Variational estimate of a breakup amplitude

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Estimates of the correction to the Born amplitude are obtained from a variational principle. A wave packet representation is used to provide an off-shell amplitude in a time-independent theory of collisions. The theory is applied numerically to a breakup reaction $p + {}^3H \rightarrow p + n + d$.

[NUCLEAR REACTIONS Time independent, off-shell amplitude, obtained from variational principle. Wave packet representation generates fragmentation exclusive cross sections.]

I. INTRODUCTION

During recent years, evidence has been gathered on the importance of multistep processes in inelastic scattering as well as in multinucleon transfer reactions in the collisions of both light[1] and heavy[2] ion projectiles on target nuclei. Whereas the evaluation of higher-order processes in the case of inelastic scattering of the target can be treated reasonably well within the framework of the coupled-channel Born approximation (CCBA), the treatment of multistep processes in rearrangement collisions is much more difficult. The proper study of reactions leading to three or more body final channels is still a difficult question.[3] It has been often dealt with in an extremely approximate fashion by merely considering the phase space available for the nuclei in the final channel. The difficulty in evaluating the amplitudes for such processes arises from the problem of constructing the correct asymptotic wave functions for the final channel. In particular, the description of the propagation of even three nuclei with a given total energy is not perfectly well understood.[4]

In a series of earlier papers,[5,6] we developed a variational approach to the evaluation of multistep amplitudes. It was pointed out in these papers that a possible method which circumvents the problem of the boundary conditions to be satisfied by the propagator is to use a wave packet description all the way. The usefulness of a wave packet description has been stressed by several authors[7] for many years, but very few calculations have explicitly employed time independent wave packets for the evaluation of scattering amplitudes. In connection with the use of wave packets, one should also employ a complex total energy in the propagator, the imaginary part of which should be commensurate with the momentum spread of the wave packet. The variational method that has been proposed was shown to be surprisingly accurate in the case of an exactly solvable model of potential scattering in the previous paper.[6]

In the present work, we formulate the problem of a breakup reaction where the final channel is a three-body channel. We describe the description of the channel states in terms of *wave packets* and demonstrate how it is possible to obtain a *practical* estimate of the multistep amplitudes with a proper treatment of the many-body propagator. The problem of the construction of the correct channel wave functions which are the true eigenfunctions of the asymptotic channel Hamiltonian is then shown to be tractable by the same method after a suitable projection.

II. THE MODEL

As an application of our variational principle we consider the breakup reaction $p + {}^3H \rightarrow p + n + d$. The wave function selected to describe the initial channel is

$$\chi = \pi^{-3}\beta^{-6}\exp - \frac{(\vec{r}_1-\vec{s}_1)^2+(\vec{r}_2-\vec{s}_2)^2+(\vec{r}_3-\vec{s}_3)^2+(\vec{r}_4-\vec{s}_4)^2+(\mathrm{Im}\vec{s}_1)^2+(\mathrm{Im}\vec{s}_2)^2+(\mathrm{Im}\vec{s}_3)^2+(\mathrm{Im}\vec{s}_4)^2}{2\beta^2}, \tag{2.1}$$

where the projectile has coordinate $\vec{r}_1$ and is assumed to be a proton spin up, while the constituents of the target are assumed to be a neutron spin up, a proton spin down, and a neutron spin down, with coordinates $\vec{r}_2$, $\vec{r}_3$, and $\vec{r}_4$, respectively. This selection of spins makes the four nucleons distinct particles; hence the unessential complications of antisymmetrization can be postponed. The complex vectors $\vec{s}_1, \ldots, \vec{s}_4$ which shift the single-nucleon Gaussians present in Eq. (2.1) are chosen with components

$$\vec{s}_1 = \begin{bmatrix} 0 \\ ik\beta^2\sin\theta \\ ik\beta^2\cos\theta \end{bmatrix}, \quad \vec{s}_2 = \begin{bmatrix} 0 \\ -\frac{1}{3}ik\beta^2\sin\theta \\ d - \frac{1}{3}ik\beta^2\cos\theta \end{bmatrix}, \quad \vec{s}_3 = \begin{bmatrix} 0 \\ d\frac{\sqrt{3}}{2} - \frac{1}{3}ik\beta^2\sin\theta \\ -\frac{1}{2}d - \frac{1}{3}ik\beta^2\cos\theta \end{bmatrix}, \quad \vec{s}_4 = \begin{bmatrix} 0 \\ -d\frac{\sqrt{3}}{2} - \frac{1}{3}ik\beta^2\sin\theta \\ -\frac{1}{2}d - \frac{1}{3}ik\beta^2\cos\theta \end{bmatrix}. \tag{2.2}$$

