

## Antisymmetrization of a mean-field theory of collisions

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For a system of  $N$  fermions with Hamiltonian  $\mathcal{H}$  we evaluate matrix elements of the  $T$  matrix between arbitrary Slater determinants  $|\chi\rangle, |\chi'\rangle$ . The resulting variational equations are driven Hartree-Fock-like equations, with source terms as right-hand sides, due to the "channels"  $|\chi\rangle, |\chi'\rangle$ . The validity of this mean-field approximation is illustrated by a numerical example.

### I. INTRODUCTION

The time-independent mean-field description of collisions which was introduced in an earlier paper<sup>1</sup> suffers from a defect common to many theories of collisions, namely a non-natural description of identical particles. This is of course due to the physical reason that, contrary to the Hartree-Fock description of bound states where all degrees of freedom play an identical role, in the case of scattering states the relative-motion degrees of freedom in the initial and final channels determine the available energy and play a role *a priori* different from the other degrees of freedom. Hence the  $T$  matrix is more often defined in terms of prior and post potential operators  $V$  and  $V'$ , respectively,

$$T_{\text{prior}} = V + V'GV, \tag{1.1a}$$

$$T_{\text{post}} = V' + V'GV, \tag{1.1b}$$

while the Green's function  $G \equiv (W - \mathcal{H})^{-1}$ , where  $W$  is a complex energy which is eventually allowed to become the on-shell energy, does retain the full symmetry of the Hamiltonian.

The restoration of the Pauli principle *a posteriori* is a straightforward although slightly tedious problem. Many solutions of this problem are known.<sup>2</sup> All told, the reconstruction of a symmetric collision amplitude as a weighted sum of exchange amplitudes is an interesting description of the reaction mechanism in terms of a hierarchy of exchanges in an increasing order. For practical purposes, however, an *a priori* symmetrized theory, which immediately provides the symmetrized amplitude, is preferable. The present paper proposes a mean-field approximation for a variational estimate of this symmetrized amplitude.

For this purpose we redefine the  $T$  matrix, or rather the  $T$  operator, in a manner similar to that considered in an earlier version of our theory;<sup>3</sup> namely, we set

$$T(E', W, E) \equiv (\overleftarrow{\mathcal{H}} - \overleftarrow{E}) + (\overleftarrow{\mathcal{H}} - \overleftarrow{E}') (W - \mathcal{H})^{-1} (\overrightarrow{\mathcal{H}} - \overrightarrow{E}), \tag{1.2}$$

where the arrows specify that  $(\mathcal{H} - E)$  and  $(\mathcal{H} - E')$

should act on the ket and bra, respectively, *before* any action of the Green's function  $G$ . Although  $E'$ ,  $W$ , and  $E$  could be considered as independent energies it is sufficient for practical purposes in the following to set  $E' = E = \text{Re}W$ , and keep  $\text{Im}W$  as finite before becoming infinitesimal at the end. The first term in the right-hand side of Eq. (1.2) being obviously related to the first Born amplitude, we concentrate in the following on the calculation of

$$\mathcal{D} \equiv \langle \chi' | (\mathcal{H} - E)G(\mathcal{H} - E) | \chi \rangle, \tag{1.3}$$

where  $|\chi\rangle$  and  $|\chi'\rangle$  are *any* square-integrable Slater determinants for  $N$  fermions.

The reasons why we set  $\chi, \chi'$  to be any square-integrable Slater determinants are obvious. On the one hand, only antisymmetric operators and wave functions appear in Eq. (1.3). On the other hand, any antisymmetrized wave function, such as the channel wave functions  $\psi, \psi'$  which are familiar in the generator coordinate theory of collisions,<sup>4</sup> can be expanded in Slater determinants  $\chi, \chi'$ . For the sake of clarity we recall that the generator coordinate theory of collisions first considers the antisymmetrized product  $\chi_0$  of projectile and target static wave functions,  $\chi^a$  and  $\chi^A$ , respectively, which are Slater determinants or simple mixtures of such,

$$\chi_0 = \mathcal{A} \chi^a(\mathbf{q}_1, \dots, \mathbf{q}_a) \chi^A(\mathbf{q}_{a+1}, \dots, \mathbf{q}_{a+A}),$$

where  $\mathcal{A}$  is the antisymmetrizer and  $\mathbf{q}_1, \dots, \mathbf{q}_a$  and  $\mathbf{q}_{a+1}, \dots, \mathbf{q}_{a+A}$  are the single-particle momenta of the projectile and target constituents, respectively. Opposite boosts are then applied to the projectile and target, generating the wave function

$$\chi_{\mathbf{k}} = \mathcal{A} \chi^a \left[ \mathbf{q}_1 - \frac{1}{a} \mathbf{k}, \dots, \mathbf{q}_a - \frac{1}{a} \mathbf{k} \right] \times \chi^A \left[ \mathbf{q}_{a+1} + \frac{1}{A} \mathbf{k}, \dots, \mathbf{q}_{a+A} + \frac{1}{A} \mathbf{k} \right],$$

where it should be stressed that the shell-model and configuration-mixing structures of  $\chi^a, \chi^A$  are not perturbed by the boosts, while only the relative motion of the

centers of mass of  $a, A$  has acquired an *average* momentum  $\mathbf{k}$  (the "generator coordinate"). This average momentum can be converted into a strict momentum  $\mathbf{K}$  via an integral

$$\psi = \int d\mathbf{k} f_{\mathbf{K}}(\mathbf{k}) \chi_{\mathbf{k}},$$

a suitable integration weight  $f_{\mathbf{K}}(\mathbf{k})$  removing the fluctuations of the relative momentum about its average value  $\mathbf{k}$ , thus converting the wave packet  $\chi_{\mathbf{k}}$  into a plane wave  $\psi$  with pure momentum  $\mathbf{K}$ . Each partition considered inside antisymmetric  $\psi, \psi'$  defines the corresponding prior or post potential  $V$  or  $V'$ , respectively, hence  $(\mathcal{H} - \bar{E})$  and  $(\mathcal{H}' - \bar{E}')$  reduce to  $V$  and  $V'$  accordingly. The complete amplitude obtained by collecting all terms is the symmetrized, physical amplitude. As  $\psi$  and  $\psi'$  are expanded in integrals or sums of  $\chi$  and  $\chi'$ , respectively, the generic calculation of  $\mathcal{D}$ , Eq. (1.3), is indeed the central problem of the theory.

