ANTISYMMETRIZATION OF A MEAN FIELD CALCULATION OF THE T-MATRIX

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ABSTRACT

The usual definition of the prior(post) interaction $V(V')$ between projectile and target (resp. ejectile and residual target) being contradictory with full antisymmetrization between nucleons, an explicit antisymmetrization projector $\mathcal{A}$ must be included in the definition of the transition operator, $T \equiv V'\mathcal{A} + V'\mathcal{A}GV$. We derive the suitably antisymmetrized mean field equations leading to a non perturbative estimate of T. The theory is illustrated by a calculation of forward α-α scattering, making use of self consistent symmetries.

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1. Introduction

Consider the usual Hamiltonian $H = \sum_i t_i + \sum_{i>j} v_{ij}$, describing a two-fragment collision a+b→c+d between N nucleons, elastic or inelastic, with or without rearrangement. It is customary to define the prior (post) interaction $V = \sum_{i\epsilon a, j\epsilon b} v_{ij}$, ($V' = \sum_{i\epsilon c, j\epsilon d} v_{ij}$), respectively, at the cost of considering as distinct the nucleons of the projectile a (resp. ejectile c) with respect to the target b (resp. residual target d) in the initial (resp. final) channel. Under this lack of antisymmetrization, one defines an initial wave χ, which is a straight product of plane waves for a and b. Similarly one defines a non antisymmetrized final wave χ' for c and d. The transition amplitude is then introduced as the on-shell matrix element $< \chi' \mid (V' + V'GV) \mid \chi >$, where G is the full $N-$nucleon Green function at the energy E of the collision.

In order to take the Pauli principle into account, the correct approach, as described for instance by Austern[1], consists in i) retaining χ, χ' as non antisymmetrized, but ii) calculating the matrix element $< \chi' \mid (V'\mathcal{A} + V'\mathcal{A}GV) \mid \chi >$, where the projector $\mathcal{A} = (N!)^{-1} \sum_{\mathcal{P}} (-)^{\mathcal{P}} \mathcal{P}$, namely the parity weighted sum of all the permutations $\mathcal{P}$ of N nucleons, takes care of the antisymmetrization. Note that the validity of the above formula for the antisymmetrized transition amplitude rests upon the assumption that initial and final wave packets χ, χ' are normalized to unity and describe non-overlapping fragments a, b and c, d, respectively. Asymptotic density and flux are then unchanged under antisymmetrization. We shall come back to this point in Section 5.

The calculation of Born terms, antisymmetrized or not, being straightforward, the present paper focusses on the following *generic* problem: Let z be any complex energy (eventually $z \to E + i0$). Let $\chi_a(\vec{r}_1 ... \vec{r}_{N_a})$ be any wave function for the projectile, with internal antisymmetrization for these N_a nucleons. For instance, χ_a may be a boosted shell model wave function, with or without configuration mixing, but it can actually differ arbitrarily from an eigenstate of the projectile Hamiltonian H_a. Let $\chi_b(\vec{r}_{N_a+1} ... \vec{r}_N)$ be an arbitrary, antisymmetrized wave function for nucleus b, and consider the straight product $\chi = \chi_a \chi_b$. For the final state, consider similarly χ'_c, χ'_d and $\chi' = \chi'_c \chi'_d$, with antisymmetrization internal to c and d, separately. We want to calculate the number

$$\mathcal{D}(z) =< \chi' \mid V'\mathcal{A}(z-H)^{-1} V \mid \chi > . \tag{1.1}$$

The main motivation for this problem is, obviously, that $\mathcal{D}$ represents the multistep transition amplitude ($T-$matrix without Born term) when χ, χ' are channel waves and z reaches the retarded on shell limit. But the validity of the arguments listed in this paper extends to all complex values of z and very general choices for χ, χ'. (The only restrictive condition for this validity is the square integrability of $V \mid \chi >$ and $V' \mid \chi' >$, so that $\mathcal{D}$ be well defined as a finite number. It is automatically satisfied for two-fragment channels and short range potentials.)

A variational calculation of $\mathcal{D}$ is described in Section 2. Then we introduce in Section 3 a time independent mean field (TIMF) approximation [2] for this calculation. Section 4 is a discussion of symmetries which can simplify the variational TIMF equations. A numerical application of the theory to α-α scattering is described in Section 5, making use of self consistent symmetries introduced in Section 4. The final Section 6 contains our discussion and conclusion. Finally we introduce in an Appendix a new formalism for the representation of nucleons in different clusters as fermions with different pseudo spins.

2. Equivalent, Antisymmetrized Variational Functionals

We will show that $\mathcal{D}$ is the stationary value of either of the following three Schwinger-like functionals of two independent trial functions Ψ, Ψ',

$$\mathcal{F} =< \Psi' \mid \mathcal{A} V \mid \chi > + < \chi' \mid V' \mid \Psi > - < \Psi' \mid (z - H) \mid \Psi >, \tag{2.1a}$$

$$\mathcal{F}' =< \Psi' \mid V \mid \chi > + < \chi' \mid V' \mathcal{A} \mid \Psi > - < \Psi' \mid (z - H) \mid \Psi >, \tag{2.1b}$$

$$F =< \Psi' \mid \mathcal{A} V \mid \chi > + < \chi' \mid V' \mathcal{A} \mid \Psi > - < \Psi' \mid (z - H) \mid \Psi >, \tag{2.1c}$$

which differ by slightly different insertions of $\mathcal{A}$. The variations of Ψ, Ψ' give the following stationarity conditions,

$$\mathcal{A} V \mid \chi > -(z - H) \mid \Psi >= 0 \text{ and } < \chi' \mid V' - < \Psi' \mid (z - H) = 0 \text{ for } \mathcal{F}, \tag{2.2a}$$

$$V \mid \chi > -(z - H) \mid \Psi >= 0 \text{ and } < \chi' \mid V' \mathcal{A} - < \Psi' \mid (z - H) = 0 \text{ for } \mathcal{F}', \tag{2.2b}$$

$$\mathcal{A} V \mid \chi > -(z - H) \mid \Psi >= 0 \text{ and } < \chi' \mid V' \mathcal{A} - < \Psi' \mid (z - H) = 0 \text{ for } F. \tag{2.2c}$$

For z complex, the full resolvent $G \equiv (z - H)^{-1}$ is a bounded, *uniquely* defined operator. Its action upon square integrable vectors $V \mid \chi >$, $\mathcal{A} V \mid \chi >$, $< \chi' \mid V'$, $< \chi' \mid V' \mathcal{A}$ returns also square integrable vectors. Thus stationarity is reached for a unique pair of trial functions,

$$\mid \Psi >= G \mathcal{A} V \mid \chi > \text{ and } < \Psi' \mid =< \chi' \mid V' G \text{ for } \mathcal{F}, \tag{2.3a}$$

$$| \Psi >= GV \mid \chi > \text{ and } < \Psi' \mid = < \chi' \mid V'\mathcal{A}G \text{ for } \mathcal{F}', \tag{2.3b}$$

$$| \Psi >= G\mathcal{A}V \mid \chi > \text{ and } < \Psi' \mid = < \chi' \mid V'\mathcal{A}G \text{ for } F. \tag{2.3c}$$

The corresponding stationary value of each functional is then

$$\widehat{\mathcal{F}} = (< \chi' \mid V'G)\mathcal{A}V \mid \chi > + < \chi' \mid V'(G\mathcal{A}V \mid \chi >) - (< \chi' \mid V'G)(z-H)(G\mathcal{A}V \mid \chi >), \tag{2.4a}$$

$$\widehat{\mathcal{F}'} = (< \chi' \mid V'\mathcal{A}G)V \mid \chi > + < \chi' \mid V'\mathcal{A}(GV \mid \chi >) - (< \chi' \mid V'\mathcal{A}G)(z-H)(GV \mid \chi >), \tag{2.4b}$$

$$\widehat{F} = (< \chi' \mid V'\mathcal{A}G)\mathcal{A}V \mid \chi > + < \chi' \mid V'\mathcal{A}(G\mathcal{A}V \mid \chi >)$$
$$-(< \chi' \mid V'\mathcal{A}G)(z-H)(G\mathcal{A}V \mid \chi >), \tag{2.4c}$$

and the idempotence of $\mathcal{A}$, together with its commutation with H and G, reduce all nine terms in the right-hand sides (r.h.s.) of Eqs.(2.4) to the same value, namely $\mathcal{D}$, see Eq.(1.1). Hence $\widehat{\mathcal{F}} = \widehat{\mathcal{F}'} = \widehat{F} = \mathcal{D}$.

We notice that six out of these nine terms are integrals confined to an interaction volume, defined by the ranges of $V \mid \chi >$, $< \chi' \mid V'$. For z reaching the on shell limit, Ψ, Ψ' are no more square integrable states, but rather purely outgoing or ingoing waves. The calculation of $\mathcal{D}(z)$, however, by means of any one among these six terms, and the calculation of its on shell limit $\mathcal{D}(E+i0)$, can be confined to a truncation of Ψ, Ψ' to this interaction volume. The remaining three terms contain both Ψ and Ψ' and can not be used to calculate $\mathcal{D}(z)$ in the on-shell limit.

