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Variational principles for exclusive and inclusive cross sections

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Density matrices and dyadic operators are systematically introduced in the definition of a T-matrix element and the square modulus of that element. This use of the density matrices and dyadic operators provides two new variational functionals in addition to the Kohn-Schwinger type functional. An equivalence between the evaluation of the inverse of an operator and a diagonalization procedure for practical calculations is also established.

The boosted shell-model (BSM) theory of collisions that has been recently proposed is based on two main ingredients, namely (i) a time-independent wave packet representation[1] of the T matrix, and (ii) a variational principle for the evaluation of each individual element[2] of the T matrix in that representation. Another approach to the practical evaluation of the transition amplitudes can be based on time-dependent theories and a recent variational principle of Balian and Veneroni[3] stresses the usefulness of the density matrix in such a theory. Besides, it focuses on the calculation of the square modulus of the transition amplitude whereas our approach[2] deals with the amplitude itself (more precisely, it deals with the correction to the Born amplitude). The purpose of this paper is to show how the BSM theory can be reformulated in terms of density matrices and dyadic operators. Besides leading to new schemes of approximation in practical calculations, this reformulation generalizes the BSM theory from exclusive cross sections to one for inclusive cross sections. Finally, this formalism may be useful in providing the connection between time-dependent and time-independent theories[4] as well as the relation to intermediate, Wigner type representations[5] thus opening the way to a systematic semiclassical description of the reaction mechanisms.

The system under consideration is a N-particle system (actually pion absorption and emission can be included in a further generalization of the BSM theory[6]) with a Hamiltonian $\mathscr{H}=\mathscr{T}+\mathscr{V}=\sum_i \mathscr{T}_i-\mathscr{T}_{\text{c.m.}}+\sum_{i>j}V_{ij}$, in obvious notations. As shown earlier,[7] antisymmetrization of the theory is straightforward and will not be explicitly treated here. Each partition of the N-particle system defines a post (prior) potential $V'(V)$.

For example, if the final channel is composed of three fragments, B', B'', and B''' with respective center-of-mass momenta $\vec{k}'$, $\vec{k}''$, and $\vec{k}'''$, the corresponding channel wave function in wave packet representation will be defined by

$$\begin{aligned}\chi'_{\vec{k}'\vec{k}''\vec{k}'''}(\vec{r}_1\cdots\vec{r}_N)=&\exp\left[i\vec{k}'\cdot\frac{(\vec{r}_1+\cdots+\vec{r}_{B'})}{B'}\right]\psi_{B'}(\vec{r}_1,\ldots,\vec{r}_{B'})\\&\times\exp\left[i\vec{k}''\cdot\frac{(\vec{r}_{B'+1}+\cdots+\vec{r}_{B'+B''})}{B''}\right]\psi_{B''}(\vec{r}_{B'+1},\ldots,\vec{r}_{B'+B''})\\&\times\exp\left[i\vec{k}'''\cdot\frac{(\vec{r}_{B'+B''+1}+\cdots+\vec{r}_N)}{B'''}\right]\psi_{B'''}(\vec{r}_{B'+B''+1},\ldots,\vec{r}_N)\ ,\end{aligned}\tag{1}$$

where $\psi_{B'}$, $\psi_{B''}$, and $\psi_{B'''}$ are the usual shell-model wave functions and $\vec{r}_1,\ldots,\vec{r}_N$ are the single particle coordinates. The description of the initial channel or any other two body channel is trivially analogous to Eq. (1). The calculation of the off-shell amplitude

$$T=\langle\chi'|[V+V'(E-\mathscr{H})^{-1}V]|\chi\rangle\ ,\tag{2}$$

where $\text{Im}E=\Gamma>0$, is thus a generalization of standard shell-model calculations. The one nontrivial step of the calculation is the multistep amplitude $\Delta T=\langle\chi'|V'GV|\chi\rangle$, with $G=(E-\mathscr{H})^{-1}$. As discussed elsewhere,[1,2,7] ΔT can be estimated as the stationary value of either of the functionals

$$F=\langle\chi'|V'|\phi\rangle+\langle\phi'|V|\chi\rangle-\langle\phi'|(E-\mathscr{H})|\phi\rangle\ ,\tag{3}$$

or

$$F_1=\frac{\langle\chi'|V'|\phi\rangle\langle\phi'|V|\chi\rangle}{\langle\phi'|(E-\mathscr{H})|\phi\rangle}\ ,\tag{4}$$