There is more to  $\mathcal{D}$ , Eq. (1.3), than just one contribution to a generator coordinate expansion of  $\langle \psi' | (\mathcal{H} - E) G (\mathcal{H} - E) | \psi \rangle$ . As a matter of fact these boosted wave packets, Slater determinants used as initial and final conditions to the time-dependent Hartree-Fock<sup>5</sup> description of collisions, are excellent approximations to channel wave functions  $\psi, \psi'$ . Indeed, as can be seen from the definitions of  $\chi_0$  and  $\chi_{\mathbf{k}}$  in the preceding paragraph, the centers of mass of  $a$  and  $A$  show only zero-point fluctuations about their shell-model centers; hence the integration with weight  $f_{\mathbf{K}}(\mathbf{k})$ , which is used to remove these fluctuations, can be omitted in those cases where the scale of these fluctuations is small compared to the mean value  $\mathbf{k}$  and expected pure value  $\mathbf{K}$ . Hence  $\mathcal{D}$  alone already gives an estimate of a physical collision amplitude.

As discussed earlier<sup>6</sup> a variational functional which provides  $\mathcal{D}$  is

$$F(\phi', \phi) \equiv \frac{\langle \phi' | (\mathcal{H} - E) | \chi \rangle \langle \chi' | (\mathcal{H} - E) | \phi \rangle}{\langle \phi' | (W - \mathcal{H}) | \phi \rangle}, \quad (1.4)$$

where  $\phi, \phi'$  are square-integrable, (anti)symmetrized trial functions. The trial functions  $\phi, \phi'$  should *a priori* be varied throughout the whole Hilbert space in order to generate the stationarity of  $F$ , but in practice they will be specialized to a restricted class of variational parameters only. The present paper sets  $\phi, \phi'$  to be Slater determinants, like  $\chi, \chi'$ . Variation of single-particle orbitals is thus the flexibility to which  $\phi, \phi'$  are restricted. The resulting variational equations are the subject of Sec. II. In Sec. III these equations are solved, and their estimate  $\mathcal{D}$  of an exact amplitude  $\mathcal{D}$  is tested in the case of an elementary two-fermion problem with a separable force. We include a discussion and conclusion in Sec. IV.

## II. VARIATIONAL EQUATIONS

We denote by  $\chi_i, \chi'_i$ , and  $\varphi_i, \varphi'_i$  the single-particle orbits which constitute  $\chi, \chi'$  and  $\phi, \phi'$ , respectively. These orbits need not *a priori* be orthonormal in any way, nor could they be in general, for these determinants are four independent determinants. Because of this lack of ortho-

normality we will need the overlap matrices  $\alpha, \alpha', \beta$  defined by

$$\alpha_{ij} = \langle \varphi'_i | \chi_j \rangle, \quad (2.1a)$$

$$\alpha'_{ij} = \langle \chi'_i | \varphi_j \rangle, \quad (2.1b)$$

$$\beta_{ij} = \langle \varphi'_i | \varphi_j \rangle. \quad (2.1c)$$

We will also need the inverse matrices

$$A = \alpha^{-1}, \quad A' = \alpha'^{-1}, \quad B = \beta^{-1}, \quad (2.2)$$

which are essential for the calculation of the cofactors of the determinants of  $\alpha, \alpha', \beta$ . For instance, the cofactor  $M_{ij}$  which corresponds to the removal of row  $i$  and column  $j$  from  $\alpha$  is

$$M_{ij} = \langle \phi' | \chi \rangle A_{ji}. \quad (2.3a)$$

The double cofactor  $M'_{ijkl}$  which corresponds first to the removal from  $\alpha'$  of row  $i$  and column  $k$  then row  $j$  and column  $l$  in that order is

$$\begin{aligned} M'_{ijkl} &= \langle \chi' | \phi \rangle (A'_{ki} A'_{lj} - A'_{kj} A'_{li}) \\ &= \langle \chi' | \phi \rangle^{-1} (M'_{ik} M'_{jl} - M'_{il} M'_{jk}). \end{aligned} \quad (2.3b)$$

The triple cofactor  $N_{ijknml}$  is defined, in obvious notation, as

$$\begin{aligned} N_{ijknml} &= \langle \phi' | \phi \rangle^{-2} [N_{il} (N_{jm} N_{kn} - N_{jn} N_{km}) \\ &\quad - N_{im} (N_{jl} N_{kn} - N_{jn} N_{kl}) \\ &\quad + N_{in} (N_{jl} N_{km} - N_{jm} N_{kl})]. \end{aligned} \quad (2.3c)$$

It is clear that these cofactors could be defined as one, two, or three-particle-hole matrix elements, at the cost of four different sets of creation and annihilation operators for the four different sets of orbitals. It is also clear that the expansion of any cofactor, including those of order zero, into any of its row or column cofactors of the next order provides the derivatives

$$\frac{\partial}{\partial \langle \varphi'_i | \varphi_j \rangle} \langle \phi' | \phi \rangle = N_{ij}, \quad (2.4a)$$

$$\frac{\partial}{\partial \langle \chi'_i | \varphi_j \rangle} M'_{kl} = M'_{kijl}, \quad (2.4b)$$

$$\frac{\partial}{\partial \langle \varphi'_i | \chi_j \rangle} M_{klmn} = M_{klijnm}, \quad (2.4c)$$

and all the other, analogous derivatives.

It must now be stressed that inspection of  $F$ , Eq. (1.4) shows that  $F$  does not depend on the norms and phases of  $\phi, \phi'$ . Since furthermore  $\phi$  is a Slater determinant, any linear rearrangement of the orbitals  $\varphi_i$  among themselves leaves  $F$  invariant. The same holds for linear rearrangements of orbitals  $\varphi'_i$  among themselves. This gauge invariance of  $F$  allows an arbitrary choice of two among the three matrices of scalar products  $\alpha, \alpha', \beta$  defined by Eq. (2.1). Actually any matrix  $\gamma$  of a nondegenerate one-body operator  $\mathcal{C}$  between  $\varphi'_i$  and  $\varphi_j$  could play the role of  $\alpha, \alpha', \beta$ .

Hence in the following we could consider among others

an auxiliary functional, made out of  $F$ , and an auxiliary operator  $\mathcal{C}$  to be defined later:

$$G = F - \sum_{i,j} \lambda_{ij} \langle \varphi'_i | \varphi_j \rangle - \sum_{i,j} \mu_{ij} \langle \varphi'_i | \mathcal{C} | \varphi_j \rangle \\ = \frac{CC'}{D} - \text{Tr} \lambda \tilde{\beta} - \text{Tr} \mu \tilde{\gamma}, \quad (2.5)$$

where in obvious notation  $C = \langle \phi' | (\mathcal{H} - E) | \chi \rangle$  and so on for  $C'$  and  $D$ . But it is as simple to just consider  $F$  and make it stationary, keeping in mind the fact that many equivalent sets of orbitals  $\{\varphi'_i, \varphi_j\}$  give the same result.