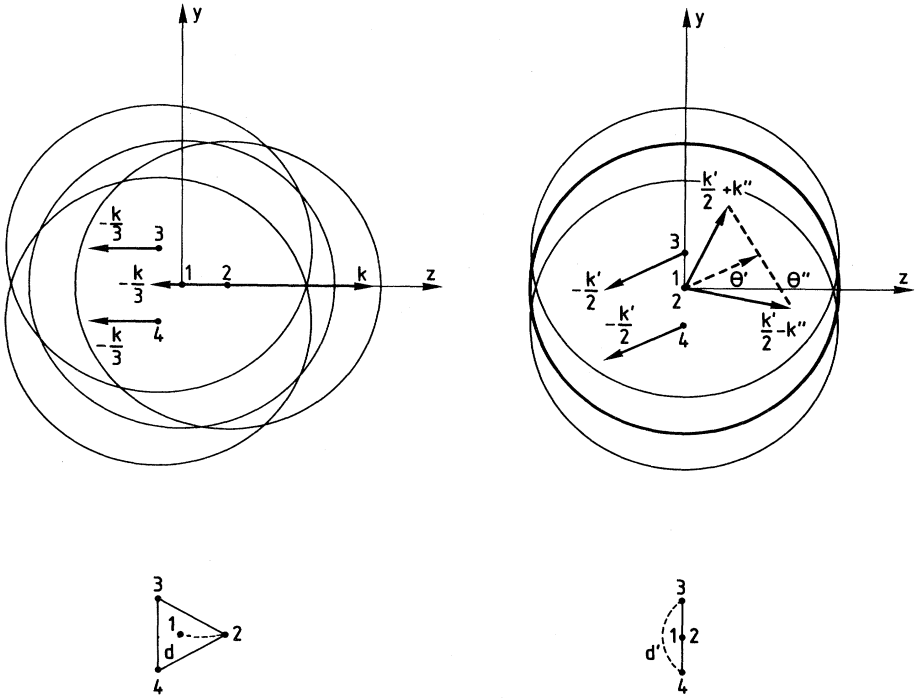

FIG. 1. Geometry of the initial (left-hand side) and final (right-hand side) wave packets. The radius of each single nucleon wave packet is scaled to show the ratio β/d or β/d'. The scales of momenta are arbitrary.

As a consequence of this choice, the projectile wave packet is boosted by an amount $\vec{k}$ and the target by the opposite momentum $-\vec{k}$. The geometry is that shown in Fig. 1, with a choice $\theta=0$ and $d\neq 0$. The reaction plane is the (y,z) plane and the triangular equilateral shape of the target is designed to prepare a forthcoming application of the model to the channel $\alpha+{}^{12}\mathrm{C}$. Nothing precludes in the following the consideration of the limit $d=0$.

With the traditional total potential

$$\mathcal{V}\equiv\sum_{i>j=1}^{4}\mathcal{V}_{ij}$$

taken as a sum of two-body interactions, the prior potential defined by this partition $1-(234)$ is, obviously,

$$V\equiv\mathcal{V}_{12}+\mathcal{V}_{13}+\mathcal{V}_{14}\,.$$

It is also obvious that χ factorizes in the representation provided by standard Jacobi coordinates, namely $\vec{R}$ for the total center of mass, $\vec{\xi}_1$ and $\vec{\xi}_2$ for the internal structure of ${}^3\mathrm{H}$, and $\vec{\rho}$ for the relative distance between p and ${}^3\mathrm{H}$. Hence,

$$\chi=\Gamma_{\mathrm{c.m.}}(\vec{R})\Gamma_{\mathrm{int}}(\vec{\xi}_1,\vec{\xi}_2)\Gamma_{\mathrm{rel}}(\vec{\rho})\exp(i\vec{k}\cdot\vec{\rho})\,, \tag{2.3}$$

where, in an obvious notation, $\Gamma_{\mathrm{c.m.}}$, Γ_{int}, and Γ_{rel} are suitably normalized Gaussians for the total center of mass, the internal structure of ${}^3\mathrm{H}$, and the channel degrees of freedom, respectively. It may be stressed at this point that this factorization is all that is needed to relate the information carried by χ to that embedded in the physically exact channel function

$$\chi^{\mathrm{ex}}=\gamma_{\mathrm{c.m.}}(\vec{R})\psi_{\mathrm{int}}(\vec{\xi}_1,\vec{\xi}_2)\exp(i\vec{k}\cdot\vec{\rho})\,, \tag{2.4}$$

where $\gamma_{\mathrm{c.m.}}$ is any center-of-mass wave function and ψ_{int} is the exact internal wave function of ${}^3\mathrm{H}$ provided by the Hamiltonian $\mathcal{H}=\mathcal{T}+\mathcal{V}$. This relation between the model wave packet χ and the physical channel function χ^{ex} will be discussed in Sec. IV.