For this reason, we now investigate an approximation in which Ψ, Ψ' are replaced by products Φ, Φ' of independent, square integrable, single particle orbitals φ_i, φ'_i, respectively, $\Phi = \prod_i \varphi_i$, $\Phi' = \prod_i \varphi'_i$, *or* antisymmetrized products of such orbitals (Slater determinants). According to Eq.(2.3a), Ψ' contains only the same partial antisymmetrization as that contained in χ', and its approximation Φ' should thus read as a product $\Phi'_c\Phi'_d$ of separate Slater determinants for the ejectile and the residual target degrees of freedom, while Ψ is fully antisymmetrized, hence Φ must be a Slater determinant. This approximation for $\mathcal{F}$ thus reads

$$\mathcal{F} = < \Phi'_c\Phi'_d \mid \mathcal{A}V \mid \chi > + < \chi' \mid V' \mid \Phi > - < \Phi'_c\Phi'_d \mid (z-H) \mid \Phi > . \tag{2.5a}$$

In the same way, the corresponding approximation for $\mathcal{F}'$ reads

$$\mathcal{F}' =< \Phi' \mid V \mid \chi > + < \chi' \mid V'\mathcal{A} \mid \Phi_a\Phi_b > - < \Phi' \mid (z-H) \mid \Phi_a\Phi_b >, \tag{2.5b}$$

with partial antisymmetrization restricted to a and b. Finally for F both Ψ, Ψ' are fully antisymmetric, and the approximation for F reads

$$F = C + C' - D, \text{ with } C =< \Phi' \mid V \mid \chi >, \; C' =< \chi' \mid V' \mid \Phi >, \; D =< \Phi' \mid (z-H) \mid \Phi >, \tag{2.5c}$$

where the insertions of $\mathcal{A}$ present in Eq.(2.1c) are useless since Φ, Φ' are Slater determinants.

We now notice that the first term in the r.h.s. of Eq.(2.5a) and the second term in the r.h.s. of Eq.(2.5b) contain an explicit $\mathcal{A}$, which projects products of Slater determinants $\Phi_a\Phi_b$, $\Phi'_c\Phi'_d$, into full determinants Φ, Φ', respectively. The same property belongs to the third term in the r.h.s. of Eq.(2.5a), because the implicit $\mathcal{A}$ contained in Φ commutes with H and carries full antisymmetrization further, into the bra. A similar argument holds again for the third term of the r.h.s. of Eq.(2.5b). It can be concluded that $\mathcal{F}, \mathcal{F}', F$, which are equivalent when Ψ, Ψ' are fully flexible trial fuctions, are still equivalent when one attempts the separation of single particle degrees of freedom.

The next Section, Sec.3, thus refers only to the variation of F, as defined by Eq.(2.5c), with Slater determinants Φ, Φ' as trial functions. For obvious technical reasons, we will investigate a slightly less general problem than that announced when introducing Eq.(1.1): only those cases are retained where χ (resp. χ') is the product of two Slater determinants χ_a, χ_b, (resp. χ'_c, χ'_d). The wave functions χ_a,...χ'_d for the nuclei involved in the collision correspond to boosted shell models, like those which define the initial states of TDHF calculations[3]. This technical restriction still defines a generic problem, however, since any matrix element of the operator $V'\mathcal{A}GV$ between correlated internal states of these nuclei can be expanded in matrix elements between uncorrelated states, via usual, static configuration mixings.

3. Time Independent Mean Field Approximation

Let $\{\chi_\alpha, \alpha = 1, ...N_a\}$ be the set of (boosted) orbitals which describes the projectile. Let $\{\chi_\beta, \beta = N_a + 1, ...N\}$, $\{\chi'_\gamma, \gamma = 1, ...N_c\}$, $\{\chi'_\delta, \delta = N_c + 1, ...N\}$ be similar sets for nuclei b, c, d. It is convenient here to define the following wave functions,

$$| \bar{\chi} > = \prod_{\alpha=1}^{N_a} | \chi_\alpha > \prod_{\beta=N_a+1}^{N} | \chi_\beta >, \; < \bar{\chi}' | = \prod_{\gamma=1}^{N_c} < \chi'_\gamma | \prod_{\delta=N_c+1}^{N} < \chi'_\delta |, \qquad (3.1a)$$

which are pure products of orbitals, and

$$| \widetilde{\Phi} >= \det \{ | \varphi_i > \} , \; < \widetilde{\Phi}' |= \det \{ < \varphi'_i | \} , \qquad (3.1b)$$

which are determinants of orbitals, without the usual $(N!)^{-1/2}$ normalizations, because it is slightly easier to calculate the contributions C, C' to the functional F as

$$C = (N_a!N_b!/N!)^{1/2} < \widetilde{\Phi}' | V | \bar{\chi} >, \; C' = (N_c!N_d!/N!)^{1/2} < \bar{\chi}' | V' | \widetilde{\Phi} > . \qquad (3.1c)$$

As usual, we consider the matrices of the overlaps of the single particle orbitals, namely the matrices $< \varphi'_i | \chi_j >, < \chi'_i | \varphi_j >, < \varphi'_i | \varphi_j >$ and their inverse matrices A_{ij}, A'_{ij}, B_{ij}, respectively. This generates the standard cofactors M_{ij}, M_{ijlk}, M_{ijknml},...M'_{ij},...N_{ijknml} such as defined by

$$< \widetilde{\Phi}' | \bar{\chi} >= \det (< \varphi'_i | \chi_j >) = \sum_j < \varphi'_i | \chi_j > M_{ij} \text{ with } M_{ij} =< \widetilde{\Phi}' | \bar{\chi} > A_{ji}, \quad (3.2a)$$

$$M'_{ik} = \sum_l < \chi'_j | \varphi_l > M'_{ijlk} \text{ with } M'_{ijlk} =< \bar{\chi}' | \widetilde{\Phi} > (A'_{ki} A'_{lj} - A'_{kj} A'_{li}), \qquad (3.2b)$$

$$N_{ijml} = \sum_n < \varphi'_k | \varphi_n > N_{ijknml} \text{ with } N_{ijknml} =< \Phi' | \Phi > \times$$

$$(B_{li} B_{mj} B_{nk} - B_{li} B_{mk} B_{nj} - B_{lj} B_{mi} B_{nk} + B_{lj} B_{mk} B_{ni} + B_{lk} B_{mi} B_{nj} - B_{lk} B_{mj} B_{ni}). \quad (3.2c)$$

Accordingly, one obtains the derivatives

$$\frac{\partial < \Phi' | \Phi >}{\partial < \varphi'_i | \varphi_j >} = N_{ij}, \qquad (3.3a)$$

$$\frac{\partial M'_{kl}}{\partial < \chi'_i | \varphi_j >} = M'_{kijl}, \qquad (3.3b)$$

$$\frac{\partial M_{klnm}}{\partial < \varphi'_i | \chi_j >} = M_{klijnm}. \qquad (3.3c)$$

A straightforward calculation then gives

$$< \widetilde{\Phi}' \mid V \mid \bar{\chi} > = \frac{1}{2} \sum_{ij\alpha\beta} < \varphi'_i \varphi'_j \mid v \mid \chi_\alpha \chi_\beta > M_{ij\beta\alpha}, \tag{3.4a}$$

$$< \bar{\chi}' \mid V \mid \widetilde{\Phi} > = \frac{1}{2} \sum_{\gamma\delta ij} < \chi'_\gamma \chi'_\delta \mid v \mid \varphi_i \varphi_j > M'_{\gamma\delta ji}, \tag{3.4b}$$

$$< \Phi' \mid (z - H) \mid \Phi >= z\det(< \varphi'_i \mid \varphi_j >) -$$

$$\sum_{ij} < \varphi'_i \mid t \mid \varphi_j > N_{ij} - \frac{1}{4} \sum_{ijkl} < \varphi'_i \varphi'_j \mid v \mid \varphi_k \varphi_l > N_{ijlk}, \tag{3.4c}$$

where Latin indices $i, j...l$ run from 1 to N, while Greek indices $\alpha, \beta, \gamma, \delta$ run only inside the labels allowed for nuclei a,b,c,d, respectively. All matrix elements of v are antisymmetrized.