The values of  $C$ ,  $C'$ , and  $D$  are easy to obtain when  $\mathcal{H}$  is, as usual, the sum of a one-body and a two-body operator:

$$\mathcal{H} = \sum_{i=1}^N t_i + \sum_{\substack{i,j \\ (i>j)}} v_{ij}, \quad (2.6)$$

where  $t$  and  $v$  can accommodate center-of-mass corrections if necessary. One finds

$$C = -E \det \alpha + \sum_{k,l} \langle \varphi'_k | t | \chi_l \rangle M_{kl} \\ + \frac{1}{4} \sum_{k,l,n,m} \langle \varphi'_k \varphi'_l | v | \chi_m \chi_n \rangle M_{klmn}, \quad (2.7a)$$

$$C' = -E \det \alpha' + \sum_{k,l} \langle \chi'_k | t | \varphi_l \rangle M'_{kl} \\ + \frac{1}{4} \sum_{k,l,n,m} \langle \chi'_k \chi'_l | v | \varphi_m \varphi_n \rangle M'_{klmn}, \quad (2.7b)$$

and

$$D = W \det \beta - \sum_{k,l} \langle \varphi'_k | t | \varphi_l \rangle N_{kl} \\ - \frac{1}{4} \sum_{k,l,n,m} \langle \varphi'_k \varphi'_l | v | \chi_m \chi_n \rangle N_{klmn}, \quad (2.7c)$$

where all the matrix elements of  $v$  are antisymmetrized as usual.

One expects the derivatives of  $C$ ,  $C'$ , and  $D$  to introduce the mean-field potentials  $S, S', U$ , defined as follows by their action upon  $\chi_j, \chi'_j, \varphi_j$ , and  $\varphi'_j$  in coordinate representation; for example,

$$\langle x | S | \chi_j \rangle = \langle \phi' | \chi \rangle^{-1} \sum_{k,l} \langle x \varphi'_k | v | \chi_j \chi_l \rangle M_{kl}, \quad (2.8a)$$

$$\langle \chi'_j | S' | \chi \rangle = \langle \chi' | \phi \rangle^{-1} \sum_{k,l} \langle \chi'_j \chi'_k | v | x \varphi_l \rangle M'_{kl}, \quad (2.8b)$$

$$\langle x | U | \varphi_j \rangle = \langle \phi' | \phi \rangle^{-1} \sum_{k,l} \langle x \varphi'_k | v | \varphi_j \varphi_l \rangle N_{kl}, \quad (2.8c)$$

$$\langle \varphi'_j | U | x \rangle = \langle \phi' | \phi \rangle^{-1} \sum_{k,l} \langle \varphi'_j \varphi'_k | v | x \varphi_l \rangle N_{kl}. \quad (2.8d)$$

The antisymmetrization of the matrix elements of  $v$  makes these potentials strict analogs of Hartree-Fock potentials, with mixed density matrices of course. It must be noticed here that  $S$ ,  $S'$ , and  $U$  are obviously insensitive to linear rearrangement inside the orbitals  $\varphi_i$  or inside the orbitals  $\varphi'_i$ . These potentials are just properties of the Slater determinants  $\phi, \phi', \chi$ , and  $\chi'$ .

The variational equations which describe the stationarity of  $F$  are now obtained as

$$\frac{\delta D}{\delta \varphi'_i} = \frac{D}{C} \frac{\delta C}{\delta \varphi'_i}, \quad (2.9a)$$

$$\frac{\delta D}{\delta \varphi_j} = \frac{D}{C'} \frac{\delta C'}{\delta \varphi_j}. \quad (2.9b)$$

The explicit calculation of the derivatives takes advantage of Eqs. (2.7) and (2.4):

$$\frac{\delta C}{\delta \varphi'_i} = \sum_j X_{ij} | \chi_j \rangle + \sum_j t | \chi_j \rangle M_{ij} \\ + \frac{1}{2} \sum_{j,l,m} \langle \cdot \varphi'_i | v | \chi_j \chi_m \rangle M_{ilmj}, \quad (2.10a)$$

$$\frac{\delta C'}{\delta \varphi_j} = \sum_i \langle \chi'_i | X'_{ij} + \sum_i M'_{ij} \langle \chi'_i | t \\ + \frac{1}{2} \sum_{i,l,m} \langle \chi'_i \chi'_l | v | \cdot \varphi_m \rangle M'_{ilmj}, \quad (2.10b)$$

$$\frac{\delta D}{\delta \varphi'_i} = \sum_j Y_{ij} | \varphi_j \rangle - \sum_j t | \varphi_j \rangle N_{ij} \\ - \frac{1}{2} \sum_{j,l,m} \langle \cdot \varphi'_i | v | \chi_j \chi_m \rangle N_{ilmj}, \quad (2.10c)$$

$$\frac{\delta D}{\delta \varphi_j} = \sum_i \langle \varphi'_i | Y_{ij} - \sum_i N_{ij} \langle \varphi'_i | t \\ - \frac{1}{2} \sum_{i,l,m} \langle \varphi'_i \varphi'_l | v | \cdot \varphi_m \rangle N_{ilmj}, \quad (2.10d)$$

The dot in the two-body matrix elements indicates that a functional derivative has been taken and stands for a free coordinate, for example,  $x$  in coordinate representation. The matrices  $X, X'$ , and  $Y$  are defined by their matrix elements

$$X_{ij} = -EM_{ij} + \sum_{k,l} \langle \varphi'_k | t | \chi_l \rangle M_{kijl} \\ + \frac{1}{4} \sum_{k,l,m,n} \langle \varphi'_k \varphi'_l | v | \chi_m \chi_n \rangle M_{klijnm}, \quad (2.11a)$$

$$X'_{ij} = -EM'_{ij} + \sum_{k,l} \langle \chi'_k | t | \varphi_l \rangle M_{kijl} \\ + \frac{1}{4} \sum_{k,l,m,n} \langle \chi'_k \chi'_l | v | \varphi_m \varphi_n \rangle M'_{klijnm}, \quad (2.11b)$$

$$Y_{ij} = WN_{ij} - \sum_{k,l} \langle \varphi'_k | t | \varphi_l \rangle N_{kijl} \\ - \frac{1}{4} \sum_{k,l,m,n} \langle \varphi'_k \varphi'_l | v | \varphi_m \varphi_n \rangle N_{klijnm}. \quad (2.11c)$$

