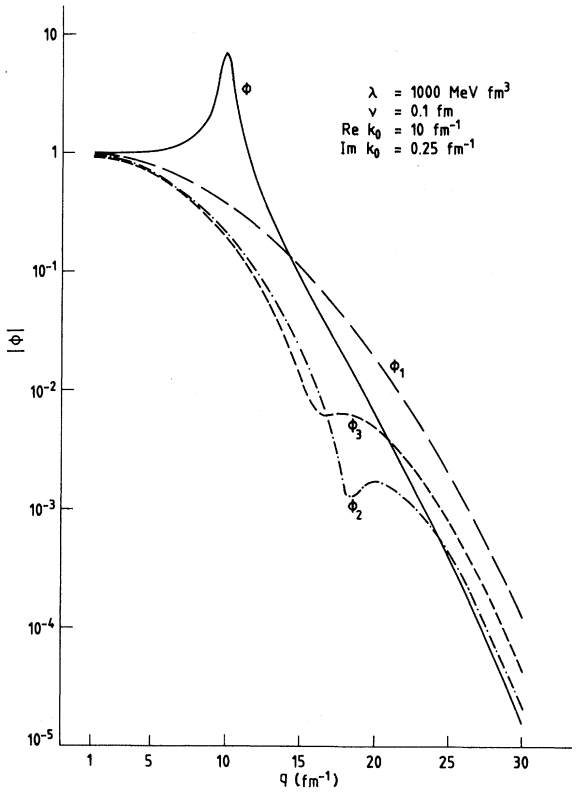

FIG. 4. The various trial functions are compared to the exact solution of the variational principle.

Eq. (2.7), has a sharp peak at $q=\mathrm{Re}k_0$, an indication of the complex pole $(E-q^2)^{-1}$. Neither trial functions Φ_1, Eqs. (3.7) and (3.13a), and Φ_2, Eqs. (3.7) and (3.13b), has a peak there. It will be noticed, however, that the variational principle takes advantage of a peak in Φ_2 at higher momentum to bring it at lower momentum in Φ_3 in order to simulate the peak of Φ. Finally, Fig. 5 shows how Φ_1 and Φ_2 are admixed in Φ_3.

IV. GENERALIZATION

For the sake of clarity, the argument will first go through an illustrative example again, say a fragmentation reaction $^{40}\mathrm{Ca}(^{16}\mathrm{O},\alpha^{12}\mathrm{C})^{40}\mathrm{Ca}^*$. Since 56 nucleons are involved, the calculation of matrix elements in a 168-dimensional space *demands* wave functions of a product type. Individual nuclei will then be described by Slater determinants or simple mixtures of Slater determinants. Channels will be described by products of such determinants (antisymmetrization will be disregarded in this section) or simple sums of such products.

It is again convenient to use a momentum representation. Let Ψ_{16} be the *s*- and *p*-closed shell Slater determinant which is a reasonable approximation for the ground state of the projectile. If one considers analogously the *s*-, *p*-, and *d*-closed shell determinant Ψ_{40} which is suitable for the target, the initial channel can be represented as

$$\chi=\Psi_{16}(\vec{p}_1-\vec{k},\ldots,\vec{p}_{16}-\vec{k})\Psi_{40}(\vec{p}_{17}+\vec{k},\ldots,\vec{p}_{56}+\vec{k})\,. \tag{4.1}$$

In so far as the shell model functions Ψ_{16} and Ψ_{40} contain no center-of-mass spuriousity, suitable Gaussian wave packets for $^{16}\mathrm{O}$ and $^{40}\mathrm{Ca}$ factorize out and one obtains

$$\chi=\psi_{16}(\vec{\xi}_{16})\psi_{40}(\vec{\xi}_{40})\left[\frac{\beta^2}{16\pi}\right]^{3/2}\left[\frac{\beta^2}{40\pi}\right]^{3/2}\exp-\frac{\beta^2(\vec{P}_{16}-\vec{k})^2}{32}\exp-\frac{\beta^2(\vec{P}_{40}+\vec{k})^2}{80}\,, \tag{4.2}$$