The functional derivatives of C and C' then read

$$\frac{\delta C}{\delta < \varphi'_i \mid} = (N_a! N_b! / N!)^{1/2} \times$$

$$\left(\sum_{j\alpha\beta} < . \ \varphi'_j \mid v \mid \chi_\alpha \chi_\beta > M_{ij\beta\alpha} + \frac{1}{2} \sum_{jmn\alpha\beta} < \varphi'_m \varphi'_n \mid v \mid \chi_\alpha \chi_\beta > M_{mnij\beta\alpha} \mid \chi_j > \right), \tag{3.5a}$$

$$\frac{\delta C'}{\delta \mid \varphi_j >} = (N_c! N_d! / N!)^{1/2} \times$$

$$\left(\sum_{i\gamma\delta} < \chi'_\gamma \chi'_\delta \mid v \mid . \ \varphi_i > M'_{\gamma\delta ij} + \frac{1}{2} \sum_{i\gamma\delta mn} < \chi'_\gamma \chi'_\delta \mid v \mid \varphi_m \varphi_n > M'_{\gamma\delta ijnm} < \chi'_i \mid \right). \tag{3.5b}$$

This suggests the definition of the following non Hermitian, channel mean field potentials,

$$< . \mid S_b \mid \chi_\alpha >=< \widetilde{\Phi}' \mid \bar{\chi} >^{-1} \sum_{j\beta} < . \ \varphi'_j \mid v \mid \chi_\alpha \chi_\beta > M_{j\beta}, \tag{3.6a}$$

$$< . \mid S_a \mid \chi_\beta >=< \widetilde{\Phi}' \mid \bar{\chi} >^{-1} \sum_{j\alpha} < . \ \varphi'_j \mid v \mid \chi_\beta \chi_\alpha > M_{j\alpha}, \tag{3.6b}$$

$$< \chi'_\gamma \mid S'_d \mid . >=< \bar{\chi}' \mid \widetilde{\Phi} >^{-1} \sum_{\delta i} < \chi'_\gamma \chi'_\delta \mid v \mid . \ \varphi_i > M'_{\delta i}, \tag{3.6c}$$

$$< \chi'_\delta \mid S'_c \mid . >=< \bar{\chi}' \mid \widetilde{\Phi} >^{-1} \sum_{\gamma i} < \chi'_\delta \chi'_\gamma \mid v \mid . \, \varphi_i > M'_{\gamma i}, \tag{3.6d}$$

which correspond to traces of v on "densities" related to nuclei b,a,d,c, respectively. It will be noticed that S_b acts upon orbitals χ_α of nucleus a only. In the same way, S_a, a trace on a "density" related to nucleus a, acts upon orbitals χ_β of nucleus b only. Accordingly, both formulae, Eqs.(3.6a,b), can be interpreted as the definition of a unique mean field potential S. Completely similar considerations are valid with Eqs.(3.6c,d), both traces on nuclei d and c defining a potential S', acting in turn on orbitals χ'_γ and χ'_δ, respectively.

The functional derivatives of D are

$$\frac{\delta D}{\delta < \varphi'_i \mid} = \sum_j (z-t) \mid \varphi_j > N_{ij} - \sum_{jkl} < \varphi'_k \mid t \mid \varphi_l > N_{kijl} \mid \varphi_j > -$$

$$\frac{1}{2} \sum_{jkl} < . \, \varphi'_k \mid v \mid \varphi_j \varphi_l > N_{iklj} - \frac{1}{4} \sum_{jmnkl} < \varphi'_m \varphi'_n \mid v \mid \varphi_k \varphi_l > N_{mnijlk} \mid \varphi_j >, \tag{3.5c}$$

$$\frac{\delta D}{\delta \mid \varphi_j >} = \sum_i < \varphi'_i \mid (z-t) N_{ij} - \sum_{ikl} < \varphi'_k \mid t \mid \varphi_l > N_{kijl} < \varphi'_i \mid -$$

$$\frac{1}{2} \sum_{ikl} < \varphi'_i \varphi'_k \mid v \mid . \, \varphi_l > N_{iklj} - \frac{1}{4} \sum_{imnkl} < \varphi'_m \varphi'_n \mid v \mid \varphi_k \varphi_l > N_{mnijlk} < \varphi'_i \mid . \tag{3.5d}$$

This suggests the definition of the following non Hermitian, mean field potential,

$$< . \mid U \mid \varphi_j >=< \Phi' \mid \Phi >^{-1} \sum_{kl} < . \, \varphi'_k \mid v \mid \varphi_j \varphi_l > N_{kl}, \tag{3.6e}$$

$$< \varphi'_i \mid U \mid . >=< \Phi' \mid \Phi >^{-1} \sum_{kl} < \varphi'_i \varphi'_k \mid v \mid . \, \varphi_l > N_{kl}. \tag{3.6f}$$

With such definitions of S, S', U, the functional derivatives now read

$$\frac{\delta C}{\delta < \varphi'_i \mid} = (N_a! N_b! / N!)^{1/2} < \widetilde{\Phi}' \mid \bar{\chi} > \times$$

$$\left[\sum_j \left(S + \sum_{kl} < \varphi'_k \mid \frac{S}{2} \mid \chi_l > A_{lk} \right) \mid \chi_j > A_{ji} - \sum_{jkl} < \varphi'_k \mid S \mid \chi_l > A_{li} A_{jk} \mid \chi_j > \right], \tag{3.7a}$$

$$\frac{\delta C'}{\delta \mid \varphi_j >} = (N_c! N_d! / N!)^{1/2} < \bar{\chi}' \mid \widetilde{\Phi} > \times$$

$$\left[\sum_i A'_{ji} < \chi'_i \mid \left(S' + \sum_{kl} < \chi'_k \mid \frac{S'}{2} \mid \varphi_l > A'_{lk} \right) - \sum_{ikl} < \chi'_k \mid S' \mid \varphi_l > A'_{li} A'_{jk} < \chi'_i \mid \right]. \tag{3.7b}$$

$$\frac{\delta D}{\delta < \varphi'_i \mid} = < \Phi' \mid \Phi > \left[\sum_j \left(z - t - U - \sum_{kl} < \varphi'_k \mid (t + \frac{U}{2}) \mid \varphi_l > B_{lk} \right) \mid \varphi_j > B_{ji} + \right.$$

$$\left. \sum_{jkl} < \varphi'_k \mid (t+U) \mid \varphi_l > B_{li} B_{jk} \mid \varphi_j > \right], \tag{3.7c}$$

$$\frac{\delta D}{\delta \mid \varphi_j >} = < \Phi' \mid \Phi > \left[\sum_i B_{ji} < \varphi'_i \mid \left(z - t - U - \sum_{kl} < \varphi'_k \mid (t + \frac{U}{2}) \mid \varphi_l > B_{lk} \right) + \right.$$

$$\left. \sum_{ikl} < \varphi'_k \mid (t+U) \mid \varphi_l > B_{li} B_{jk} < \varphi'_i \mid \right]. \tag{3.7d}$$

We now take advantage of the fact that a Slater determinant is invariant, except for an inessential change of phase and norm, under the linear rearrangement of its orbitals. Hence a linear rearrangement of orbitals φ_j can diagonalize one out the four matrices $< \varphi'_i \mid \varphi_j >$, $< \varphi'_i \mid h \mid \varphi_j >$, $< \chi'_i \mid \varphi_j >$, $< \chi'_i \mid S' \mid \varphi_j >$. In the same way, a linear rearrangement of orbitals φ'_i can diagonalize one out of the four matrices $< \varphi'_i \mid \varphi_j >$, $< \varphi'_i \mid h \mid \varphi_j >$, $< \varphi'_i \mid \chi_j >$, $< \varphi'_i \mid S \mid \chi_j >$. In a representation where both overlap matrices $< \varphi'_i \mid \chi_j >$ and $< \chi'_i \mid \varphi_j >$ are diagonal, these formulae reduce to

$$\frac{\delta C}{\delta < \varphi'_i \mid} = (N_a! N_b! / N!)^{1/2} < \widetilde{\Phi}' \mid \bar{\chi} > < \varphi'_i \mid \chi_i >^{-1} \times$$

$$\left[\left(S + \frac{1}{2} \sum_k \frac{< \varphi'_k \mid S \mid \chi_k >}{< \varphi'_k \mid \chi_k >} \right) \mid \chi_i > - \sum_j \frac{< \varphi'_j \mid S \mid \chi_i >}{< \varphi'_j \mid \chi_j >} \mid \chi_j > \right], \tag{3.8a}$$

$$\frac{\delta C'}{\delta \mid \varphi_j >} = (N_c! N_d! / N!)^{1/2} < \bar{\chi}' \mid \widetilde{\Phi} > < \chi'_j \mid \varphi_j >^{-1} \times$$

$$\left[< \chi'_j \mid \left(S' + \frac{1}{2} \sum_k \frac{< \chi'_k \mid S' \mid \varphi_k >}{< \chi'_k \mid \varphi_k >} \right) - \sum_i \frac{< \chi'_j \mid S' \mid \varphi_i >}{< \chi'_i \mid \varphi_i >} < \chi'_i \mid \right], \tag{3.8b}$$

where one finds that the reference energy for S, resp. S', is $< \Phi' \mid V \mid \chi > / < \Phi' \mid \chi >$, resp. $< \chi' \mid V' \mid \Phi > / < \chi' \mid \Phi >$, see also Eq.(3.9). Alternately, in a representation where both matrices $< \varphi'_i \mid \varphi_j >$ and $< \varphi'_i \mid h \mid \varphi_j >$, with $h \equiv t + U$, are diagonal, the simplification reads