These equations, (2.11) and (2.10), can be further simplified upon taking advantage of Eqs. (2.3) and (2.8) and the symmetry properties of the cofactors and matrix elements of  $v$ . One finds first

$$X_{ij} = M_{ij} \left[ -E + \sum_{k,l} \langle \varphi'_k | (t + \frac{1}{2}S) | \chi_l \rangle M_{kl} \langle \phi' | \chi \rangle^{-1} \right] \\ - \sum_{k,l} \langle \varphi'_k | (t + S) | \chi_l \rangle M_{il} M_{kj} \langle \phi' | \chi \rangle^{-1}, \quad (2.12a)$$

$$X'_{ij} = M'_{ij} \left[ -E + \sum_{k,l} \langle \chi'_k | (t + \frac{1}{2} S') | \varphi_l \rangle M_{kl} \langle \chi' | \phi \rangle^{-1} \right] \\ - \sum_{k,l} \langle \chi'_k | (t + S') | \varphi_l \rangle M'_{il} M'_{kj} \langle \chi' | \phi \rangle^{-1}, \quad (2.12b)$$

$$Y_{ij} = N_{ij} \left[ W - \sum_{k,l} \langle \varphi'_k | (t + \frac{1}{2} U) | \varphi_l \rangle N_{kl} \langle \phi' | \phi \rangle^{-1} \right] \\ + \sum_{k,l} \langle \varphi'_k | (t + U) | \varphi_l \rangle N_{il} N_{kj} \langle \phi' | \phi \rangle^{-1}, \quad (2.12c)$$

where one recognizes the following Hartree-Fock matrices:

$$h_{kl} = \langle \varphi'_k | (t + S) | \chi_l \rangle, \quad (2.13a)$$

$$h'_{kl} = \langle \chi'_k | (t + S') | \varphi_l \rangle, \quad (2.13b)$$

$$H_{kl} = \langle \varphi'_k | (t + U) | \varphi_l \rangle. \quad (2.13c)$$

Assume then that Eqs. (2.9) have been solved, namely, that  $\{\varphi'_i, \varphi_j\}$  are self-consistent orbitals. Because of the freedom of rearrangement available for these orbitals, nothing prevents the choice of a representation in which the following *two* conditions are simultaneously satisfied:

$$\beta_{ij} = \beta_{ii} \delta_{ij}, \quad (2.14a)$$

$$H_{ij} = \epsilon_{ij} \beta_{ii} \delta_{ij}. \quad (2.14b)$$

An immediate consequence of Eq. (2.14a) is that the matrix  $N$  also becomes diagonal,

$$N_{ij} = \frac{\langle \phi' | \phi \rangle}{\beta_{ii}} \delta_{ij}. \quad (2.15)$$

In this representation the variational equations (2.9) become simply

$$\langle \phi' | \phi \rangle \beta_{ii}^{-1} \left[ W - \sum_k \langle \varphi'_k | (t + \frac{1}{2} U) | \varphi_k \rangle \beta_{kk}^{-1} \right. \\ \left. + \epsilon_i - t - U \right] | \varphi_i \rangle = \frac{D}{C} \frac{\delta C}{\delta \varphi'_i}, \quad (2.16a)$$

$$\langle \phi' | \phi \rangle \beta_{jj}^{-1} \langle \varphi'_j | \left[ W - \sum_k \langle \varphi'_k | (t + \frac{1}{2} U) | \varphi_k \rangle \beta_{kk}^{-1} \right. \\ \left. + \epsilon_j - t - U \right] = \frac{D}{C'} \frac{\delta C'}{\delta \varphi_j}. \quad (2.16b)$$

A further simplification occurs if one notices that the norms of  $\varphi_i, \varphi'_i$  are arbitrary. As a matter of fact, the "off-diagonal" freedom of orbital rearrangement has already been taken into account by the representation which diagonalizes the matrices  $\beta$  and  $H$ , see Eqs. (2.1c), (2.13c) and (2.14), and it is now possible to use the norm and phase freedom of these orbitals ("diagonal" freedom) to reduce Eqs. (2.16) into

$$(\eta_i - t - U) | \varphi_i \rangle = \left| \frac{\delta C}{\delta \langle \varphi'_i |} \right\rangle, \quad (2.17a)$$

$$\langle \varphi'_i | (\eta_i - t - U) = \left\langle \frac{\delta C'}{\delta | \varphi_i \rangle} \right\rangle, \quad (2.17b)$$

where one recognizes that

$$\eta_i = W - \frac{\langle \phi' | \mathcal{H} | \phi \rangle}{\langle \phi' | \phi \rangle} + \frac{\langle \varphi'_i | (t + U) | \varphi_i \rangle}{\langle \varphi'_i | \varphi_i \rangle}. \quad (2.18)$$

This choice of norms and phases corresponds to the conditions

$$\beta_{ii} = \frac{\langle \phi' | \phi \rangle \langle \phi' | (\mathcal{H} - E) | \chi \rangle}{\langle \phi' | (W - \mathcal{H}) | \phi \rangle} \\ = \frac{\langle \phi' | \phi \rangle \langle \chi' | (\mathcal{H} - E) | \phi \rangle}{\langle \phi' | (W - \mathcal{H}) | \phi \rangle} \quad (2.19)$$

hence at the stationary point  $C = C'$  and also  $\beta_{ii}$  is independent of  $i$ .

The special solutions  $\{\varphi_i, \varphi'_i\}$  described by Eqs. (2.17) will be retained as reference solutions in the following. Their compatibility with Eqs. (2.14) derives from the following lemma and theorem.