where ψ_{16} and ψ_{40} are the internal wave functions of the projectile and target, respectively, and $\vec{\xi}_{16}$ and $\vec{\xi}_{40}$

denote the corresponding 15 and 39 Jacobi coordinates or momenta. The center-of-mass momenta $\vec{P}_{16}$ and $\vec{P}_{40}$ of these nuclei are assumed to occur in wave packets with widths $\beta/\sqrt{16}$ and $\beta/\sqrt{40}$ corresponding to the equal shell model width parameter β for both nuclei. Such an approximation is known to be tolerable in the shell model for nuclei whose masses do not differ too much.

From Eq. (4.2) one finds

$$\chi=\psi_{16}\psi_{40}\left[\frac{7\beta^2}{160\pi}\right]^{3/2}\exp-\frac{7\beta^2(\vec{q}-\vec{k})^2}{160}\left[\frac{\beta^2}{28\pi}\right]^{3/2}\exp-\frac{\beta^2P^2}{112}\,, \tag{4.3}$$

to be compared with Eq. (3.5). Once again the relative momentum $\vec{q}$ acquires a spreading around its center value $\vec{k}$. It is here of order $\sqrt{2\mu\beta^{-1}}$, where μ is the reduced mass $\frac{80}{7}$.

In the same way one may use for the final channel a product of boosted Slater determinants for the three nuclei. For instance, with a closed s shell for the α particle, closed s and $p_{3/2}$ shells for ^{12}C, and closed p, s, d shells for ^{40}Ca, one finds

$$\chi'=\Psi_4(\vec{p}_1-\vec{k}'_1,\ldots,\vec{p}_4-\vec{k}'_1)\Psi_{12}(\vec{p}_5-\vec{k}'_2,\ldots,\vec{p}'_{16}-\vec{k}'_2)\Psi_{40}(\vec{p}_{17}+\vec{k}'_1+\vec{k}'_2,\ldots,\vec{p}_{56}+\vec{k}'_1+\vec{k}'_2)\,. \tag{4.4}$$

Hence, if $\vec{q}'_{12}$ is the relative momentum between α and ^{12}C, and $\vec{q}'_3$ is the relative momentum between the pair α-^{12}C and the residual nucleus ^{40}Ca, Eq. (4.4) becomes

$$\chi'=\psi_4(\vec{\xi}_4)\psi_{12}(\vec{\xi}_{12})\psi_{40}(\vec{\xi}_{40})\left[\frac{\beta^2}{6\pi}\right]^{3/2}\exp-\frac{(\vec{q}'_{12}-\vec{k}'_{12})^2}{6\beta^2}\left[\frac{7\beta^2}{160\pi}\right]^{3/2}\exp-\frac{7\beta^2(\vec{q}'_3-\vec{k}'_3)^2}{160}$$

$$\times\left[\frac{\beta^2}{14\pi}\right]^{3/2}\exp-\frac{\beta^2P^2}{112}\,, \tag{4.5}$$

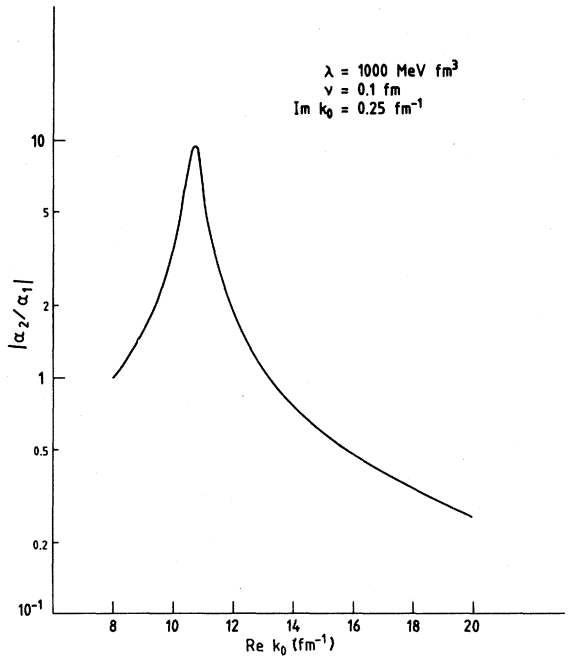

FIG. 5. Behavior of the admixture ratio of the first two variational solutions inside the third solution.