where ϕ and ϕ' are trial functions. In what follows, we shall use the abbreviations

$$\sigma=V|\chi\rangle\langle\chi|V\ ,$$
$$\sigma'=V'|\chi'\rangle\langle\chi'|V'\ ,$$
$$\hat{\sigma}=V|\chi\rangle\langle\chi'|V'\ ,$$

and define the density operators $\rho=|\phi\rangle\langle\phi|$, $\rho'=|\phi'\rangle\langle\phi'|$ and $\hat{\rho}=|\phi\rangle\langle\phi'|$.

The functional F_1, Eq. (4), can be reexpressed as

$$F_1=\frac{\text{Tr}\hat{\rho}\hat{\sigma}}{\text{Tr}\hat{\rho}(E-\mathscr{H})}\ ,\tag{5}$$

with the constraint

$$\hat{\rho}^2=\hat{\rho}\,\text{Tr}\hat{\rho}\ ,\tag{6}$$

where Tr is the symbol of trace. The constraint, Eq. (6), is necessary to ensure that $\hat{\rho}$ is a dyadic operator. It thus allows us to consider the functional of a trial operator,

$$F_2 = \mathrm{Tr}\hat{\rho}\hat{\sigma} - f\,\mathrm{Tr}\hat{\rho}(E-\mathscr{H}) - \mathrm{Tr}\Lambda(\hat{\rho}^2 - \hat{\rho}t) \ , \tag{7}$$

where f and t are two C-number Lagrange multipliers and Λ is an operator Lagrange multiplier. The stationarity condition of F_2 with respect to $\hat{\rho}$ reads

$$\hat{\sigma} - f(E-\mathscr{H}) - \Lambda\hat{\rho} - \hat{\rho}\Lambda + \Lambda t = 0 \ , \tag{8}$$

which has the form of a set of linear, nonhomogeneous equations for the matrix elements of $\hat{\rho}$ and Λ. Depending upon the choice of the trial operators $\hat{\rho}$, a large class of models is thus available. Once $\hat{\rho}$ has been determined as a function of Λ from Eq. (8), the parameters f and t have to be adjusted self-consistently so that they satisfy $f = F_1$ and $t = \mathrm{Tr}\hat{\rho}$, respectively. Finally Λ has to be adjusted to satisfy Eq. (6) as well as possible.

To summarize this section, the amplitude ΔT is obtained as the stationary value of a functional of a trial operator $\hat{\rho}$ which takes into account the two trial functions $|\phi\rangle$ and $|\phi'\rangle$ considered in Eqs. (3) and (4). It may be worth remarking that F_1 becomes equal to ΔT, Eq. (4), as soon as the stationarity with respect to $|\phi\rangle$ alone, or $|\phi'\rangle$ alone, is reached. Thus, a special problem of interest in the future will be the behavior of F_2, Eq. (7), and of Eq. (8), when $\hat{\rho} = GV|\chi\rangle\langle\phi'|$ or $\hat{\rho} = |\phi\rangle\langle\chi'|V'G$.

The square modulus of ΔT can be expressed in terms of σ and σ' as

$$|\Delta T|^2 = \mathrm{Tr}G\sigma G^{\dagger}\sigma' \ , \tag{9}$$

with the same notations. It is trivial to verify that the functional of two trial density operators ρ and ρ',

$$F_3 = \mathrm{Tr}\sigma'\rho + \mathrm{Tr}\rho'\sigma + \mathrm{Tr}(E^* - \mathscr{H})\rho'(E-\mathscr{H})\rho \ , \tag{10}$$

becomes equal to $|\Delta T|^2$ when stationarity with respect to ρ and ρ' is reached. This is not subject to the constraints such as $\rho = \rho^{\dagger}$ and $\rho^2 = \rho\,\mathrm{Tr}\rho$ as can be seen by considering the derivative of F_3 with respect to ρ',

$$0 = \frac{\delta F_3}{\delta\rho'} = \tilde{\sigma} - (E^* - \tilde{\mathscr{H}})\tilde{\rho}(E - \tilde{\mathscr{H}}) \ , \tag{11}$$

where the tilde $\sim$ represents transposition. Equation (11) is the same as

$$\rho = G\sigma G^{\dagger} = GV|\chi\rangle\langle\chi|VG^{\dagger} \ , \tag{12}$$

which is automatically a diagonal dyadic operator. Similarly, the stationarity of F_3 with respect to ρ leads to $\rho' = G^{\dagger}\sigma' G$ which is a diagonal dyadic operator as well.