$$\frac{\delta D}{\delta < \varphi_i' \mid} = \frac{< \Phi' \mid \Phi >}{< \varphi_i' \mid \varphi_i >} \left(z - h - \sum_k \frac{< \varphi_k' \mid (t + \frac{U}{2}) \mid \varphi_k >}{< \varphi_k' \mid \varphi_k >} + \frac{< \varphi_i' \mid h \mid \varphi_i >}{< \varphi_i' \mid \varphi_i >} \right) \mid \varphi_i >, \tag{3.8c}$$

$$\frac{\delta D}{\delta \mid \varphi_j >} = \frac{< \Phi' \mid \Phi >}{< \varphi_j' \mid \varphi_j >} < \varphi_j' \mid \left(z - h - \sum_k \frac{< \varphi_k' \mid (t + \frac{U}{2}) \mid \varphi_k >}{< \varphi_k' \mid \varphi_k >} + \frac{< \varphi_j' \mid h \mid \varphi_j >}{< \varphi_j' \mid \varphi_j >} \right), \tag{3.8d}$$

where one finds the reference energy for h,

$$\bar{E} \;=\; \frac{< \Phi' \mid H \mid \Phi >}{< \Phi' \mid \Phi >} \;=\; \sum_k \frac{< \varphi_k' \mid (t + \frac{U}{2}) \mid \varphi_k >}{< \varphi_k' \mid \varphi_k >}, \tag{3.9}$$

and self energies for φ_i, φ_i',

$$\eta_i \;=\; z - \;\bar{E}\; + \;\frac{< \varphi_i' \mid h \mid \varphi_i >}{< \varphi_i' \mid \varphi_i >}. \tag{3.10}$$

We notice that the unknown orbitals φ_i are much less coupled to one another in Eq.(3.8c) than in Eq.(3.7c), and the same remark holds for the φ_j' when Eq.(3.7d) simplifies into Eq.(3.8d). Hence, among all the possible rearrangements which could technically simplify practical calculations, we choose those representations which simultaneously diagonalize $< \varphi_i' \mid \varphi_j >$ and $< \varphi_i' \mid h \mid \varphi_j >$. The remaining four matrices will in general be non diagonal. Eqs.(3.8c), (3.8d) also have the advantage that they are close to the traditional, homogeneous Hartree-Fock scheme.

The stationarity conditions,

$$\frac{\delta (C - D)}{\delta < \varphi_i' \mid} = 0\,, \;\frac{\delta (C' - D)}{\delta \mid \varphi_j >} = 0 \tag{3.11}$$

then read

$$(\eta_i - h) \mid \varphi_i > = \; \frac{(N_a! N_b! / N!)^{1/2} \;\; < \widetilde{\Phi}' \mid \bar{\chi} > < \varphi_i' \mid \varphi_i >}{< \Phi' \mid \Phi >} \times$$

$$\left[\sum_j \left(S + \sum_{kl} < \varphi_k' \mid \frac{S}{2} \mid \chi_l > A_{lk} \right) \mid \chi_j > A_{ji} - \sum_{jkl} < \varphi_k' \mid S \mid \chi_l > A_{li} A_{jk} \mid \chi_j > \right], \tag{3.12a}$$

and

$$< \varphi'_j \mid (\eta_j - h) = \frac{(N_c!N_d!/N!)^{1/2} \ \ < \bar{\chi}' \mid \widetilde{\Phi} > < \varphi'_j \mid \varphi_j >}{< \Phi' \mid \Phi >} \times$$

$$\left[\sum_i A'_{ji} < \chi'_i \mid \left(S' + \sum_{kl} < \chi'_k \mid \frac{S'}{2} \mid \varphi_l > A'_{lk} \right) - \sum_{ikl} < \chi'_k \mid S' \mid \varphi_l > A'_{li} A'_{jk} < \chi'_i \mid \right] . \tag{3.12b}$$

A slight simplification of the r.h.s. of Eqs.(3.12) is further possible: because χ_a and χ_b are Slater determinants, a linear rearrangement of the orbitals χ_α among themselves, and a separate rearrangement of the orbitals χ_β, can partly diagonalize the matrix $< \varphi'_i \mid \chi_j >$, but the simplicity of Eq.(3.8a) cannot be obtained under such a partial diagonalization. The same holds for separate rearrangements of χ'_γ and χ'_δ, which can induce the simplified r.h.s., Eq.(3.8b), partly only.

It will be interesting, in future numerical applications, to investigate whether the residual off-diagonal parts of $< \varphi'_i \mid \chi_j >$ and $< \chi'_i \mid \varphi_j >$ can be neglected. If so, the corresponding approximation would create a representation where all four equations, Eqs.(3.8), would be almost compatible. This "one-orbital-partner" approximation would represent the many-body collision by single-particle transitions $\chi_i \to \varphi'_i$, $\varphi_i \to \chi'_i$, with a conservation of the label i.

For the sake of completeness, we recall here a result, shown earlier[4] in a slightly different context where both χ, χ' are full Slater determinants rather than products of such determinants. The result is still valid for the present paper:
Theorem: The solutions φ_i, φ'_j of Eqs.(3.12) are consistent with the ansatz that both matrices $< \varphi'_i \mid \varphi_j >$ and $< \varphi'_i \mid h \mid \varphi_j >$ are diagonal.
Proof: For $i \neq j$, multiply Eq.(3.12a) by $< \varphi'_j \mid$ and Eq.(3.12b) by $\mid \varphi_i >$, respectively. Both resulting r.h.s. vanish, because the antisymmetries of Φ' and Φ with respect to their respective orbitals induce

$$< \varphi'_j \mid \frac{\delta C}{\delta < \varphi'_i \mid} >= 0 \, , < \frac{\delta C'}{\delta \mid \varphi_j >} \mid \varphi_i >= 0. \tag{3.13}$$

Variation of C and C' with respect to $< \varphi'_i \mid$ and $\mid \varphi_j >$ and subsequent scalar multiplication by $< \varphi'_j \mid$ and $\mid \varphi_i >$ will for $j \neq i$ create two identical rows (or columns) in the determinantal structure of C and C'.

4. Self Consistent Symmetries

In practical calculations one often uses channel wave functions which have some symmetry. Then one can choose trial functions having the same symmetry, without destroying the self consistency of the mean field equations, if some commutation relations are fulfilled. Using such self consistent symmetries could be called a "projection before variation" and may reduce the number of coupled mean field equations enormously.

Let us first consider a unitary operator P acting in single-particle space, which relates the χ_i's through

$$P|\chi_i>= e^{i\theta_i}|\chi_{\sigma(i)}> \text{ and } <\chi'_i|P^\dagger =<\chi'_{\sigma(i)}|e^{-i\theta_i}, \tag{4.1}$$

where σ indicates a permutation among the orbitals and θ_i is an arbitrary i-dependent phase. Then one can choose

$$P|\varphi_i>= e^{i\theta_i}|\varphi_{\sigma(i)}> \text{ and } <\varphi'_i|P^\dagger =<\varphi'_{\sigma(i)}|e^{-i\theta_i}, \tag{4.2}$$

if the following commutation relations are valid

$$[t,P]=0\,,\ [v,P\otimes P]=0, \tag{4.3a}$$

and if furthermore the transformation P leaves the orbitals in the same fragment or transfers all orbitals from one fragment to the other, as we shall prove below.

For the overlap matrices $\beta_{ij}=<\varphi'_i|\varphi_j>$, $\alpha_{ij}=<\varphi'_i|\chi_j>$, $\alpha'_{ij}=<\chi'_i|\varphi_j>$, the unitarity of P implies

$$\beta_{ij}=e^{i(\theta_j-\theta_i)}\beta_{\sigma(i)\sigma(j)}\,,\ \alpha_{ij}=e^{i(\theta_j-\theta_i)}\alpha_{\sigma(i)\sigma(j)}\,,\ \alpha'_{ij}=e^{i(\theta_j-\theta_i)}\alpha'_{\sigma(i)\sigma(j)}. \tag{4.4}$$

Next let us study the transformation properties of cofactors and inverse matrices. Writing the generalized cofactor expansion of $\det\beta$, which is invariant under Eq.(4.2), as

$$\delta_{ki}\det\beta=\sum_j\beta_{ij}N_{kj}=\sum_j e^{i(\theta_j-\theta_i)}\beta_{\sigma(i)\sigma(j)}N_{kj}, \tag{4.5}$$

and comparing with

$$\delta_{\sigma(k)\sigma(i)}\det\beta=\sum_j\beta_{\sigma(i)j}N_{\sigma(k)j}=\sum_j\beta_{\sigma(i)\sigma(j)}N_{\sigma(k)\sigma(j)}, \tag{4.6}$$

one finds :

$$N_{ij}=e^{-i(\theta_j-\theta_i)}N_{\sigma(i)\sigma(j)}, \tag{4.7a}$$

and for the inverse of the overlap matrix β

$$B_{ij} = e^{i(\theta_j - \theta_i)} B_{\sigma(i)\sigma(j)}. \tag{4.7b}$$

In the same way one gets

$$M_{ij} = e^{-i(\theta_j - \theta_i)} M_{\sigma(i)\sigma(j)}\,,\; M'_{ij} = e^{-i(\theta_j - \theta_i)} M'_{\sigma(i)\sigma(j)}. \tag{4.7c}$$