where

$$\vec{k}'_{12}=(12\vec{k}'_1-4\vec{k}'_2)/16$$

and

$$\vec{k}'_3=\vec{k}'_1+\vec{k}'_2\,.$$

Although Eqs. (4.3) and (4.5) are written in a Jacobi representation for the sake of understanding and identifying center-of-mass motions, all practical calculations have to use the single momentum representation, as provided by Eqs. (4.1) and (4.4).

Once χ and χ' have been defined, as in Eqs. (4.1) and (4.4), from products of boosted single particle orbitals or products of boosted Slater determinants, matrix elements $\langle\chi'\,|\,V'\,|\,\Phi\rangle$, $\langle\Phi'\,|\,V\,|\,\chi\rangle$, and $\langle\Phi'\,|\,(E-H)\,|\,\Phi\rangle$ are straightforward, even though sometimes tedious, to calculate if Φ' and Φ are also product-type. Let us assume, for instance, that Φ is the product $\Phi_{16}\Phi_{40}$ of two determinants, like χ, and Φ' is the product of three determinants $\Phi'_4\Phi'_{12}\Phi'_{40}$ like χ'. It must be pointed out that from their definitions, Eqs. (2.2) and (2.3), the permutation symmetries of V and V' are those of χ and χ', respec-

tively. Since H is a completely symmetric operator, one finds from Eqs. (2.7) that Φ and Φ' also have the same symmetries as χ and χ', respectively.

The situation where Φ, χ, Φ', and χ' are products of single particle orbitals or of Slater determinants then leads to standard techniques for the calculation of all matrix elements involved by the variational principle. All integrals in the many-dimensional space essentially factorize into products of single-particle overlaps, or related quantities, and at most one two-body matrix element.

It is now trivial to generalize the theory to any number of clusters in the continuum. Any isolated nucleon, for instance, will be represented by a boosted Gaussian wave packet, and so on.

V. TREATMENT OF ANTISYMMETRIZATION EFFECTS

The discussion in the preceding section dealt with the case wherein only the evaluation of the direct term was considered. In the energy range of 10 MeV $< E/A <$ 100 MeV, it is often prudent to consider antisymmetry effects, which are necessarily going to be relevant when there is an overlap of the densities of the colliding nuclei.

For a rearrangement collision of the type $a+A \rightarrow b+B$, with $a=(b+x)$ and $B=(A+x)$, if we label the nucleons in a, A, b, and B, the direct term is defined as one where the light final product b has the nucleon labels already contained in a and the target A has the nucleon labels contained in the residual nucleus B. Since the physical wave functions of the nuclei a, A, b, and B are antisymmetric with respect to the exchange of their constituent nucleons, there are

$$\begin{bmatrix} b \\ a \end{bmatrix} \begin{bmatrix} B \\ A \end{bmatrix}$$

equivalent terms contributing to the direct transition. Thus, the cross section evaluated for a given labeling, as described in Sec. IV, has to be multiplied by this number in order to obtain the total direct cross section. To be explicit, one defines the direct Born transition amplitude by

$$T_{\beta\alpha}^{B(0)}(\vec{k}_\beta,\vec{k}_\alpha)=\left[\begin{bmatrix} B \\ A \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix}\right]^{1/2} \times\left\langle \psi_b(1\cdots b)\psi_B(b+1\cdots a+1\cdots a+A)\chi_\beta \left| \sum_{i\in a}\sum_{j\in A} \mathscr{V}_{ij} \right| \psi_a(1\cdots b,b+1\cdots a) \times\psi_A(a+1\cdots a+A)\chi_\alpha \right\rangle , \quad (5.1)$$