For the final channel we choose the model wave packet

$$\chi'=\pi^{-3}\beta^{-6}\times\exp-\frac{(\vec{r}_1-\vec{s}\,'_1)^2+(\vec{r}_2-\vec{s}\,'_2)^2+(\vec{r}_3-\vec{s}\,'_3)^2+(\vec{r}_4-\vec{s}\,'_4)^2+(\mathrm{Im}\vec{s}\,'_1)^2+(\mathrm{Im}\vec{s}\,'_2)^2+(\mathrm{Im}\vec{s}\,'_3)^2+(\mathrm{Im}\vec{s}\,'_4)^2}{2\beta^2}\,, \tag{2.5}$$

where again $\vec{r}_1$, $\vec{r}_2$, $\vec{r}_3$, and $\vec{r}_4$ are the coordinates of a proton spin up, a neutron spin up, a proton spin down, and a neutron spin down, respectively. The complex shift vectors are now

$$\vec{s}\,'_1=\begin{bmatrix}0\\ i\beta^2(\frac{1}{2}k'\sin\theta'+k''\sin\theta'')\\ i\beta^2(\frac{1}{2}k'\cos\theta'+k''\cos\theta'')\end{bmatrix},$$

$$\vec{s}\,'_2=\begin{bmatrix}0\\ i\beta^2(\frac{1}{2}k'\sin\theta'-k''\sin\theta'')\\ i\beta^2(\frac{1}{2}k'\cos\theta'-k''\cos\theta'')\end{bmatrix},$$

$$\vec{s}\,'_3=\begin{bmatrix}0\\ \frac{1}{2}(d'-i\beta^2k'\sin\theta')\\ -\frac{1}{2}i\beta^2k'\cos\theta'\end{bmatrix},\qquad(2.6)$$

$$\vec{s}\,'_4=\begin{bmatrix}0\\ -\frac{1}{2}(d'+i\beta^2k'\sin\theta')\\ -\frac{1}{2}i\beta^2k'\cos\theta'\end{bmatrix},$$

inducing the geometry shown by Fig. 1. The projectile leaves with momentum $\frac{1}{2}\vec{k}\,'+\vec{k}\,''$ after knocking out the neutron spin up with momentum $\frac{1}{2}\vec{k}\,'-\vec{k}\,''$ and the deuteron spin down remains with momentum $-\vec{k}\,'$. A distance d' is taken for the deuteron extension and all the geometry has been confined to the (y,z) reaction plane. An extension of the model to an $\alpha+\alpha+{}^8$Be channel is obviously in order.

The "post" potential is now $V'=\mathscr{V}-\mathscr{V}_{34}$ and it is again trivial to check that χ factorizes as

$$\chi'=\Gamma_{\text{c.m.}}(\vec{R})\Gamma'_{\text{int}}(\vec{\xi}\,')\Gamma'_{\text{rel}}(\vec{\rho}\,')\times\exp(i\vec{k}\,'\cdot\vec{\rho}\,')\Gamma''_{\text{rel}}(\vec{\rho}\,'')\exp(i\vec{k}\,''\cdot\vec{\rho}\,''),\qquad(2.7)$$

where $\Gamma_{\text{c.m.}}$ is the same center-of-mass wave packet as in Eq. (2.3), and Γ'_{int}, Γ'_{rel}, and Γ''_{rel} are Gaussians related to the internal structure of the deuteron, and the two relative motions of the channel with

$$\vec{\rho}\,'=\tfrac{1}{2}(\vec{r}_1+\vec{r}_2-\vec{r}_3-\vec{r}_4)$$

and $\rho''=\vec{r}_1-\vec{r}_2$. The relation of χ' with

$$\chi'^{\text{ex}}=\gamma_{\text{c.m.}}(\vec{R})\psi'_{\text{int}}(\vec{\xi}\,')\exp[i(\vec{k}\,'\cdot\vec{\rho}\,'+\vec{k}\,''\cdot\vec{\rho}\,'')],\qquad(2.8)$$

where ψ'_{int} is the exact deuteron internal wave function provided by $\mathscr{H}$, will also be discussed in Sec. IV.

The operators V and V' define a T operator

$$T=V+V'(E-\mathscr{H})^{-1}V\qquad(2.9a)$$

or

$$T=V'+V'(E-\mathscr{H})^{-1}V,\qquad(2.9b)$$

depending upon the usual "prior" or "post" definition. This is a perfectly well defined operator in the Hilbert space of the present four-body problem as long as E is complex and one calculates matrix elements such as $\langle\chi'\,|\,T\,|\,\chi\rangle$ between smooth and fastly decreasing wave packets. As a matter of fact, the physical amplitude is

$$\langle\chi'^{\text{ex}}\,|\,T\,|\,\chi^{\text{ex}}\rangle,$$

where E is on shell. The quantity of interest in the present theory is the off-shell matrix element

$$\langle\chi'\,|\,T(E+i\Gamma)\,|\,\chi\rangle,$$

where the finite imaginary part Γ has been made explicit. Because of our use of wave packets the legitimate order of magnitude of Γ is automatically given by the zero point energies carried by Γ_{rel}, Γ'_{rel}, and Γ''_{rel}. With obvious notations the zero-point kinetic energy for each degree of freedom is

$$\epsilon_0=\frac{3\hbar^2}{4m\beta^2},\qquad(2.10)$$

where m is the nucleon mass.