It should be pointed out that the above variational formalism for the square modulus is not restricted to exclusive reactions. This is because σ and σ' in Eqs. (9) and (10) can be generalized into measure operators for inclusive reactions. Indeed, as can be seen from Eq. (1), a dyadic $\sigma' = V'|\chi'\rangle\langle\chi'|V'$ carries labels $\vec{k}'$, $\vec{k}''$, ... and so on. An integration over a part of these variables, properly weighted for energy and momentum conservation, defines an inclusive measure. For instance, one could define in a three fragment case, the "inclusive density operator"

$$\bar{\sigma}'(\vec{k}') = \int d\vec{k}''d\vec{k}'''\delta(\vec{k}'+\vec{k}''+\vec{k}''')\delta\left(E - \frac{k'^2}{2mB'} - \frac{k''^2}{2mB''} - \frac{k'''^2}{2mB'''}\right) V'|\chi'_{\vec{k}'\vec{k}''\vec{k}'''}\rangle\langle\chi'_{\vec{k}'\vec{k}''\vec{k}'''}|V' \ . \tag{13}$$

It is thus obvious that $\bar{\sigma}'$ can be substituted for σ' in Eqs. (9) and (10) and that F_3 remains a variational functional for the corresponding inclusive $|\Delta T|^2$. Any other definition of $\bar{\sigma}'$ by improvements or generalizations of Eq. (13) will retain the same relationship between Eqs. (9) and (10).

The same argument can be applied to the cross terms which express the interference between the Born amplitude and ΔT. Consider for instance

$$I = \langle\chi|V'|\chi'\rangle\langle\chi'|V'GV|\chi\rangle = \mathrm{Tr}V|\chi\rangle\langle\chi|\sigma'G \ . \tag{14}$$

It can be shown that it is the stationary value of the functional

$$F_4 = \mathrm{Tr}\sigma'\rho + \mathrm{Tr}V|\chi\rangle\langle\chi|\rho' - \mathrm{Tr}\rho'(E-\mathscr{H})\rho \ . \tag{15}$$

One of the variational functionals to estimate the multistep amplitude ΔT was of the form [Eq. (4)]

$$F_1 = \frac{\langle\chi'|V'|\phi\rangle\langle\phi'|V|\chi\rangle}{\langle\phi'|(E-\mathscr{H})|\phi\rangle|} \ . \tag{16}$$

At the stationary value of the functional, one can rewrite Eq. (16) as

$$\langle\phi'|[(E-\mathscr{H}) - f^{-1}V|\chi\rangle\langle\chi'|V']|\phi\rangle = 0 \ . \tag{17}$$

If, in Eq. (17), the stationary value f^{-1} of F_1^{-1} was used, it is valid for arbitrary variation of ϕ'. Hence, one can consider the following "eigenvalue equation,"

$$[E - \mathscr{H} - f^{-1}V|\chi\rangle\langle\chi'|V']|\phi\rangle = 0 \ . \tag{18}$$

For a given value of f, one can determine a (complex) eigenvalue E and an eigenstate $|\phi\rangle$. If the normalization of $|\phi\rangle$ is chosen such that

$$f^{-1}\langle\chi'|V'|\phi\rangle = 1 \ , \tag{19}$$

Eq. (18) is equivalent to

$$(E-\mathscr{H})|\phi\rangle = V|\chi\rangle \ , \tag{20}$$

i.e., $|\phi\rangle$ is the difference of the exact off-shell wave function at energy E and the Born term $|\chi\rangle$. If one uses Eq. (18), with the normalization constraint (19), one can consider the energy E as the stationary value of the functional

$$J = \frac{\langle\phi'|[\mathscr{H} + f^{-1}V|\chi\rangle\langle\chi'|V']|\phi\rangle}{\langle\phi'|\phi\rangle} \ . \tag{21}$$

Equation (21) has the form of a generalized Ritz variational principle for off-diagonal matrix elements. The energy E and the "correction amplitude" f are conjugate quantities which are derivable from the same variational principle. It can be seen that f is a function of the energy E, Eq. (4), and E is a function of f, Eq. (21), and only if the stationary value of F_1 in Eq. (4) is used in Eq. (21) will one obtain the correct energy E.