where $\vec{k}_\alpha$ and $\vec{k}_\beta$ are the channel momenta for the initial and final relative waves χ_α, χ_β and can be used to boost Ψ_a, Ψ_A, Ψ_b, Ψ_B suitably. When the variational principle is used to calculate the correction to the Born amplitude, the same normalization factor is to be carried through. The single nucleon exchange amplitude is defined by

$$T_{\beta\alpha}^{B(1)}(\vec{k}_\beta,\vec{k}_\alpha) =\left[\begin{bmatrix} B \\ A-1 \end{bmatrix}\begin{bmatrix} a \\ b-1 \end{bmatrix}\begin{bmatrix} A \\ 1 \end{bmatrix}\begin{bmatrix} b \\ 1 \end{bmatrix}\right]^{1/2} \times\left\langle \Psi_b(1\cdots b)\Psi_B(b+1\cdots a+1\cdots a+A) \left| P_{l'k'}\sum_{i\in a}\sum_{j\in A} \mathscr{V}_{ij} \right| \Psi_a(1\cdots a)\Psi_A(a+1\cdots a+A) \right\rangle , \quad l'\in(a,b),\ k'\in(A,B) , \quad (5.2)$$

where the operator $P_{l'k'}$ exchanges the particles l' and k' with the condition that l' is a label common to b and a, and k' is a label common to A and B. The many nucleon exchange contributions are to be evaluated in a similar manner.[12] We have used the suffixes 0 and 1 for the transition amplitudes to denote the number of nucleons exchanged. The general expression for the antisymmetrized Born transition amplitude is

$$T_{\beta\alpha}^{B}(\vec{k}_\beta,\vec{k}_\alpha)=\sum_{n=0}^{b}\left[\begin{bmatrix} B \\ A-n \end{bmatrix}\begin{bmatrix} a \\ b-n \end{bmatrix}\begin{bmatrix} A \\ n \end{bmatrix}\begin{bmatrix} b \\ n \end{bmatrix}\right]^{1/2}(-)^n T_{\beta\alpha}^{B(n)}(\vec{k}_\alpha,\vec{k}_\beta) . \quad (5.3)$$

The expression retains the same form for the exact transition amplitude also. It should be noted that we have

used the prior version for the transition amplitude.[13] This is due to the fact that in an experiment the initial channel is a two body channel so that the interaction is easier to handle.

To calculate the correction to the Born amplitude, the method discussed in Sec. IV is immediately applicable to what we have termed the direct amplitude $T^{(0)}_{\beta\alpha}$ and has to be multiplied by the same normalization factor, i.e.,

$$\Delta T^{(0)}_{\beta\alpha}=\left[\begin{bmatrix}B\\A\end{bmatrix}\begin{bmatrix}a\\b\end{bmatrix}\right]^{1/2} F^{st}(\Phi',\Phi)\ . \tag{5.4}$$

It is easy to generalize this for the case of exchange amplitudes. Let us consider the single nucleon exchange amplitude. The exact single nucleon exchange amplitude is

$$T^{(1)}_{\beta\alpha}=N_1\langle\Psi_b(1\cdots b)\Psi_B(b+1\cdots a+1\cdots a+A)\left|\left[1+\left[\sum_{i\in b}\sum_{j\in B}\mathscr{V}_{ij}\right]\frac{1}{E-H}\right]\right.$$

$$\times P_{l'k'}\left[\sum_{i\in a}\sum_{j\in A}\mathscr{V}_{ij}\right]\left|\Psi_a(1\cdots a)\Psi_A(a+1\cdots a+A)\right\rangle\ ,\quad l'\in(a,b),\ \ k'\in(A,B)\ . \tag{5.5}$$

Thus the correction term is

$$\Delta T^{(1)}_{\beta\alpha}=N_1\langle\Psi_b(1\cdots b)\Psi_B(b+1\cdots a+1\cdots a+A)\left|\left[\sum_{i\in b}\sum_{j\in B}\mathscr{V}_{ij}\right]\frac{1}{E-H}\right.$$

$$\times P_{l'k'}\left[\sum_{i\in a}\sum_{j\in A}\mathscr{V}_{ij}\right]\left|\Psi_a(1\cdots a)\Psi_A(a+1\cdots a+A)\right\rangle\ ,\quad l'\in(a,b),k'\in(A,B)\ . \tag{5.6}$$