A central, spin- and isospin-independent interaction has been chosen as the sum of a short-range repulsion and middle-range attraction, both Gaussians

$$\mathscr{V}_{ij}=v_+\exp-\frac{(\vec{r}_i-\vec{r}_j)^2}{\mu_+^2}-v_-\exp-\frac{(\vec{r}_i-\vec{r}_j)^2}{\mu_-^2}.\qquad(2.11)$$

The Hamiltonian $\mathscr{H}=\mathscr{T}+\mathscr{V}$ contains only the internal kinetic energy,

$$\mathscr{T}=\sum_{i=1}^{4}-\frac{\hbar^2}{2m}\Delta_i+\frac{\hbar^2}{8m}\Delta_{\vec{R}}.\qquad(2.12)$$

Hence the formalism is free from any center-of-mass spuriosity, as long as all wave functions which appear in the calculations factorize, like χ,χ', into the same center-of-mass wave packet $\Gamma_{\text{c.m.}}$ and an internal wave function.

For the sake of completeness it is recalled that, while the prior and post Born amplitudes

$$T_B=\langle\chi'\,|\,V\,|\,\chi\rangle\qquad(2.13a)$$

and

$$T'_B=\langle\chi'\,|\,V'\,|\,\chi\rangle,\qquad(2.13b)$$

are trivial to calculate from Eqs. (2.1), (2.5), and (2.11), the multistep amplitude

$$\Delta T=\langle\chi'\,|\,V'(E+i\Gamma-\mathscr{H})^{-1}V\,|\,\chi\rangle\qquad(2.14)$$

is here estimated as the stationary value of a functional of two trial functions ϕ and ϕ'. This functional F may be selected either as

$$F=\langle\phi'\,|\,V\,|\,\chi\rangle+\langle\chi'\,|\,V'\,|\,\phi\rangle-\langle\phi'\,|\,(E+i\Gamma-\mathscr{H})\,|\,\phi\rangle\qquad(2.15a)$$

or

$$F=\frac{\langle\phi'\,|\,V\,|\,\chi\rangle\langle\chi'\,|\,V'\,|\,\phi\rangle}{\langle\phi'\,|\,(E+i\Gamma-\mathscr{H})\,|\,\phi\rangle}.\qquad(2.15b)$$

In both possible choices for F, the variational conditions with respect to ϕ and ϕ' read

$$|\,\phi\rangle=(E+i\Gamma-\mathscr{H})^{-1}V\,|\,\chi\rangle\qquad(2.16a)$$

or

$$|\,\phi'\rangle=(E-i\Gamma-\mathscr{H})^{-1}V'\,|\,\chi'\rangle.\qquad(2.16b)$$

(In a space of restricted trial wave functions these equations must of course be projected into the subspace of allowed variation of ϕ' and ϕ, respectively.) It is clear from Eqs. (2.16) that ϕ and ϕ' will be off-shell approximations

to purely outgoing and ingoing waves, respectively. It can be stressed that ϕ and ϕ' are square integrable, like $V\chi$ and $V\chi'$. This is an obvious consequence of the choice of χ and χ' as wave packets and of a nonvanishing Γ.

In the present paper the variational parameters of ϕ and ϕ' are chosen as linear, i.e.,

$$|\phi\rangle=\sum_{n=1}^{2N}\alpha_n|\psi_n\rangle\ , \tag{2.17a}$$

$$|\phi'\rangle=\sum_{n=1}^{2N}\alpha'_n|\psi_n\rangle\ , \tag{2.17b}$$

namely an expansion basis of wave packets ψ_n is chosen. This choice of trial functions has the advantage of converting the variational principle into a straightforward linear algorithm. It can indeed be checked that the variational estimate of ΔT is then

$$\Delta T=\sum_{nn'}\langle\chi'|V'|\psi_{n'}\rangle\mathscr{G}_{n'n}\langle\psi_n|V|\chi\rangle\ , \tag{2.18}$$

where $\mathscr{G}$ is the inverse of the matrix $\mathscr{A}$ whose matrix element is

$$\mathscr{A}_{n'n}=\langle\psi_{n'}|(E+i\Gamma-\mathscr{H})|\psi_n\rangle\ . \tag{2.19}$$

Although physically less flexible than a nonlinear set of trial functions, the choice, Eq. (2.17), has the further advantage that it can incorporate the coupled-channel approximation. Indeed, in the present work, the first N functions of the basis ψ_n are just taken as wave packets similar to χ, Eq. (2.1). Instead of the physical modulus k and the physical angle $\theta=0$, running values K and θ are taken in Eq. (2.2). In the same way the last N basis vectors ψ_n have been chosen to take the form of χ', Eq. (2.5). For the sake of simplicity, $\vec{k}''$ remains fixed, and only $\vec{k}'$ is converted into a running $\vec{K}''$. The summations, Eq. (2.17), can also be interpreted as discretizations of integrals. Hence the formalism also relates to the generator coordinate method, with $\vec{K}$ and $\vec{K}'$ as generator coordinates. The nonorthogonality of the basis is known to be a minor difficulty. The numerical application which follows shows how this scheme seems to be convergent in a practical way.