Eq.(4.2) together with Eq.(4.3a) give

$$< \varphi'_i|t|\varphi_j >= e^{i(\theta_j - \theta_i)} < \varphi'_{\sigma(i)}|t|\varphi_{\sigma(j)} > . \tag{4.8a}$$

and

$$< \varphi'_i\varphi'_k|v|\varphi_j\varphi_l >= e^{i(\theta_j + \theta_l - \theta_i - \theta_k)} < \varphi'_{\sigma(i)}\varphi'_{\sigma(k)}|v|\varphi_{\sigma(j)}\varphi_{\sigma(l)} > . \tag{4.8b}$$

From (4.8a,b) together with (4.7a,b) we find for the self consistent one-body operators U and h

$$< \varphi'_i|U|\varphi_j >= e^{i(\theta_j - \theta_i)} < \varphi'_{\sigma(i)}|U|\varphi_{\sigma(j)} > \text{ and } < \varphi'_i|h|\varphi_j >= e^{i(\theta_j - \theta_i)} < \varphi'_{\sigma(i)}|h|\varphi_{\sigma(j)} >, \tag{4.9a}$$

or extending to the full Hilbert space of single-particle motion

$$[U, P] = 0\,,\; [h, P] = 0. \tag{4.9b}$$

Eqs.(4.9a) and (4.9b) together with Eq.(4.7b) will prove sufficient for the l.h.s. of the mean field equations (3.12) to be invariant. We will now turn to the inhomogeneous terms on their r.h.s..

To this end, let us define ρ (resp. ρ') as a matrix with elements equal to 0 if the orbitals χ_i and χ_j (resp. χ'_i and χ'_j) are from the same fragment and 1 if they are from different fragments. Then if P satisfies

$$\rho_{ij} = \rho_{\sigma(i)\sigma(j)} \text{ and } \rho'_{ij} = \rho'_{\sigma(i)\sigma(j)}, \tag{4.3b}$$

we have

$$< \cdot\, |[S, P]|\chi_i >= 0\,,\; < \chi'_i|[S', P]|\,\cdot >= 0, \tag{4.10a}$$

where

$$S|\chi_i >= (\det \alpha)^{-1} \sum_{kl} \rho_{il} < \cdot\; \varphi'_k|v|\chi_i\chi_l > M_{kl}, \tag{4.10b}$$

$$< \chi'_i|S' = (\det \alpha')^{-1} \sum_{kl} \rho'_{ki} < \chi'_i\chi'_k|v| \cdot \varphi_l > M'_{kl}, \tag{4.10c}$$

use having been made of Eq.(4.7c) and the analogue of Eq.(4.8b) for the channel potentials.

To prove the self consistency of the ansatz (4.2), one has to show that

$$P\frac{\delta F}{\delta < \varphi_i'|} = e^{i\theta_i}\frac{\delta F}{\delta < \varphi_{\sigma(i)}'|} \ . \tag{4.11}$$

This is exemplified for Eq. (3.7c) where the symbol $\bar{\eta}$ is used for the i-independent part of the self energy

$$P \det\beta \left[\sum_j (z-h-\bar{\eta})B_{ji} + \sum_{jkl} < \varphi_k'|h|\varphi_l > B_{li}B_{jk}\right] |\varphi_j >=$$

$$e^{i\theta_i}\det\beta \left[\sum_j (z-h-\bar{\eta})B_{\sigma(j)\sigma(i)} + \sum_{jkl} < \varphi_{\sigma(k)}'|h|\varphi_{\sigma(l)} > B_{\sigma(l)\sigma(i)}B_{\sigma(j)\sigma(k)}\right] |\varphi_{\sigma(j)} >, \tag{4.12}$$

using (4.7b) and (4.9a,b). This is the desired result because in the sum $\sigma(j)$ can be replaced by j for every summation index. The same can be done for the r.h.s. of the mean field equations (3.7a) and for Eqs.(3.7b,d), which completes the proof of the self consistency of the ansatz (4.2).

The second case are antiunitary symmetries like time reversal. Let us recall the properties of antiunitary operators A,

$$A(\lambda|\varphi >) = \lambda^* A|\varphi >, \tag{4.13a}$$

$$< \varphi'|(A|\varphi >) = (< \varphi'|A)|\varphi >^* \tag{4.13b}$$

and

$$A^\dagger A = AA^\dagger = 1 \text{ or } < \varphi'|\varphi >= \left[(< \varphi'|A^\dagger)(A\varphi >)\right]^* . \tag{4.13c}$$

Let us consider a situation where

$$A|\chi_i >= e^{i\theta_i}|\chi_{\sigma(i)}' > \text{ and } < \chi_i'|A^\dagger =< \chi_{\sigma(i)}|e^{-i\theta_i}. \tag{4.14}$$

Then one can choose

$$A|\varphi_i >= e^{i\theta_i}|\varphi_{\sigma(i)}' > \text{ and } < \varphi_i'|A^\dagger =< \varphi_{\sigma(i)}|e^{-i\theta_i}, \tag{4.15}$$

to fulfill the mean field equations provided A obeys the following relations

$$At = t^\dagger A\,,\ (A\otimes A)v = v^\dagger(A\otimes A), \tag{4.16a}$$

and leaves the orbitals in the same fragment or transfers all orbitals from one fragment to the other such that

$$\rho_{ij} = \rho'_{\sigma(j)\sigma(i)}\,,\; \rho'_{ij} = \rho_{\sigma(j)\sigma(i)}. \tag{4.16b}$$

For Hermitian t and v, Eqs.(4.16a) reduce to commutator relations. From (4.13c) it can be seen that

$$\beta_{ij} = e^{i(\theta_i-\theta_j)}\beta_{\sigma(j)\sigma(i)}\,,\; \alpha_{ij} = e^{i(\theta_i-\theta_j)}\alpha'_{\sigma(j)\sigma(i)}\,,\; \alpha'_{ij} = e^{i(\theta_i-\theta_j)}\alpha_{\sigma(j)\sigma(i)} \tag{4.17a}$$

and

$$\det\alpha = \det\alpha'. \tag{4.17b}$$

Like in (4.5) and (4.6), one has for example

$$\delta_{ki}\det\alpha = \sum_j \alpha_{ij}M_{kj} = \delta_{\sigma(k)\sigma(i)}\det\alpha' = \sum_j e^{i(\theta_i-\theta_j)}\alpha'_{\sigma(j)\sigma(i)}M'_{\sigma(j)\sigma(k)}, \tag{4.18}$$

hence we can conclude

$$M_{ij} = e^{-i(\theta_i-\theta_j)}M'_{\sigma(j)\sigma(i)}\,,\; M'_{ij} = e^{-i(\theta_i-\theta_j)}M_{\sigma(j)\sigma(i)}, \tag{4.19a}$$

similarly

$$N_{ij} = e^{-i(\theta_i-\theta_j)}N_{\sigma(j)\sigma(i)}\,,\; B_{ij} = e^{i(\theta_i-\theta_j)}B_{\sigma(j)\sigma(i)}. \tag{4.19b}$$

For the matrix elements of t one calculates

$$<\varphi'_i|t|\varphi_j> = e^{i(\theta_i-\theta_j)} <\varphi'_{\sigma(j)}|t|\varphi_{\sigma(i)}>, \tag{4.20}$$

while for v

$$<\varphi'_i\varphi'_k|v|\varphi_j\varphi_l> = <\varphi'_i\varphi'_k|\left[v(A\otimes A)^\dagger(A\otimes A)|\varphi_j\varphi_l>\right] =$$

$$\left(\left[<\varphi'_i\varphi'_k|(A\otimes A)^\dagger\right]v^\dagger\left[(A\otimes A)|\varphi_j\varphi_l>\right]\right)^* = e^{i(\theta_i+\theta_k-\theta_j-\theta_l)} <\varphi'_{\sigma(j)}\varphi'_{\sigma(l)}|v|\varphi_{\sigma(i)}\varphi_{\sigma(k)}> . \tag{4.21}$$

Therefore

$$<\varphi'_i|U|\varphi_j> = e^{i(\theta_i-\theta_j)} <\varphi'_{\sigma(j)}|U|\varphi_{\sigma(i)}>\,,\; <\varphi'_i|h|\varphi_j> = e^{i(\theta_i-\theta_j)} <\varphi'_{\sigma(j)}|h|\varphi_{\sigma(i)}>, \tag{4.22}$$

whereas S is related to S'

$$<\varphi'_i|S|\chi_j> = e^{i(\theta_i-\theta_j)} <\chi'_{\sigma(j)}|S'|\varphi_{\sigma(i)}>\,,\; <\chi'_i|S'|\varphi_j> = e^{i(\theta_i-\theta_j)} <\varphi'_{\sigma(j)}|S|\chi_{\sigma(i)}> . \tag{4.23}$$

Now we are able to express the commutation relations for S, S' and U, h with A as

$$AU = U^\dagger A\,,\; Ah = h^\dagger A, \tag{4.24a}$$

$$< \cdot\, |(AS|\chi_i >) =< \cdot\, |(S'^\dagger A|\chi_i >)\,,\; (< \chi_i'|AS')|\, \cdot >= (< \chi_i'|S^\dagger A)|\, \cdot >, \tag{4.24b}$$

and as in (4.12) we can conclude

$$A \det \beta \left[\sum_j (z - h - \bar{\eta}) B_{ji} + \sum_{jkl} < \varphi_k'|h|\varphi_l > B_{li} B_{jk} \right] |\varphi_j >=$$

$$e^{i\theta_i} \det \beta \left[\sum_j (z^* - h^\dagger - \bar{\eta}^*) B^*_{\sigma(i)j} + \sum_{jkl} < \varphi_k'|h|\varphi_l >^* B^*_{lj} B^*_{\sigma(i)k} \right] |\varphi_j' > . \tag{4.25}$$

Apart from a phase factor we recognize the l.h.s. of the complex conjugate mean field equation resulting from $\delta F/\delta|\varphi_{\sigma(i)} >$. Doing the same for the r.h.s. proves the consistency of the ansatz (4.15). It is worth noting that the above proofs simplify if one uses the diagonal representation in channel-spin formalism (see Appendix).