Using the shorthand notation $|\chi\rangle$ for the initial state and $\langle\chi'|$ for the final state and V and V' for the prior interaction and postinteraction, it can be seen that the functional

$$F^{(1)}(\Phi',\Phi)=\frac{\langle\Phi'|V|\chi\rangle\langle\chi'|V'P_{l'k'}|\Phi\rangle}{\langle\Phi'|(E-H)|\Phi\rangle}\ , \tag{5.7}$$

when multiplied by N_1, yields an estimate for $\Delta T^{(1)}_{\beta\alpha}$. Here we have used N_1 to represent the normalization factor

$$N_1=\left[\begin{bmatrix}B\\A-1\end{bmatrix}\begin{bmatrix}a\\b-1\end{bmatrix}\begin{bmatrix}A\\1\end{bmatrix}\begin{bmatrix}B\\1\end{bmatrix}\right]^{1/2}.$$

Thus the estimate for the total correction to the antisymmetrized transition amplitude is obtained as

$$\Delta T_{\beta\alpha}(\vec{k}_\beta,\vec{k}_\alpha)=\sum_{n=0}^{b}\left[\begin{bmatrix}B\\A-n\end{bmatrix}\begin{bmatrix}A\\n\end{bmatrix}\begin{bmatrix}a\\b-n\end{bmatrix}\begin{bmatrix}b\\n\end{bmatrix}\right]^{1/2}(-)^nF^{(n)}_{\beta\alpha}(\vec{k}_\beta,\vec{k}_\alpha)\ . \tag{5.8}$$

In a practical calculation involving heavy ions, it would in general be difficult to include all the exchange terms and a physical insight has to be used as a guide to the possible dominant exchange mechanisms. The variational principle which has just been discussed can provide such an insight in order to find dominant terms. The case of many-cluster channels goes along the same lines, in a straightforward but more tedious way.

VI. TRIAL FUNCTIONS AND REACTION MECHANISMS

It has been seen that the class of trial functions must be restricted, for obvious technical reasons, to product-type wave functions, or sums of such. This restriction does not prevent the investigation of a large body of mechanisms.

As a first example, deformed orbitals can be used for the single particle orbitals in Φ and Φ'. The

variational parameters are then trivially chosen as orientation angles or deformation parameters, not to mention cranking parameters.

As a second example, density effects can be investigated through a scaling parameter converting an orbital $\varphi(r)$ into an orbit $\varphi(\lambda r)$. A variable constraint on the mean-square radius provides a Lagrange multiplier as the variational parameter. Any constraint on any multipole can further be considered.

A third example is that of a shock-wave mechanism, although in principle it should rather occur at higher energies. Static orbits centered around the origin of the integration mesh can be boosted by a factor

$$\exp[i\vec{r}\cdot\vec{\mathscr{K}}(\vec{r})] ,$$

where the position-dependent momentum function $\vec{\mathscr{K}}(r)$ could be chosen as $\mathscr{K}_x=\mathscr{K}_y=0$ and

$$\mathscr{K}_z=\mathscr{K}\left[1+\exp\frac{-(z+\mathscr{R})^2+(tg^2\theta)(x^2+y^2)}{b^2}\right]^{-1} , \tag{6.1}$$

where $\mathscr{R}$ is the nuclear radius, hence defining the tip of the shock-wave cone at position $(0,0,-\mathscr{R})$, and θ and b are variational parameters defining the angle and thickness of the wave front, respectively.

Implosion-explosion mechanisms can be also investigated by means of radial boosting of the orbitals, the momentum function $\vec{\mathscr{K}}(\vec{r})$ being a radial vector depending only on the distance r to the mesh center.

Since combinations of mechanisms are always possible, one has to design a procedure for practical calculations. As seen in the illustrative example, Sec. III, trial functions just depending on one variational parameter, i.e., $\vec{K}$, already provide more than one stationary solution. This will occur in general every time the trial function depends nonlinearly on the parameter, even though the exact variational equations, Eqs. (2.7), are linear.