*Lemma.* The orbitals which are solutions of Eqs. (2.17) satisfy the relations

$$C = \left\langle \varphi'_i \left| \frac{\delta C}{\delta \langle \varphi'_i |} \right. \right\rangle, \quad C' = \left\langle \frac{\delta C'}{\delta | \varphi_i \rangle} \left| \varphi_i \right. \right\rangle, \quad (2.20a)$$

and, for  $i \neq j$ ,

$$0 = \left\langle \varphi'_j \left| \frac{\delta C}{\delta \langle \varphi'_i |} \right. \right\rangle = \left\langle \frac{\delta C'}{\delta | \varphi_j \rangle} \left| \varphi_i \right. \right\rangle. \quad (2.20b)$$

*Proof.* Since  $C$  and  $C'$  are strictly linear with respect to each of the orbitals  $\varphi'_i$  and  $\varphi_i$ , respectively, the validity of Eq. (2.20a) is trivial. Besides, one finds that  $C = C'$  by left multiplying Eq. (2.17a) by  $\langle \varphi'_i |$  and right multiplying Eq. (2.17b) by  $| \varphi_i \rangle$ , then equating the results. As regards Eqs. (2.20b), it suffices to remember that  $C$  is a strictly bilinear and *antisymmetric* functional of any pair of its orbitals  $\varphi'_i, \varphi'_j$ ,  $i \neq j$ . Hence the saturation of  $\delta C / \delta \langle \varphi'_i |$  by  $\varphi'_j$  corresponds to the expansion of  $\phi'$  with respect to row  $i$ , for instance, by means of (wrong) cofactors corresponding to row  $j$ . The same obvious cancellation occurs for the saturation of  $\delta C' / \delta | \varphi_i \rangle$  by  $\varphi_j$ .

*Theorem.* The orbitals which are solutions of Eq. (2.17) form a biorthogonal set of left and right eigenstates of the matrix  $H$ .

*Proof.* From Eqs. (2.20b) and (2.17a) one finds, for  $i \neq j$ ,

$$\eta_i \langle \varphi'_j | \varphi_i \rangle - \langle \varphi'_j | (t + U) | \varphi_i \rangle = 0. \quad (2.21a)$$

From Eqs. (2.20b) and (2.17b) one finds, for  $i \neq j$ ,

$$\eta_j \langle \varphi'_j | \varphi_i \rangle - \langle \varphi'_j | (t + U) | \varphi_i \rangle = 0. \quad (2.21b)$$

In general  $\eta_i \neq \eta_j$ , hence both  $\langle \varphi'_j | \varphi_i \rangle$  and  $\langle \varphi'_j | (t+U) | \varphi_i \rangle$  vanish. If  $\eta_i = \eta_j$ , one can also calculate  $\langle \varphi'_i | \varphi_j \rangle$  and  $\langle \varphi'_i | (t+U) | \varphi_j \rangle$ , mix  $\varphi_i$  with  $\varphi_j$  to cancel the new overlap  $\langle \varphi'_i | \varphi_j \rangle$ , then use Eq. (2.21a) to find that the new matrix element  $\langle \varphi'_i | (t+U) | \varphi_j \rangle$  vanishes. The details are left as an exercise for the interested reader.

As a final result of this section we notice that the propagation self-energy  $\eta_i$  defined by Eq. (2.18) differs from the traditional Hartree-Fock energy  $\epsilon_i$  defined by Eqs. (2.14b) and (2.13c). This is because in general in the present case

$$W - \frac{\langle \phi' | \mathcal{H} | \phi \rangle}{\langle \phi' | \phi \rangle} \neq 0,$$

contrary to the traditional Hartree-Fock case, where  $\phi$  and  $\phi'$  are the same and  $W$  is the physical, real energy.

### III. AN ILLUSTRATIVE EXAMPLE

For the sake of simplicity we consider a two-body one-dimensional, elastic collision. The channel wave packet reads, in momentum representation,

$$\chi(q_1, q_2; k) = \frac{1}{\sqrt{2}} \pi^{-1/2} b \{ \exp\{-\frac{1}{2}b^2[(q_1-k)^2 + (q_2+k)^2]\} - \exp\{-\frac{1}{2}b^2[(q_1+k)^2 + (q_2-k)^2]\} \}, \tag{3.1}$$

where one recognizes that particles 1 and 2 have been prepared in normalized Gaussian wave packets  $\chi_1$  and  $\chi_2$ , boosted by  $\pm k$ , respectively, and antisymmetrized. An alternate representation of  $\chi$  is as a product of  $\chi_{c.m.} \chi_r$  of center-of-mass and relative wave packets, respectively,

$$\chi(q, Q; k) = \pi^{-1/4} \left[ \frac{b}{\sqrt{2}} \right]^{1/2} \exp(-\frac{1}{4}b^2Q^2) \frac{1}{\sqrt{2}} \pi^{-1/4} (b\sqrt{2})^{1/2} \{ \exp[-b^2(q-k)^2] - \exp[-b^2(q+k)^2] \}, \tag{3.2}$$

with obvious notations for the center-of-mass and relative momenta  $Q = q_1 + q_2$  and  $q = \frac{1}{2}(q_1 - q_2)$ , respectively. The Hamiltonian for the model is defined by its matrix elements

$$\begin{aligned} \langle q_1 q_2 | \mathcal{H} | q'_1 q'_2 \rangle &= \left[ \frac{q_1^2}{2} + \frac{q_2^2}{2} - \frac{(q_1 + q_2)^2}{4} \right] \delta(q_1 - q'_1) \delta(q_2 - q'_2) - \frac{1}{4} \lambda_0 v^2 (q_1 - q_2) \exp[-\frac{1}{4}v^2(q_1 - q_2)^2] \\ &\times (q'_1 - q'_2) \exp[-\frac{1}{4}v^2(q'_1 - q'_2)^2] \delta(q_1 + q_2 - q'_1 - q'_2), \end{aligned} \tag{3.3}$$

or  
 In the special case of two particles, the permutation symmetry of  $v_{12}\chi$  is the same as that of  $\chi$ , hence the Pauli principle is correctly taken into account.

$$\begin{aligned} \langle qQ | \mathcal{H} | q'Q' \rangle &= \delta(Q - Q') [q^2 \delta(q - q') - \lambda_0 v^2 q q'] \\ &\times \exp(-v^2 q^2) \exp(-v^2 q'^2). \end{aligned} \tag{3.4}$$

As seen from Eq. (3.2),  $\chi$  factorizes as a product  $\chi_r \chi_{c.m.}$  of relative and center-of-mass wave packets, the former being normalized to unity in  $L_2$  norm. The exact amplitude being obviously

$$\mathcal{D} = \langle \chi | v_{12} | \psi \rangle, \tag{3.6}$$

with  $\psi$  defined by

$$\mathcal{D} = \langle \chi | v_{12} (W - \mathcal{H})^{-1} v_{12} | \chi \rangle \tag{3.5} \quad (W - \mathcal{H})\psi = v_{12}\chi, \tag{3.7}$$

it is clear from Eq. (3.4) that  $\mathcal{H}$  leaves the center-of-mass invariant, hence  $\psi$  also factorizes into a product  $\psi_r \chi_{c.m.}$ . A reduction of Eq. (3.7) is thus