It is possible to generalize (4.1) or (4.14). We consider the case where the unitary operator P acts only inside the given set of orbitals χ_i and χ_i' such that

$$P|\chi_i >= \sum_j L_{ji}|\chi_j > \text{ and } < \chi_i'|P^\dagger = \sum_j < \chi_j'|L^\dagger_{ij} \;\; . \tag{4.26}$$

Then the following ansatz is self consistent

$$P|\varphi_i >= \sum_j L_{ji}|\varphi_j > \text{ and } < \varphi_i'|P^\dagger = \sum_j < \varphi_j'|L^\dagger_{ij} \;\; , \tag{4.27}$$

i.e. it fulfills

$$P \frac{\delta F}{\delta < \varphi_i'|} = \sum_j L_{ji} \frac{\delta F}{\delta < \varphi_j'|} = \frac{\delta F}{\delta(< \varphi_i'|P^+)} \;\; , \tag{4.28}$$

provided the commutator conditions (4.3a) are satisfied together with

$$[\rho, L] = [\rho', L] = 0. \tag{4.29}$$

If (4.28) is valid then P generates out of the i-th mean field equation the equation for the transformed orbital, which therefore can be left out of the actual calculation. The proof starts by noting that

$$\beta_{ij} = \sum_{kl} L^\dagger_{ik} L_{lj} \beta_{kl}, \tag{4.30a}$$

in short

$$\beta = L^{\dagger}\beta L, \tag{4.30b}$$

which leads to

$$[\beta, L] = 0\,,\ \ [\tilde{N}, L] = 0 \ \text{ and } \ [B, L] = 0. \tag{4.31a}$$

Here $\tilde{N}$ is the transpose of the cofactor matrix N_{ij}. By the same argument

$$[\tilde{M}, L] = 0 \,\text{and}\ \ [\tilde{M}', L] = 0. \tag{4.31b}$$

Using (4.3a) one finds

$$U \det\beta = \sum_{kl} <\cdot\,\varphi_k'|v|\cdot\varphi_l> N_{kl} = P^{\dagger}\left(\sum_{kl}\sum_{mn} L_{kn}^{\dagger} L_{ml} <\cdot\,\varphi_k'|v|\cdot\ \varphi_l> N_{kl}\right) P, \tag{4.32}$$

and applying (4.31a) results in

$$U = P^{\dagger}\left((\det\beta)^{-1}\sum_{mn} N_{nm} <\cdot\,\varphi_n'|v|\cdot\varphi_m>\right) P = P^{\dagger} U P. \tag{4.33}$$

Thus one can list the following properties

$$[U, P] = 0\,,\ [S, P] = [S', P] = 0 \,\text{and}\, [h, P] = 0, \tag{4.34}$$

which lead to

$$[\bar{U}, L] = 0\,,\ [\bar{S}, L] = [\bar{S}', L] = 0\,,\ \text{and}\, [\bar{h}, L] = 0. \tag{4.35}$$

$\bar{U}$, $\bar{S}$, $\bar{S}'$ and $\bar{h}$ are defined as the matrices $U_{ij} =< \varphi_i'|U|\varphi_j >$ etc. With these relations the proof of (4.28) is simple. For the example (3.7c) the l.h.s. of (4.28) can be written as

$$(\det\beta)\sum_j \left[(z - h - \bar{\eta})\,(LB)_{ji} + \left(LB\bar{h}B\right)_{ji}\right] |\varphi_j >=$$

$$= (\det\beta)\sum_j \left[(z - h - \bar{\eta})\,(BL)_{ji} + \left(B\bar{h}BL\right)_{ji}\right] |\varphi_j >, \tag{4.36}$$

where one recognizes the r.h.s. of (4.28). The same generalization can be done for anti-unitary transformations. On the other hand, the invariance of a Slater determinant under unitary transformations u of the orbitals, with $\det u = 1$, makes it possible to choose orbitals $u\chi_i$ so that (4.26) transforms into (4.1). The conditions (4.29) tell us that L has to be a block matrix like

$$\text{a)}\begin{pmatrix} l_1 & 0 \\ 0 & l_2 \end{pmatrix} \ \text{or}\ \ \text{b)}\begin{pmatrix} 0 & l_1 \\ l_2 & 0 \end{pmatrix}, \tag{4.37}$$

while u is restricted to type a), because the χ_i and χ_i''s are only partially antisymmetrized. With L, l_1 and l_2 unitary there exists a unitary matrix which diagonalizes them. Choosing such a u brings (4.26) into the form (4.1), with the $e^{i\theta_i}$ as eigenvalues. For case a) one finds $\sigma(i) = i$ while in case b) one has $\sigma^2(i) = i$ where $\sigma(i)$ and i refer to different fragments. In the next Section we use self consistent symmetries to reduce the 16 equations for the alpha-alpha system.

5. The α-α system

The elastic alpha-alpha collision has been studied by many authors [5] as a test bench of microscopic theories of collisions. As an application of antisymmetrized TIMF we consider elastic $\alpha-\alpha$ scattering in forward direction. A central, spin- and isospin-independent interaction is chosen as a sum of a short-range repulsion and a middle-range attraction, both Gaussians

$$v(\vec{r}, \vec{r'}) = V_a \exp(-\frac{|\vec{r} - \vec{r'}|^2}{r_a^2}) + V_r \exp(-\frac{|\vec{r} - \vec{r'}|^2}{r_r^2}) . \tag{5.1}$$

As potential depths V_a, V_r and ranges r_a, r_r we use the parameters proposed by Volkov [6]

$$V_a = -83.34\text{MeV}\ r_a = 1.6\text{fm}\ V_r = 144.86\text{MeV}\ r_r = 0.82\text{fm}\ .$$

The channel wavefunctions are described by boosted single nucleon Gaussians

$$\chi(\vec{r}, \vec{k}) = \pi^{-\frac{3}{4}}\beta^{-\frac{3}{2}} \exp(i\vec{k}\cdot\vec{r} - \frac{r^2}{2\beta^2}) , \tag{5.2}$$

where $\vec{k}$ is the single particle boost. Let $\vec{r}_1, \vec{r}_5$ denote the coordinates of the proton with spin up in the projectile and the target, respectively. In the same way, let $\vec{r}_2, \vec{r}_6, \vec{r}_3, \vec{r}_7, \vec{r}_4, \vec{r}_8$ denote the protons spin down, the neutrons spin up and the neutrons spin down, respectively. The 8-particle channel wavefunction is therefore given by

$$\chi(\vec{r}_1, ..., \vec{r}_8, \vec{k}) = \chi_1(\vec{r}_1, \vec{k}) \times ... \times \chi_4(\vec{r}_4, \vec{k}) \times \chi_5(\vec{r}_5, -\vec{k}) \times ... \times \chi_8(\vec{r}_8, -\vec{k}) . \tag{5.3}$$

Our problem has the following symmetries:

a. Spin Isospin symmetries within each cluster imply

$$\chi_1 = \chi_2 = \chi_3 = \chi_4 \text{ and } \chi_5 = \chi_6 = \chi_7 = \chi_8 . \tag{5.4}$$

b. Elastic scattering in forward direction, bra-ket symmetry:

$$\chi_i(\vec{r}) = \chi_i'(\vec{r}) \text{ for all i} \tag{5.5}$$

c. Forward scattering together with time reversal:

$$\chi_1^*(\vec{r}) = \chi_5'(\vec{r}), \quad \chi_5^*(\vec{r}) = \chi_1'(\vec{r}) \tag{5.6}$$

d. Parity:

$$\chi_1(\vec{r}) = \chi_5(-\vec{r}), \quad \chi_5'(\vec{r}) = \chi_1'(-\vec{r}). \tag{5.7}$$

Following Section 4, we can choose trial functions which are consistent with our variational equations

$$\varphi_1(\vec{r}) = \varphi_5(-\vec{r}), \quad \varphi_5'(\vec{r}) = \varphi_1'(-\vec{r}) \tag{5.8}$$

$$\varphi_1^*(\vec{r}) = \varphi_5'(\vec{r}), \quad \varphi_5^*(\vec{r}) = \varphi_1'(\vec{r})\,. \tag{5.9}$$