The first step of a general mechanism investigation seems therefore to select one class of trial functions for each mechanism and only one variational parameter in each class. It is indeed very impractical to search for the stationary points of the *complex* functional F, Eq. (2.6), in a parameter space of too large a dimension. This yields a set of stationary solutions $\{\Phi_n^m,\Phi_n'^m\}$ for each mechanism m. A suitable linear mixture of the Φ_n^m on one hand, and $\Phi_n'^m$ on the other hand, then provides an additional improvement of the theory. As seen from Eqs. (3.22) and (3.23), the linear combination parameters inserted in the functional G, Eq. (2.9), are defined *uniquely* by linear variational equations.

In a more general way, it might be sometimes convenient to avoid using the functional F as an optimization procedure for the basis in which Φ,Φ' will be expanded. A variational parameter such as $\vec{K}$ can be used directly as a generator coordinate, under the ansatz

$$\Phi=\int d\vec{K} f(\vec{K})\Phi_{\vec{K}} , \tag{6.2}$$

and the variational equation provided by the functional G then reads

$$\langle\Phi'_{\vec{K}'}\,|\,V\,|\,\chi\rangle-\int d\vec{K}\langle\Phi'_{\vec{K}'}\,|\,(E-H)\,|\,\Phi_{\vec{K}}\rangle f(\vec{K})=0 . \tag{6.3}$$

The other trial function Φ' obeys an analogous equation for its expansion in terms of a basis $\Phi'_{\vec{K}'}$. As discussed earlier,[14] time can be used as a special case of a generator coordinate provided by TDHF solutions.

Although the channel wave packets χ,χ' have been obtained by plane-wave boosting, one may also attempt to boost single particle orbitals in a way similar to a distorted wave formalism. The question of corrections to DWBA then arises. Consider a rearrangement collision. The distorted wave transition amplitude can be written as

$$T_{\beta\alpha}^{\mathrm{DW}}=\langle\chi_\beta^{(-)}\,|\,V_\beta\,|\,\chi_\alpha^{(+)}\rangle$$

or

$$\langle\chi_\beta^{(-)}\,|\,V_\alpha\,|\,\chi_\alpha^{(+)}\rangle .$$

One can define V_α and V_β in the projection operator formalism,[15] with P a projection operator on the elastic channel, and $Q=1-P$, as

$$V_\alpha=Q_\alpha HP_\alpha$$

and (6.4)

$$V_\beta=P_\beta HQ_\beta ,$$

if we assume that the distorting potentials used in $\chi_\alpha^{(+)},\chi_\beta^{(-)}$ are the folded potentials.

The variational principle yields a correction to the amplitude $T_{\beta\alpha}^{\mathrm{DW}}$ in the form

$$F_{\beta\alpha}=\frac{\langle\chi_\beta^{(-)}\,|\,P_\beta HQ_\beta\,|\,\Phi_\alpha\rangle\langle\Phi_\beta\,|\,Q_\alpha HP_\alpha\,|\,\chi_\alpha^{(+)}\rangle}{\langle\Phi_\beta\,|\,(E-H)\,|\,\Phi_\alpha\rangle} . \tag{6.5}$$

If, in the space (Q_α, Q_β), one introduces a basis χ_i, χ'_i, i.e.,

$$|\Phi_\alpha\rangle = \sum_i C_i^{(\alpha)} |\chi_i\rangle, \quad \langle\Phi_\beta| = \sum_i C_i^{(\beta)} \langle\chi'_i| \ , \tag{6.6}$$

one can show that the stationary value of $F_{\beta\alpha}$ for variations about the C's is

$$J_{\beta\alpha} = S'^T_\beta M^{-1} S_\alpha \ , \tag{6.7}$$

where S_α is a column vector with components

$$S_{i\alpha} = \langle\chi'_i | Q_\alpha H P_\alpha | \chi^{(+)}_\alpha\rangle \ ,$$