III. NUMERICAL APPLICATION

A. Parameters

The single-nucleon Gaussian width is chosen as $\beta=2$ fm. This induces a momentum fluctuation $\Delta k=0.5$ fm^{-1}, hence zero-point energies of order $\epsilon_0=7.8$ MeV. This is to be compared with the Ganil energies in which we are interested, namely 10 to 80 MeV per nucleon. Hence the imaginary part of the energy has been set to the value $\Gamma=10$ MeV throughout this numerical application.

For the sake of simplicity the geometrical parameters have been taken as $d=1/\sqrt{3}$ fm and $d'=1$ fm. To show that the formalism can incorporate interactions with a non-negligible repulsion, the parameters of the force, Eq. (2.11), have been taken as

$$\begin{aligned} &v_+=350\text{ MeV},\ \mu_+=1\text{ fm},\\ &v_-=60\text{ MeV},\ \mu_-=3\text{ fm}\ . \end{aligned} \tag{3.1}$$

This induces for the "triton" described by Eq. (2.1) a self-energy

$$\epsilon_t=2\epsilon_0+3\langle v_{34}\rangle=-15.0\text{ MeV} \tag{3.2}$$

and for the "deuteron" described by Eq. (2.5) a self-energy

$$\epsilon_d=\epsilon_0+\langle v_{34}\rangle'=-2.4\text{ MeV}\ . \tag{3.3}$$

These are tolerable orders of magnitude, although Γ_{int} [see Eq. (2.3)] and Γ'_{int} [see Eq. (2.7)] obviously differ from strict eigenstates of $\mathscr{H}$. As will be seen, the prior and post Born amplitudes remain very much compatible, however. This indicates that the deviation from eigenstates is not drastic.

Finally, the relative momentum $\vec{k}''$ between the proton and neutron spin up (particles 1 and 2) in the final channel has been frozen to modulus $k''=0.5$ fm and angle $\theta''=3\pi/2$. The kinetic energy of the pair is thus

$$\epsilon_b=\hbar^2k''^2/m=10.4\text{ MeV}\ . \tag{3.4}$$

B. Rule for energy conservation

The total center of mass being subtracted, there are three zero-point kinetic energies. For the initial channel, the self-energy ϵ_t includes two of them. The third zero-point energy occurs in the channel relative motion. The energy to occur in the propagator is thus chosen as

$$E=\epsilon_t+\epsilon_0+\frac{2\hbar^2k^2}{3m}\ . \tag{3.5}$$

For the final channel, however, there are two degrees of freedom in the continuum, hence the wave packet representation introduces two zero-point energies. This problem of course disappears as $\beta\to\infty$. In the present case, as a matter of convention, we have taken only one ϵ_0 into account. Namely, energy conservation is assumed to occur if

$$E=\epsilon_d+\epsilon_b+\epsilon_0+\frac{\hbar^2k'^2}{2m}\ . \tag{3.6}$$

C. Bases

Substituting K for k in Eq. (3.5), we select for the basis of expansion (2.17) of ϕ and ϕ' in functions of the forms (2.1) and (2.5) the values $K=1$ fm^{-1}, 1.5 fm^{-1}, 2 fm^{-1}, and so on, with an increment of 0.5 fm^{-1}. The corresponding values of E are, respectively, 20.5 MeV, 55.1 MeV, 103.6 MeV, and so on. For each value of K, a value of K' is derived from Eq. (3.6) with K' substituted for k'.

As regards angles, a sequence of values $-2\pi/3$, $-\pi/2,-\pi/3,-\pi/6,0,\pi/6,\ldots,2\pi/3$ is considered for θ, then for θ'. It is expected that the mechanism of forward scattering is dominant. Hence the basis is always symmetrically centered around the values $\theta=0$ and $\theta'=0$.

Five bases have been considered to study the convergence properties and the component admixtures of ϕ and ϕ'. One of these bases corresponds, for instance, to eight energies and three angles. Namely for this (8,3) basis, θ runs from $-\pi/6$ to $\pi/6$ and K runs from 1 to 4.5 fm for the specification of ψ_n according to Eq. (2.1). Then θ' runs from $-\pi/6$ to $\pi/6$ and K' follows K by energy conservation to specify ψ_n according to Eq. (2.5). This makes

an expansion of ϕ and ϕ' into 48 components. In an obvious notation, the other bases investigated in the calculation are (15,3) (9,5), (5,9), and (9,7). In the special case of the (9,5) basis, the angular values are actually $-\pi/6$, $-\pi/12$, 0, $\pi/12$, and $\pi/6$.