Spin and isospin symmetries are assumed again, naturally. As described in Section 3, it is convenient to use a biorthogonal representation : If we rearrange the trial functions into parity eigenstates, such a representation can be introduced as

$$\begin{aligned}
\tilde{\varphi}_+(\vec{r}) &= \sqrt{\frac{1}{2}}\,(\varphi_1(\vec{r}) + \varphi_5(\vec{r})) \\
\tilde{\varphi}_-(\vec{r}) &= \sqrt{\frac{1}{2}}\,(-\varphi_1(\vec{r}) + \varphi_5(\vec{r})) \\
\tilde{\varphi}_+'(\vec{r}) &= \sqrt{\frac{1}{2}}\,(\varphi_1'(\vec{r}) + \varphi_5'(\vec{r})) \\
\tilde{\varphi}_-'(\vec{r}) &= \sqrt{\frac{1}{2}}\,(-\varphi_1'(\vec{r}) + \varphi_5'(\vec{r}))\,.
\end{aligned} \tag{5.10}$$

The symmetries and the spin-isospin independence of the chosen interaction reduce the 16 coupled equations to only two coupled, non linear equations for $\tilde{\varphi}_+$ and $\tilde{\varphi}_-$ which have to be solved self consistently.

Because of our use of wave packets, zero point energies have to be taken into account. The zero point energy of a single nucleon is

$$<\chi_i'|t_i|\chi_i>_{k=0} = \; E_0 \; = \; \frac{3}{4}\frac{\hbar^2}{m\beta^2}\,, \tag{5.11}$$

where m is the nucleon mass. Note that E_0 is also the center-of-mass zero point energy of an alpha particle. The binding energy of the alpha particle consists of the internal nucleon-nucleon interaction and three zero point energies,

$$E_\alpha \; = \; 3E_0 \; + \; 6 <\chi_1'\chi_2'|v|\chi_1\chi_2> \;. \tag{5.12}$$

We adjust the width of the wave packet to 1.4 fm to get the experimental binding energy of the alpha particle. With wave packets the relative motion of the two alpha particles is not a pure plane wave, but also a wave packet of Gaussian shape. For that reason, a zero point correction for the relative motion is necessary.

Because of the Galilean invariance of our many particle system, the unphysical kinetic energy of the center-of-mass motion has to be subtracted. Hence the relative motion Hamiltonian reads

$$H_r \;=\; H - T_{CM} \;=\; H - \frac{1}{16m} \sum_{i=1}^{8} \vec{p_i}^{\,2} \,. \tag{5.13}$$

The problem of T_{CM} subtraction is the occurence of non diagonal terms , such as $\vec{p}_1 \cdot \vec{p}_2$. It is much simpler to approximate the center-of-mass kinetic energy operator T_{CM} by its zero point expectation value,

$$< T_{CM} > = \; E_0 \,. \tag{5.14}$$

With all these arguments, the total asymptotic energy consists of the kinetic energy of the relative motion and the binding energy of the two alpha particles as well as the zero point correction of relative motion and the center-of-mass subtraction

$$E \;=\; \frac{\hbar^2}{4m}(4k)^2 + 2E_\alpha + 2E_0 \,. \tag{5.15}$$

The two coupled equations for $\tilde{\varphi}_+$ and $\tilde{\varphi}_-$ are solved numerically, using a scaled Hamiltonian and the channel wavefunction as starting points. With the help of the Hamiltonian

$$H_\lambda = \sum_i t_i + \lambda \sum_{i,j} \frac{1}{2} v_{ij} \tag{5.16}$$

we modify the stationarity conditions (2.2c) by introducing an additional term

$$\lambda \mathcal{A} V|\chi> + (\lambda - 1)\, \mathcal{A} \sum_{\substack{i,j\epsilon 1,\cdots,4 \\ i,j\epsilon 5,\cdots,8}} \frac{1}{2} v_{ij}|\chi> - \; (z - H_\lambda)|\Phi> = \; 0 \,. \tag{5.17}$$

We start with a large scaling parameter λ, when Eq.(5.17) implies $|\,\Phi> \sim |\,\chi>$, and reduce this parameter to the physical value $\lambda = 1$. We also start with complex energies $E + i\Gamma$ and decrease Γ to zero to get the on-shell limit of $<\chi'|\Delta T|\chi>$. A partial wave expansion for the mean field solution is useful to reduce the numerical expense. Choosing $\vec{k}$ along the z-axis, one can expand the channel wave functions in partial waves with just magnetic quantum number $m = 0$:

$$r\chi_1(\vec{r}) = \sum_l \chi_l(r)\, Y_l^0(\hat{r}), \tag{5.18}$$

with

$$\chi_l(r) = r\,\pi^{-\frac{3}{4}}\beta^{-\frac{3}{2}}\hat{l}(4\pi)^{\frac{1}{2}}i^l j_l(kr)\exp(-\frac{r^2}{2\beta^2})\,. \tag{5.19}$$

In analogy we consider the following expansions of $\tilde{\varphi}_+$ and $\tilde{\varphi}_-$, see Eqs.(5.10),

$$r\tilde{\varphi}_+(\vec{r}) = \sum_{l\,even} \varphi_{l+}(r)\,Y_l^0(\hat{r}),$$

$$r\tilde{\varphi}_-(\vec{r}) = \sum_{l\,odd} \varphi_{l-}(r)\,Y_l^0(\hat{r}), \tag{5.20}$$

where the summation can be restricted to even and odd numbers, respectively. E.g., the left hand side of our mean field Equation (3.12a) in partial wave expansion for $\tilde{\varphi}_+$ then reads

$$\left[\eta_+ + \frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{\hbar^2 l(l+1)}{2mr^2}\right]\ \varphi_{l+}(r) - 3\sum_{l'} U_{ll'}^{++}(r)\varphi_{l'+}(r) - 4\sum_{l'} U_{ll'}^{--}(r)\varphi_{l'+}(r)$$

$$+\sum_{l'} U_{ll'}^{-+}(r)\varphi_{l'-}(r), \tag{5.21}$$

where

$$U_{ll'}^{\pi\nu}(r) = \sum_L \hat{L}\hat{l}\hat{l}'\begin{pmatrix} l\ l'\ L \\ 0\ 0\ 0\end{pmatrix}^2 U_L^{\pi\nu}(r), \tag{5.22}$$

$$U_L^{\pi\nu}(r) = \int dr' C_L(r,r')\sum_j\sum_{j'}\hat{j}\hat{j}'\hat{L}\begin{pmatrix} j\ j'\ L \\ 0\ 0\ 0\end{pmatrix}^2$$

$$\times\begin{cases} \varphi_{j+}(r')\varphi_{j'+}(r')/n_{++}, & \text{for } (\pi\nu)=(++); \\ \varphi_{j-}(r')\varphi_{j'-}(r')/n_{--}, & \text{for } (\pi\nu)=(--); \\ \varphi_{j-}(r')\varphi_{j'+}(r')/n_{--}, & \text{for } (\pi\nu)=(-+), \end{cases} \tag{5.23}$$

$$C_L(r,r') = V_a\,I_L(\frac{2rr'}{r_a^2})\exp(-\frac{r^2+r'^2}{r_a^2}) + V_r\,I_L(\frac{2rr'}{r_r^2})\exp(-\frac{r^2+r'^2}{r_r^2}), \tag{5.24}$$

$$n_{++} = <\tilde{\varphi}'_+|\tilde{\varphi}_+>,\ n_{--} = <\tilde{\varphi}'_-|\tilde{\varphi}_->, \tag{5.25}$$

and η_+ is the self energy corresponding to $\tilde{\varphi}_+$. Note that in general η_- is different from η_+ because of the chosen representation. Here I_L denotes the modified spherical Bessel function of order L. Also note that in Eq.(5.21), when written with explicit parity coupling, only local potential terms appear.

Corresponding to the expansion of the l.h.s. of Eq.(3.12a) an expansion of the source term is possible by using χ instead of $\tilde{\varphi}$. A channel potential $S_{ll'}^{+,1}$ acting on $\chi_{l'1}$ can be defined as

$$S_{ll'}^{+,1}(r) = \sum_L \hat{L}\hat{l}\hat{l}'\begin{pmatrix} l\ l'\ L \\ 0\ 0\ 0\end{pmatrix}^2 S_L^{+,1}(r), \tag{5.26}$$

with

$$S_L^{+,1}(r) = \int dr' C_L(r,r') \sum_j \sum_{j'} \hat{j}\hat{j}'\hat{L} \begin{pmatrix} j & j' & L \\ 0 & 0 & 0 \end{pmatrix}^2 \varphi_{j+}(r')\chi_{j'1}(r'). \tag{5.27}$$

The spin and isospin symmetry reduces the large amount of cofactors of first, second and third order to only cofactors between nucleons with same spin and isospin. The convergence of our method is usually fast. On the way to the on-shell limit neither bifurcation nor crossing occurred. As described in [7], solutions with incoming waves sometimes creep in. Standard relaxation techniques [8] change these solutions into outgoing ones. Relaxation techniques are also useful to speed up the convergence of our iterative method and remove other unphysical solutions.