As it has just been established, $|\phi\rangle$ and $\langle\phi'|$ are, respectively, right and left eigenstates at eigenvalue E of the operator $\mathscr{H} + f^{-1}\hat{\sigma}$, a non-Hermitian operator indeed. In order to bring the theory closer to the hermiticity of the Bloch theory of collisions,[8] it is tempting to convert the dyadic "source operator" $\hat{\sigma}$ into a Hermitian operator. This can be achieved as follows.

Let Σ be the generalization of $\hat{\sigma}$ defined by

$$\Sigma = (V|\chi\rangle + \alpha V'|\chi'\rangle)(\langle\chi|V + \alpha^*\langle\chi'|V') , \tag{22}$$

with four independent values of α, for instance 0, 1, 50, and $-i$. Then the replacement of $\hat{\sigma}$ by Σ in Eq. (5) defines a variational principle for a linear combination of the four amplitudes $\langle\chi|VGV|\chi\rangle$, $\langle\chi'|V'GV|\chi\rangle$, $\langle\chi|VGV'|\chi'\rangle$, and $\langle\chi'|V'GV'|\chi'\rangle$. Each individual amplitude can be later recovered by suitable admixtures of the results obtained for those independent values of α considered above.

A first property of this symmetrized variational principle is that, insofar as the wave packets $|\chi\rangle$ and $|\chi'\rangle$ are close to channel wave functions, then

$$V|\chi\rangle + \alpha V'|\chi'\rangle \simeq (\mathscr{H} - \mathrm{Re}E)(|\chi\rangle + \alpha|\chi'\rangle) , \tag{23}$$

hence one formulates the theory in terms of *forward elastic* amplitudes only for the "double channel" $|\chi\rangle + \alpha|\chi'\rangle$. Another property is that $|\phi\rangle$ and $|\phi'\rangle$ are now eigenstates of $\mathscr{H} + f^{-1}\Sigma$, whose nonhermiticity is now carried by just the complex amplitude f^{-1}. It can be checked finally that, in case practical calculations are performed in a representation where $\mathscr{H}$ and $|\gamma\rangle = V|\chi\rangle + \alpha V'|\chi'\rangle$ are real, then $|\phi\rangle$ and $|\phi'\rangle$ are just complex conjugates, hence the Euclidean functionals

$$F_5 = (\gamma|\phi) + (\phi|\gamma) - (\phi|(E-\mathscr{H})|\phi) , \tag{24}$$

$$F_6 = \frac{(\gamma|\phi)(\phi|\gamma)}{(\phi|(E-\mathscr{H})|\phi)} , \tag{25}$$

$$F_7 = \frac{(\phi|[\mathscr{H} + f^{-1}|\gamma)(\gamma|]|\phi)}{(\phi|\phi)} , \tag{26}$$

and so on, where the round bracket $(|)$ now denotes the Euclidean scalar product already familiar in Kohn-type variational principles. It may be stressed, however, that ϕ remains square integrable, both in the Hermitian and the Euclidean metrics.

Although the replacement of the perturbation $\hat{\sigma}$ of $\mathscr{H}$ by Σ increased the apparent rank of that perturbation from 1 to 4, this symmetrization seems therefore to show significant advantages. Generalizations of optical theorems might be in order, and also a complete hermitization of the theory should be investigated, for ϕ and ϕ' are square integrable eigenstates of $\mathscr{H} + f^{-1}\Sigma$ (we notice, however, that they become purely outgoing and ingoing waves when E becomes real and relations with the approach of Hahn[9] are likely).

Two classes of results have been found in this paper. The first one is the set of functionals F_2, F_3, and so on. Their flexibility is somewhat remarkable since they generalize the theory to (i) a very large class of trial density matrices, (ii) the calculation of inclusive processes, and finally, (iii) a highly symmetrized and Euclidean formalism. More important might be the second class of results, whereby the complex energy and the amplitude have been found to behave like dual quantities. The latter enters the definition of an auxiliary Hamiltonian, the former is the physically relevant eigenvalue, and the corresponding eigenfunction is *square integrable*. This relation between the transition amplitude and the energy has thus transformed the usual continuum formulation of scattering into one of a discrete quantization, Eq. (18).

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