D. Orthogonality defect

Table I shows a few matrix elements of the overlap matrix

$$\mathcal{N}_{n'n} \equiv \langle \psi_{n'} | \psi_n \rangle ,$$

as an illustration of the density of the basis. As soon as energies and angles carried by ψ_n and ψ'_n differ by two or three steps in the basis parameters, these vectors are practically orthogonal. In any case, as shown by Eq. (2.19), this overlap matrix enters trivially into the calculation of the Green's function.

E. Level density

The straightforward estimate of the resolvent $(E+i\Gamma-\mathscr{H})^{-1}$ which is here obtained by matrix inversion demands a justification, since the continuum has been discretized. For that purpose, the spectrum of the Hamiltonian when projected on the basis (9,7) has been calculated. It is found that about 90 eigenvalues spread between 0 and 500 MeV. Although these eigenvalues turn out to cluster rather than spread evenly with the kind of basis we used, the average level density is thus of order 1 level per 5 MeV. Since Γ has been taken of order 10 MeV, the discretization then appears to be tolerable. For a basis such as (8,3) the average level spacing is no longer smaller than Γ, and it is indeed found that convergence is not achieved. For intermediate cases like (15,3), (9,5), and (5,9) the level density seems to be just sufficient.

F. Convergence

The values obtained for ΔT, Eq. (2.18), for a typical energy $E=103.6$ MeV and three observation angles $\theta'=-\pi/6$, 0, and $\pi/6$ ($\theta=0$), are listed in Table II for the various bases considered. A tolerable level of convergence seems to be reached. It can be noticed, however, that ΔT systematically turns out to be of the same order of magnitude as the Born amplitudes and opposite in sign to them, as if, for instance, one had obtained $\phi \simeq -\chi$. This is because, insofar as

$$V|\chi\rangle \simeq (\mathscr{H}-E)|\chi\rangle , \tag{3.7}$$

then the discretization induces

$$|\phi\rangle = (E+i\Gamma-\mathscr{H})^{-1}V|\chi\rangle \simeq (E-\mathscr{H})^{-1}(\mathscr{H}-E)|\chi\rangle . \tag{3.8}$$

It will thus be of great interest in the future to investigate numerical applications with higher level densities and smaller values of Γ, so that ϕ becomes closer to an on-shell outgoing wave. Then the compensation between ΔT and the Born amplitudes will become less systematic.

G. Final results

These are shown on Fig. 2, for three energies present in our bases, namely 55.1, 103.6, and 165.9 MeV. Not

TABLE I. Overlaps and couplings of the vector of form χ with $k=2$ fm^{-1} ($E=103.6$) and $\theta=0$, with other vectors of the basis. A sequence of χ vectors is first considered, then a sequence of χ' vectors. In the χ subspace the matrix elements are either strictly real, or their imaginary parts hardly exceed 10^{-1}. All values are given in MeV, the vectors being square normalized to unity. The diagonal energy 73.0 MeV differs from the asymptotic energy 103.6 MeV because of the three additional bounds $\langle \mathscr{V}_{12}\rangle+\langle \mathscr{V}_{13}\rangle+\langle \mathscr{V}_{14}\rangle$. It is seen that the matrices of overlap and coupling are significantly decreasing away from the diagonal in the present numerical application.

	χ									χ'			
$\theta(\theta')$	$-\frac{\pi}{3}$	$-\frac{\pi}{6}$	0	$-\frac{\pi}{3}$	$-\frac{\pi}{6}$	0	$-\frac{\pi}{3}$	$-\frac{\pi}{6}$	0	0	$-\frac{\pi}{6}$	0	0
E	20.5	20.5	20.5	55.1	55.1	55.1	103.6	103.6	103.6	165.9	165.9	242	
Overlap	0.02	0.13	0.26	0.01	0.25	0.72	0.01	0.24	1.00	0.12	0.72	0.26	
										55.1	103.6	103.6	165.9
										$(4+2i)$	$(1+i)$	$(2+2i)$	$i10^{-3}$
										10^{-3}	10^{-3}	10^{-3}	
Coupling	3.2	5.7	8.7	3.2	12.5	34.1	2.5	18.0	73.0	14.3	73.8	37.9	
										5.8	18.8	3.7	1.5
										$+0.2i$	$+0.3i$	$+0.8i$	$+0.5i$

TABLE II. Numerical estimates obtained for the multistep correction amplitude ΔT when different expansion bases are considered. The asterisk for the (9,5) basis shows that an angle step of $\pi/12$ rather than $\pi/6$ has been used. The results seem to show a larger sensitivity to the number of energies included than to the number of angles. All values are listed in MeV, the wave packets being square normalized to unity. The prior and post Born amplitudes are also listed for comparison.