S^T_β is the row vector with elements

$$S'_{\beta j} = \langle\chi^{(-)}_\beta | P_\beta H Q_\beta | \chi_j\rangle \ ,$$

and M is a square matrix with elements

$$M_{ji} = \langle\chi'_j | (E - H) | \chi_i\rangle \ . \tag{6.8}$$

The method is similar to Feshbach's approach to elastic and inelastic scattering. What is worthwhile to point out is that one does not obtain any term similar to the nonorthogonality term in $J_{\beta\alpha}$.[16] This is due to the fact that the variational principle avoids using a perturbation expansion and directly tries to evaluate the representation of the total Green's function $(E-H)^{-1}$. In the particular case that we wish to consider, one explicit rearrangement channel which is coupled strongly to both the incident and exit channel, i.e., $\langle\Phi_\beta = \langle\chi_\gamma|$ and $|\Phi_\alpha\rangle = |\chi_\gamma\rangle$, we can introduce momenta $\vec{K}_\gamma$ as variational parameters and determine the best possible combinations of sets of functions

$$|\chi_\gamma(\vec{K}_{\gamma i})\rangle, i = 1 \cdots N \ ,$$

which yield a representation for $(E-H)^{-1}$. This method is equivalent to determining a "classical" path for the propagator for the intermediate state.

Alternatively, one can use the solution of the time dependent Hartree-Fock for the collision of nuclei. This method generates a single Slater determinant at each instant of time which has so far failed to yield a procedure for calculating cross sections. We can consider the TDHF solutions for a time interval $t_1 \le t \le t_2$ during which the two colliding systems are in close contact. By choosing the trial functions $|\Phi_\alpha\rangle$ and $\langle\Phi_\beta|$ to be linear superpositions of the type

$$|\Phi_\alpha\rangle = \sum_{n=1}^{N} C_n |\phi_\alpha^{\mathrm{TDHF}}(\vec{x}, t_n)\rangle \ ,$$

$$\langle\Phi_\beta| = \sum_{n=1}^{N} C'_n \langle\phi_\beta^{\mathrm{TDHF}}(\vec{x}, t_n)| \ ,$$

where we have discretized the time interval into N steps, we can again obtain expressions of the type of Eq. (6.7) for the correction to DWBA. This possibility of using Slater determinants again opens the immense possibility of studying various effects which might show up as precursors in TDHF such as the effect of shock waves, strong deformation, or large densities due to compression, on the measured transition amplitudes.

VII. DISCUSSION AND CONCLUSION

A first characteristic of this theory is the simulation of channel wave functions by wave packets. This prevents the calculation of exact on-shell amplitudes, but has the advantage of reducing all calculations to square integrable functions. As a matter of fact, the experimental energy and momentum resolutions do allow for a certain amount of averaging, and the theory is suited for that, through the calculation of off-shell amplitudes.

If the study of a narrow resonance makes it necessary to sharpen the wave packets in momentum space, a generator coordinate formalism can be used to define the channels. Distorted waves are also easy to express in this formalism. It is clear, however, that a sum or integral of factorized wave functions provides a less tractable calculation scheme than just one factorized wave packet. This subtlety does not seem to be necessary at present.

It has been seen how exchange effects can be investigated in this theory. It is remarkable that the permutational symmetry of the trial functions Φ and Φ' is identical to that of the channel functions χ and χ', respectively. Besides serving as guide for the choice of trial functions, this symmetry rule provides insight into the importance of various orders of exchange.

The theory is obviously nonperturbative. This is essentially due to the nondiagonal matrix element $\langle\Phi'|(E-H)|\Phi\rangle$, whence the variational principle derives a representation of the Green's function. Complicated rearrangement processes from χ to χ' are thus expected to be not more complicated to calculate than simpler processes.

The main feature of the theory is the possibility of making practical calculations through factorizable trial functions. Multicentered Hartree-Fock and shell model techniques are now familiar in the literature, and a large number of orbits creates only a nuisance in the calculation, not an impossibility. It has been seen how a large number of mechanisms

can be investigated with factorizable wave functions, or limited sums of such. The theory now needs to be tested against a typical fragmentation case. This is under study.

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