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$$\begin{aligned}
(W - q^2)\psi_r(q) &= -\lambda_0 v q \exp(-v^2 q^2) \\
&\quad \times \int dq' v q' \exp(-v^2 q'^2) [\psi_r(q') + \chi_r(q')] , \quad (3.8)
\end{aligned}$$

where one identifies, in the integral on the right-hand side, the scalar products  $\langle v | \psi_r \rangle$  and  $\langle v | \chi_r \rangle$  of  $|\psi_r\rangle$  and  $|\chi_r\rangle$ , respectively, with the form factor  $|v\rangle$  of the non-local potential, Eq. (3.4). Because of the separability of the potential, the integral in the right-hand side of Eq. (3.8) is just a sum of two numbers  $\langle v | \psi_r \rangle$  and  $\langle v | \chi_r \rangle$ ,

$$\begin{aligned}
\langle v | \chi_r \rangle &= \frac{v}{\sqrt{2}} \int dq q \exp(-v^2 q^2) \pi^{-1/4} (b\sqrt{2})^{1/2} \{ \exp[-b^2(q-k)^2] - \exp[-b^2(q+k)^2] \} \\
&= 2^{3/4} \pi^{1/4} \left[ \frac{v^2 b}{v^2 + b^2} \right]^{1/2} \frac{b^2 k}{v^2 + b^2} \exp \left[ -\frac{b^2 v^2 k^2}{v^2 + b^2} \right] , \quad (3.9b)
\end{aligned}$$

one finds easily

$$\psi_r(q) = -\lambda_0 v q \frac{\exp(-v^2 q^2)}{W - q^2} (\langle v | \chi_r \rangle + \langle v | \psi_r \rangle) , \quad (3.10)$$

hence

$$\langle v | \psi_r \rangle = \frac{-\lambda_0 \langle v | \chi_r \rangle \Delta(W)}{1 + \lambda_0 \Delta(W)} , \quad (3.11)$$

and finally

$$\mathcal{D} = \lambda_0^2 \langle v | \chi_r \rangle^2 \frac{\Delta(W)}{1 + \lambda_0 \Delta(W)} . \quad (3.12)$$

Incidentally the Born term is

hence  $\psi_r$  is found as

$$\psi_r(q) = -\lambda_0 (\langle v | \psi_r \rangle + \langle v | \chi_r \rangle) \frac{v q \exp(-v^2 q^2)}{W - q^2} .$$

We just have to integrate again  $\psi_r$  with the form factor  $v$  to obtain an equation for  $\langle v | \psi_r \rangle$ , see Eq. (3.11) below. Defining the function

$$\Delta(W) = v^2 \int dq \frac{q^2 \exp(-2v^2 q^2)}{W - q^2} , \quad (3.9a)$$

and the number

$$\mathcal{T}_B = -\lambda_0 \langle v | \chi_r \rangle^2 ,$$

hence the exact  $T$ -matrix amplitude is

$$\mathcal{T} = \mathcal{T}_B + \mathcal{D} = \frac{\langle \chi_r | v | \chi_r \rangle}{1 + \lambda_0 \Delta(W)} .$$

We now turn to the mean-field approximation. The one-body part of  $\mathcal{H}$  is, see Eq. (3.3),

$$T = \frac{q_1^2}{4} + \frac{q_2^2}{4} , \quad (3.13a)$$

while the two-body part is

$$V = -\frac{1}{2} q_1 q_2 + v_{12} . \quad (3.13b)$$

Hence

$$\begin{aligned}
D = \langle \phi' | (W - \mathcal{H}) | \phi \rangle &= W (\langle \phi'_1 | \phi_1 \rangle \langle \phi'_2 | \phi_2 \rangle - \langle \phi'_1 | \phi_2 \rangle \langle \phi'_2 | \phi_1 \rangle) \\
&\quad - \frac{1}{4} (\langle \phi'_1 | q_1^2 | \phi_1 \rangle \langle \phi'_2 | \phi_2 \rangle + \langle \phi'_2 | q_2^2 | \phi_2 \rangle \langle \phi'_1 | \phi_1 \rangle) \\
&\quad - \langle \phi'_1 | q_1^2 | \phi_2 \rangle \langle \phi'_2 | \phi_1 \rangle - \langle \phi'_2 | q_2^2 | \phi_1 \rangle \langle \phi'_1 | \phi_2 \rangle) \\
&\quad + \frac{1}{2} (\langle \phi'_1 | q_1 | \phi_1 \rangle \langle \phi'_2 | q_2 | \phi_2 \rangle - \langle \phi'_1 | q_1 | \phi_2 \rangle \langle \phi'_2 | q_2 | \phi_1 \rangle) - \langle \phi'_1 \phi'_2 | v | \phi_1 \phi_2 \rangle . \quad (3.14)
\end{aligned}$$

while

$$C = \langle \phi' | v | \chi \rangle = \langle \phi'_1 \phi'_2 | v | \chi_1 \chi_2 \rangle . \quad (3.15)$$

In Eqs. (3.14) and (3.15) and the following, the notation  $v_{12}$  is shortened to  $v$ .

The functional derivatives are obtained readily as

$$\begin{aligned}
\frac{\delta D}{\delta \phi'_1} &= \langle \phi'_2 | \phi_2 \rangle \left[ W - \frac{1}{4} q_1^2 - \frac{1}{4} \frac{\langle \phi'_2 | q_2^2 | \phi_2 \rangle}{\langle \phi'_2 | \phi_2 \rangle} \right] | \phi_1 \rangle \\
&\quad + \frac{1}{4} | \phi_2 \rangle \langle \phi'_2 | q_2^2 | \phi_1 \rangle \\
&\quad + \langle \phi'_2 | (\frac{1}{2} q_1 q_2 - v) | \phi_1 \phi_2 \rangle \quad (3.16)
\end{aligned}$$

and

$$\frac{\delta C}{\delta \phi'_1} = \langle \phi'_2 | v | \chi_1 \chi_2 \rangle . \quad (3.17)$$