Basis \ Angle θ'	$-\frac{\pi}{6}$	0	$\frac{\pi}{6}$
(8,3)	$-0.92+0.98i$	$-2.41+2.03i$	$-0.85+0.92i$
(15,3)	$-1.36+0.42i$	$-3.00+1.20i$	$-1.28+0.56i$
(9,5)*	$-1.31+0.39i$	$-3.04+1.27i$	$-1.16+0.45i$
(5,9)	$-1.43+0.41i$	$-3.30+1.32i$	$-1.31+0.45i$
(9,7)	$-1.34+0.42i$	$-3.04+1.28i$	$-1.23+0.50i$
T_B	$1.56-0.21i$	$3.20-0.68i$	$1.58-0.23i$
T'_B	$1.80-0.21i$	$3.53-0.66i$	$1.65-0.21i$

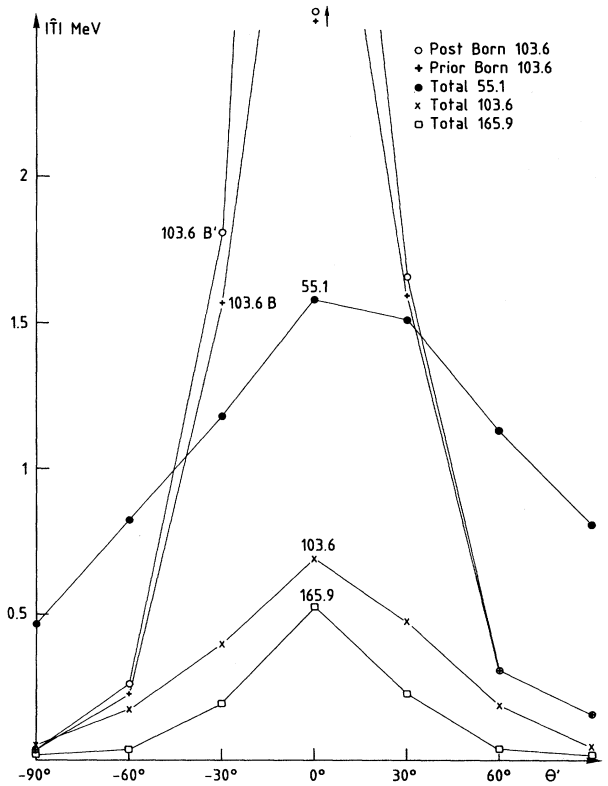

FIG. 2. Post and prior Born amplitudes for $k=2$ fm^{-1} and estimates of breakup amplitudes for $k=1.5$, 2, and 2.5 fm^{-1}. Thin lines have been drawn to guide the eye. At 0° in the recoil angle θ' the Born amplitudes are of order 3.5 and 3.2 MeV, respectively. The wave packets which simulate the channels have the geometry displayed by Fig. 1.

surprisingly, one observes a forward peaking of the amplitude, although the choice $\theta''=2\pi/3$ induces a slight left-right asymmetry. The values shown take into account an average between the post and prior Born amplitudes, namely the calculated final amplitudes are

$$\overline{T}=\tfrac{1}{2}(T_B+T'_B)+\Delta T\ . \tag{3.9}$$

For comparison the post and prior Born amplitudes at 103.6 MeV are also shown in Fig. 2. For the sake of simplicity only the modulus $|\overline{T}|$ is displayed in Fig. 2. The interested reader would be supplied upon request with the separate real and imaginary parts of the amplitudes, together with the computation code.

As the T operator, defined by Eqs. (2.9), has the same dimension as the Hamiltonian $\mathscr{H}$, the theory provides all amplitudes in MeV, since square-normalized wave packets have been used. The usual representation of amplitudes, however, makes use of plane waves of unit flux. A conversion factor is thus in order.

On one hand, in the present theory, any degree of freedom related to the continuum, see for instance $\vec{\rho}$ in Eq. (2.3), occurs with a wave packet

$$\hat{\Gamma}(\vec{\rho})=\pi^{-3/4}(\beta\sqrt{\mu})^{-3/2}\exp-\frac{\mu\rho^2}{2\beta^2}\exp(i\vec{k}\cdot\vec{\rho})\ , \tag{3.10}$$

where μ is the reduced mass number of $\vec{\rho}$.