In Eq. (3.16) we have already taken advantage of the cancellation of  $\langle \phi'_2 | \phi_1 \rangle$  and in both equations the dot expresses the free coordinate coming from the functional derivation. It will be noticed, for instance, that

$$\langle \phi'_2 | v | \chi_1 \chi_2 \rangle = M_{11} \langle \cdot | S | \chi_1 \rangle + M_{12} \langle \cdot | S | \chi_2 \rangle , \quad (3.18)$$

see Eq. (2.8a). It will also be noticed that, in the special case of two particles, mean-field matrix elements such as  $\langle \varphi'_2 | U | \varphi_1 \rangle$  and  $\langle \varphi'_2 | S | \chi_1 \rangle$  vanish identically, because the two-body matrix elements entering the definitions of  $U$  and  $S$ , Eqs. (2.8), are antisymmetrized *a priori*. Hence the only nontrivial exchange coupling between  $\varphi_1$  and  $\varphi_2$  in Eq. (3.16) comes from  $\langle \varphi'_2 | q_2^2 | \varphi_1 \rangle$ . The special representation discussed at the end of Sec. II must therefore

cancel that matrix element. Finally, we take advantage of two symmetries of the problem, namely, (i) parity since  $\chi_1$  and  $\chi_2$  are deduced from each other by opposite boosts  $k$  and  $-k$ , respectively, hence  $\varphi_1$  and  $\varphi_2$  may be taken as strictly even and odd, respectively, and (ii) Euclidean symmetry since  $\mathcal{D}$  is a diagonal matrix element, hence  $|\phi'\rangle$  is just the complex conjugate of  $|\phi\rangle$ . The "reference" mean-field equation for  $\varphi_1$  is thus

$$\begin{aligned} (W - \frac{1}{4}q_1^2 - \frac{1}{4}\theta_2)\varphi_1(q_1) - \frac{1}{2}\kappa_2 q_1 \varphi_2(q_1) - \int dq'_1 w_2(q_1 q'_1) \varphi_1(q'_1) \\ = -\frac{1}{4}\lambda_0 v^2 \int dq_2 dq'_1 dq'_2 \delta(q_1 + q_2 - q'_1 - q'_2) \exp[-\frac{1}{4}v^2(q_1 - q_2)^2] (q_1 - q_2) \exp[-\frac{1}{4}v^2(q'_1 - q'_2)^2] (q'_1 - q'_2) \\ \times \varphi_2(q_2) [\chi_1(q'_1) \chi_2(q'_2) - \chi_2(q'_1) \chi_1(q'_2)], \end{aligned} \quad (3.19)$$

$$\theta_2 = n_2^{-1} \int dq_2 q_2^2 [\varphi_2(q_2)]^2, \quad (3.20a)$$

$$\kappa_2 = n_2^{-1} \int dq_2 \varphi_2(q_2) q_2 \varphi_1(q_2), \quad (3.20b)$$

$$\begin{aligned} w_2(q_1 q'_1) = -\frac{1}{2} n_2^{-1} \lambda_0 v^2 \int dq_2 dq'_2 \delta(q_1 + q_2 - q'_1 - q'_2) (q_1 - q_2) (q'_1 - q'_2) \varphi_2(q_2) \\ \times \exp[-\frac{1}{4}v^2(q_1 - q_2)^2] \exp[-\frac{1}{4}v^2(q'_1 - q'_2)^2] \varphi_2(q'_2), \end{aligned} \quad (3.20c)$$

and

$$n_2 = \int dq_2 [\varphi_2(q_2)]^2. \quad (3.20d)$$

Because of the  $p$ -wave interaction which has been chosen the direct and exchange contributions to  $w$ , Eq. (3.20c), are equal. The same holds also for the right-hand side of Eq. (3.19). The term  $q_1 | \varphi_1 \rangle$  which should be present with  $\kappa_2 q_1 | \varphi_2 \rangle$  and  $w$  on the left-hand side of Eq. (3.19), because of the  $q_1 q_2$  term in Eq. (3.13b), actually vanishes. This is because it is weighted by the Euclidean matrix element  $\langle \varphi_2 | q_2^2 | \varphi_1 \rangle$  which obviously vanishes when  $\varphi_1$  and  $\varphi_2$  have opposite parities.

The right-hand side of Eq. (3.19) slightly simplifies, because of the factorization of  $\chi$  into a product  $\chi_r \chi_{c.m.}$ ,

$$\frac{\delta C}{\delta \varphi'_1} = -\frac{1}{\sqrt{2}} \lambda_0 v \langle v | \chi_r \rangle \int dq_2 \varphi_2(q_2) (q_1 - q_2) \exp[-\frac{1}{4}v^2(q_1 - q_2)^2] \pi^{-1/4} \left[ \frac{b}{\sqrt{2}} \right]^{1/2} \exp[-\frac{1}{4}b^2(q_1 + q_2)^2]. \quad (3.21)$$

In the same way the reference mean-field equation for  $\varphi_2$  is

$$\begin{aligned} (W - \frac{1}{4}q_2^2 - \frac{1}{4}\theta_1)\varphi_2(q_2) - \frac{1}{2}\kappa_1 q_2 \varphi_1(q_2) - \int dq'_2 w_1(q_2 q'_2) \varphi_2(q'_2) \\ = -\frac{1}{\sqrt{2}} \lambda_0 v \langle v | \chi_r \rangle \int dq_1 \varphi_1(q_1) (q_1 - q_2) \exp[-\frac{1}{4}v^2(q_1 - q_2)^2] \pi^{-1/4} \left[ \frac{b}{\sqrt{2}} \right]^{1/2} \exp[-\frac{1}{4}b^2(q_1 + q_2)^2], \end{aligned} \quad (3.22)$$

where  $\theta_1$ ,  $\kappa_1$ , and  $w_1$  are obtained from the substitution of  $\varphi_1$  for  $\varphi_2$  in Eqs. (3.20a), (3.20b), and (3.20d).

Equations (3.21) and (3.22) have been numerically solved on the CISI Cray computer by a brute-force iterative algorithm, where an initial guess for  $\varphi_1$  and  $\varphi_2$  generates mean-field kernels  $w_1, w_2$  and kinetic parameters  $\theta_1, \kappa_1, \theta_2, \kappa_2$ , and hence new orbitals  $\varphi_1, \varphi_2$  after inversion of the left-hand sides of Eqs. (3.21) and (3.22). Typical integration meshes correspond to 35 points ranging from  $-7b^{-1}$  to  $7b^{-1}$  in momentum space and a boost momentum  $k$  of order 2 or 3 times  $b^{-1}$ . Both parameters  $b$  and  $v$  are taken of order  $1fm$ . With  $\hbar^2/m$  as a unit, a typical value of the energy is taken as 6, with an imaginary part ranging from 1, which is truly off shell, down to 0.1, which is practically on shell. The strength constant  $\lambda_0$  is also taken of order 1. Depending on the parameters, con-

vergence towards self-consistency may or may not need relaxation in the iterative algorithm. Convergence is sometimes reached in 10 steps and sometimes demands 400 steps.

We have not made a systematic investigation of all possible solutions, as in Ref. 7. The comparison shown in Table I, between mean-field amplitudes and those exact amplitudes obtained from Eq. (3.12), is just meant as an illustration of the method. For a more systematic numerical analysis in two simpler cases (not antisymmetrized) we refer to earlier works.<sup>7,8</sup> The agreement shown by Table I is good enough to definitely justify the use of the mean-field approximation in its present antisymmetrized formulation.

Besides numerical agreement between the exact  $\mathcal{D}$  and the mean field  $\overline{\mathcal{D}}$  a main result of the numerical applica-

TABLE I. Comparison of the exact ( $\mathcal{D}$ ) and mean-field amplitudes ( $\mathcal{T}$ ) for various values of  $\text{Re}E$  and a fixed value of  $\text{Im}E = 0.1$ . The system of units and the values of the other parameters are defined in Sec. III.

$\text{Re}E$	$\text{Re}\mathcal{D}$	$\text{Re}\mathcal{T}$	$\text{Im}\mathcal{D}$	$\text{Im}\mathcal{T}$
6.25	$4.1 \times 10^{-4}$	$4.0 \times 10^{-4}$	$-7.5 \times 10^{-6}$	$-6.2 \times 10^{-6}$
6.00	$5.3 \times 10^{-4}$	$5.2 \times 10^{-4}$	$-1.1 \times 10^{-5}$	$-7.3 \times 10^{-6}$
5.76	$6.8 \times 10^{-4}$	$6.6 \times 10^{-4}$	$-1.8 \times 10^{-5}$	$-8.7 \times 10^{-6}$
5.72	$8.7 \times 10^{-4}$	$8.3 \times 10^{-4}$	$-1.9 \times 10^{-5}$	$-1.0 \times 10^{-5}$
5.29	$1.1 \times 10^{-3}$	$1.1 \times 10^{-3}$	$-2.5 \times 10^{-5}$	$-2.7 \times 10^{-5}$
5.06	$1.4 \times 10^{-3}$	$1.3 \times 10^{-3}$	$-3.3 \times 10^{-5}$	$-2.4 \times 10^{-5}$
4.84	$1.8 \times 10^{-3}$	$1.7 \times 10^{-3}$	$-4.5 \times 10^{-5}$	$-2.7 \times 10^{-5}$
4.62	$2.2 \times 10^{-3}$	$2.1 \times 10^{-3}$	$-6.1 \times 10^{-5}$	$-2.9 \times 10^{-5}$
4.41	$2.8 \times 10^{-3}$	$2.6 \times 10^{-3}$	$-8.7 \times 10^{-5}$	$-8.7 \times 10^{-5}$
4.20	$3.5 \times 10^{-3}$	$3.2 \times 10^{-3}$	$-1.4 \times 10^{-4}$	$-1.0 \times 10^{-4}$
4.00	$4.4 \times 10^{-3}$	$4.0 \times 10^{-3}$	$-3.4 \times 10^{-4}$	$-7.1 \times 10^{-5}$
3.80	$4.8 \times 10^{-3}$	$4.8 \times 10^{-3}$	$-5.9 \times 10^{-4}$	$-7.0 \times 10^{-5}$
3.61	$6.1 \times 10^{-3}$	$5.9 \times 10^{-3}$	$-3.2 \times 10^{-4}$	$-2.7 \times 10^{-4}$
3.42	$7.6 \times 10^{-3}$	$7.3 \times 10^{-3}$	$-3.5 \times 10^{-4}$	$-3.0 \times 10^{-4}$

tion is the check of the theorem proven in Sec. II. Test cases were run where the initial guesses for  $\varphi_1, \varphi_2$  were not orthogonal. The self-consistent orbitals turned out to restore orthogonality.

The code MIRCAR is available on request to any interested reader. We intend in the future to map out the variational space in order to identify the likely multiplicity of solutions and the corresponding bifurcation points.

The numerical agreement found in Table I is strikingly systematic, despite slight inconsistencies in the imaginary amplitudes. (These inconsistencies are clearly due to the fact that  $\text{Im}\mathcal{D}$  is at least one order of magnitude smaller than  $\text{Re}\mathcal{D}$  in the present case, hence a 3% inaccuracy in  $\text{Re}\mathcal{D}$  is compatible with a 30% inaccuracy for  $\text{Im}\mathcal{D}$ . They disappeared in another case where  $\text{Im}\mathcal{D}$  and  $\text{Re}\mathcal{D}$  are of the same order.) We find this good behavior of the mean-field method very encouraging for many-body problems, where the mean field is expected to be even better justified than it is in a two-body problem. A systematic search for the solutions and bifurcations of the mean-field equations is in order. This should shed light on the shell models provided by the present theory, these shell models having obviously a dynamical interpretation in terms of reaction mechanisms. Preliminary results on this problem of bifurcations seem to show that there is one well-defined physical branch, which is obtained as the most stable solution when  $\text{Im}W/\text{Re}W$  is large. When one lets  $\text{Im}W$  tend towards zero, and one follows this solution by continuity, no bifurcation has yet been observed numerically.

#### IV. DISCUSSION AND CONCLUSION

Several results have been obtained here. The main result is a representation of the many-body Green's function for fermions in a way where antisymmetrization appears

technically very easy. (The case of bosons would be as easy.) A subsidiary result of some importance is the existence of a canonical representation of the mean-field orbitals, in which these orbitals make a dynamically biorthogonal set. Furthermore, these generalized Hartree-Fock equations turn out to provide an excellent approximation to exact results in a solvable model. *The on-shell limit of the calculated amplitude is smooth.* This opens the way towards realistic calculations for systems with many fermions.

In any attempt towards realistic calculations a great deal of attention should be paid to the possibility of several, competing solutions of the system of nonlinear equations proposed in this paper. Their discovery and interpretation may be the most stimulating aspect of the theory. This demands, of course, the optimization of the numerical algorithms which will be in this numerical solution.

A last remark is in order. While we have used the gauge (rearrangement) freedom of Slater determinants  $\phi', \phi$  to define a canonical representation of  $\varphi'_i, \varphi_i$ , we still have some freedom for an additional canonical representation of  $\chi'_i, \chi_i$ . If such an additional representation can be found, it will provide shell models not just for the trial functions, but also for the channel wave packets. This intriguing conjecture may deserve some attention.

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