On the other hand, the Fourier transform of $\hat{\Gamma}$ is

$$\Gamma(\vec{\sigma})=\pi^{-3/4}(\beta/\sqrt{\mu})^{3/2}\exp\left[-\frac{\beta^2(\vec{\sigma}-\vec{k})^2}{2\mu}\right]\ , \tag{3.11}$$

with $\vec{\sigma}$ the conjugate variable of $\vec{\rho}$. This is to be compared with the Fourier transform of the unit-flux plane wave

$$(2\pi)^{-3/2}\int d\vec{\rho}\exp(-i\vec{\rho}\cdot\vec{\sigma})\exp(i\vec{k}\cdot\vec{\rho})$$
$$=(2\pi)^{3/2}\delta(\vec{\sigma}-\vec{k})\ . \tag{3.12}$$

To be normalized like the δ function in Eq. (3.12), the Gaussian in Eq. (3.11) must be integrated without any squaring. It is trivial that

$$\int d\vec{\sigma} \exp -\frac{\beta^2(\vec{\sigma}-\vec{k})^2}{2\mu} = \left[\frac{2\mu\pi}{\beta^2}\right]^{3/2}, \tag{3.13}$$

hence each degree of freedom with reduced mass number μ brings the need of a multiplicative factor

$$C_\mu = \left[\frac{\pi\beta^2}{\mu}\right]^{3/4}. \tag{3.14}$$

In the present case, the conversion factor from the wave packet amplitude to the plane-wave amplitude is thus

$$C_{3/4}C_1C_{1/2} = \pi^{9/4}\beta^{9/2}(\tfrac{8}{3})^{3/4}. \tag{3.15}$$

IV. DISCUSSION AND CONCLUSION

The purpose of this paper was to illustrate the flexibility and applicability of the variational principle, Eqs. (2.15). This has been achieved by the consideration of a full-fledged four-body problem, involving a two-body initial channel and a three-body final channel. In the process, the theory has been shown to incorporate the cluster model (with nontrivial geometries), the generator coordinate method, and the coupled channel method. The distorted wave Born approximation would be a special case of the latter. An additional property of the theory is a correct treatment of center-of-mass motion when a suitable control of χ and χ' by Gaussians is implemented.

In a forthcoming paper a model of the $\alpha+{}^{12}\mathrm{C} \rightarrow \alpha+\alpha+{}^{8}\mathrm{Be}$ reaction will be considered in order to illustrate applicability of the theory to the calculation of exchange terms. It is already obvious at this stage that exchange terms, either in the internal symmetrization of a cluster or in the reaction mechanism, are made easy to calculate through the single-particle factorization of χ and χ'. This is only a slightly tedious, but straightforward extension of the theory.

Another question in order is the optimization of the expansion basis of ϕ and ϕ'. Although a definite amount of convergence was obtained in the present calculation, it must be borne in mind that this convergence is likely to be basis dependent. The basis itself can be optimized if it is included in the variational principle. This problem is now under investigation.[8]

A final question to clarify is the relation of the present time-independent wave packet theory (TIWP) with the more usual time-independent theories of nuclear collisions. The conversion factors such as described by Eq. (3.15) are only a first step for such a relation. The solution is provided by a comparison of, e.g., Eq. (2.3) with Eq. (2.4). The point is, a large number of adjustable parameters, such as θ, K, β, and d, can be introduced inside the model wave packet χ. As a matter of fact, an overcomplete basis can even be made of such TIWP. Let λ denote generically the parameter set of such a basis. It is then always possible to reconstruct the exact channel wave function χ^{ex} by an expansion

$$\chi^{\mathrm{ex}} = \int d\lambda f(\lambda)\chi_\lambda, \tag{3.16}$$

where $f(\lambda)$ is a suitable mixture coefficient. Hence a usual T-matrix amplitude would be given by the expansion

$$\langle \chi'^{\mathrm{ex}} \mid V'(E+i\Gamma-\mathscr{H})^{-1}V \mid \chi^{\mathrm{ex}}\rangle = \int d\lambda' d\lambda f'^{*}(\lambda')\langle \chi'_{\lambda'} \mid V'(E+i\Gamma-\mathscr{H})^{-1}V \mid \chi_\lambda\rangle f(\lambda), \tag{3.17}$$

where, in obvious notations, one also recognizes a reconstruction of the exact final channel wave function χ'^{ex}.

When sharp resonances are not investigated a finite value of Γ can be retained. In the present paper, only qualitative estimates of amplitudes were looked for. Hence a reconstruction of χ^{ex} and χ'^{ex} is not needed. It is much easier to take advantage of the fact that χ and χ^{ex}, for instance, have an identical factorization scheme; see Eqs. (2.3) and (2.4). The free parameters β and d, for instance, could be adjusted to make $\Gamma_{\mathrm{int}}(\vec{\xi}_1, \vec{\xi}_2)$ as close as possible to the true eigenstate $\psi_{\mathrm{int}}(\vec{\xi}_1, \vec{\xi}_2)$.

In conclusion, a systematic simulation of channel wave functions by time-independent wave packets reduces the calculation of exclusive amplitudes to the techniques of the microscopic theory of bound states.

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