The Born terms of both the antisymmetrized ($\diamond$) and the non-antisymmetrized ($\circ$) theories, respectively, are shown in Figure 1. Note their different behaviours when the boost k diminishes. This is an obvious illustration of the importance of exchange terms at low energies, whereas the Pauli principle may be neglected at high energies. One should, however, realize that the wave packets χ, χ' whose widths are related to the sizes of the fragments, may poorly correspond, at low energy, to well separated asymptotic fragments as required when using the above formula for the antisymmetrized transition amplitude. In consequence, the antisymmetrized wavepacket $\mathcal{A}|\chi>$ has vanishing norm as k tends to zero, and the antisymmetrization effect seen in $<\chi'|V\mathcal{A}|\chi>$ is likely to be too strong at low k-values: If the relative motion part of χ were a plane wave, one would only have to exclude $k=0$ where the fragments fully overlap; since we deal with wave packets, we have to exercise care in a finite region around $k=0$. This defect can be remedied completely by taking suitable superpositions [9] at different k-values on both the bra and the ket sides in the transition amplitude. Rather than going into such an elaborate calculation we restrict ourselves to estimating the correction by dividing $<\chi'|V\mathcal{A}|\chi>$ by the required* normalization factor $\sqrt{<\chi|\mathcal{A}|\chi>}$ on the ket side. As a result the antisymmetrized Born term is modified at low k-values as shown by the ($\triangle$) curve in Fig.1. The limiting value remains zero nevertheless.

Figure 2 displays the real parts of $<\chi'|\Delta T|\chi>$ as a function of the total asymptotic energy E for both the antisymmetrized and the non antisymmetrized calculations. In the same way, Figure 3 shows the energy dependence of the relative difference Δ between the antisymmetrized and non antisymmetrized results for the imaginary part of the multistep

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* Note that V and $\mathcal{A}$ do not commute, $<\chi'|V\mathcal{A}|\chi> \neq <\chi'|\mathcal{A}V\mathcal{A}|\chi>$, and renormalization is not required on the bra side.

amplitude

$$\Delta = \frac{<\chi'|\mathrm{Im}\Delta T|\chi>_{NA} - <\chi'|\mathrm{Im}\Delta T|\chi>_{AS}}{<\chi'|\mathrm{Im}\Delta T|\chi>_{NA}} \,. \tag{5.28}$$

As expected, antisymmetrization is important in the low-energy region. Regarding the defect of the channel waves χ, χ' at low energies, the same arguments apply as given above for the Born term.

Finally we show on Fig.4 an example of one of the wave functions φ generated by our code. It is remarkable that it is a square integrable state, although we are dealing with a theory of collisions. The reason for this is not only that the source terms χ, χ' are wave packets. Rather, a main feature of this formalism is the ocurrence of retarded self energies η with *finite* imaginary parts even when the imaginary part of the many body energy E vanishes on shell. We notice on Fig.4 the damped oscillations of φ_- away from the center of the interaction region. The damping is indeed due to the retardation expressed by Im η.

6. Discussion and Conclusion

At low energies not exceeding a few MeV per nucleon, previous microscopic theories of collisions [5] have been quite successful in the description of nuclear collisions. This success can be understood, to a large extent at least, from the limited number of channels open to the reaction mechanisms, as analyzed, e.g. by Tang [10]. Conversely, at large energies, beyond those corresponding to the Fermi momentum, effective theories have been also successfully proposed [11] for the derivation of optical potentials between the colliding nuclei. There is still room for a new microscopic approach, as shown by the present paper.

Indeed we have proved here that the TIMF antisymmetrized theory can be implemented numerically, although it seems to be somewhat demanding and ambitious in activating *all* degrees of freedom. The TIMF equations involve all the single particle wave functions on the same footing, while we can insist that low energy [5] as well as high energy [11] theories essentially privilege the wave functions and/or the interactions governing the relative degrees of freedom between the clusters. These TIMF equations generate *non perturbatively* intermediate states Φ, Φ' which parametrize the multistep transition amplitude and give a picture of the reaction mechanism, as illustrated by Fig.4.

Once again we want to stress the fact that we are using a wave packet representation of the T-matrix rather than the more physical plane wave representation of relative motion. The conversion of one representation into another [9] is a typical generator coordinate [12] problem, which we intend to study.

Finally, it is clear that the mean field calculation which has been presented here can accomodate higher order corrections. An advantage of the TIMF technique is its close connection with the traditional techniques of the shell model. Therefore Tamm-Dancoff corrections and even RPA corrections are available.

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Appendix Channel Spin

The prior and post interactions V, V' are symmetric under nucleon exchange *within* the respective fragments but unsymmetric when nucleon exchange *between* fragments is included. Under this partial lack of permutation symmetry, only pure product or intrafragment antisymmetrized wave functions χ, χ' were used so far in this paper. This is similar to the second quantized formulation of TDMF by Reinhardt [13]. We shall now show that there exists an equivalent "channel spin" formulation which works with totally antisymmetrized, two-component channel wave functions. For the sake of clarity of presentation, we shall slightly modify our notation of Sections 2 and 3 in the following way: We denote the pure products of (normalized) single-particle wave functions in initial and final channels, eq(3.1a), by round brackets $|\chi)$ and $(\chi'|$, respectively. Curly brackets are used for channel wave functions

$$|\chi\} = \sqrt{N_a!N_b!}\,\mathcal{A}_a\mathcal{A}_b|\chi)\ , \qquad (A.1a)$$

$$\{\chi'| = \sqrt{N_c!N_d!}\,(\chi'|\mathcal{A}_c\mathcal{A}_d\ , \qquad (A.1b)$$

which are normalized and antisymmetrized *within* the fragments a, b, c, d, in obvious notation. Angular brackets, like in $|\Phi>$, are reserved for fully antisymmetrized wave functions,

$$|\chi>= \frac{1}{\sqrt{N!}}\sum_{\mathcal{P}}(-)^{\mathcal{P}}\mathcal{P}|\chi). \qquad (A.1c)$$

With such $|\chi\}$, $\{\chi'|$ it is in general not possible to diagonalize all three overlap matrices $\alpha_{ij} =< \varphi'_i|\chi_j >$, $\alpha'_{ij} =< \chi'_i|\varphi_j >$, $\beta_{ij} =< \varphi'_i|\varphi_j >$ by rearrangement of orbitals within the four sets of wave functions $\{\chi_i\}$, $\{\chi'_i\}$, $\{\varphi_i\}$, $\{\varphi'_i\}$. This would correspond to solve the following set of equations for the matrices M, M' and B, B' where the latter two have block structures which do not mix orbitals of different fragments,

$$\begin{aligned} M'\beta M &= d_\beta\ ,\\ M'\alpha B &= d_\alpha\ ,\\ B'\alpha' M &= d_{\alpha'}\ , \end{aligned} \qquad (A.2)$$

with diagonal matrices d_α, $d_{\alpha'}$, d_β. This means that $B^{-1}\alpha^{-1}\beta\alpha'^{-1}B'^{-1} = d_\alpha^{-1}d_\beta d_{\alpha'}^{-1}$ has to be diagonal, which is not possible in general because of the block structure of B and B', which is a consequence of partial antisymmetrization. To diagonalize all three overlap matrices one has to work with totally antisymmetrized channel wave functions χ and χ'.

Because the actions of V and $(H-E)$ on an exact channel eigenstate are equivalent, one could replace V by $(H-E)$ which commutes with the total antisymmetrizer $\mathcal{A}$. However, the equivalence of $(H-E)$ and V (or V') is destroyed if approximate channel wave functions χ, χ' are used, like in the mean field approximation, when $(H-E)|\chi>$ and $V|\chi>$ may differ by long-ranged terms. Because V is normally short-ranged, V should be used. In order to alleviate the clumsy partial antisymmetrization imposed by V and V', the concept of channel (pseudo-)spin is introduced in this Appendix.

Inside the matrix elements which involve χ or χ', the single-particle wave functions χ_i, χ_i' and φ_i, φ_i' are translated into two-component (channel spin) wave functions

$$|\chi_i> \to |\chi_i^{cs}> = \left| \begin{matrix} \chi_i \\ 0 \end{matrix} \right\rangle, \qquad \text{for } i\,\epsilon\, a, \tag{A.3a}$$

$$|\chi_i> \to |\chi_i^{cs}> = \left| \begin{matrix} 0 \\ \chi_i \end{matrix} \right\rangle, \qquad \text{for } i\,\epsilon\, b, \tag{A.3b}$$

$$< \chi_i'| \to < \chi_i'^{cs}| = \left\langle \begin{matrix} \chi_i' \\ 0 \end{matrix} \right|, \qquad \text{for } i\,\epsilon\, c, \tag{A.3c}$$

$$< \chi_i'| \to < \chi_i'^{cs}| = \left\langle \begin{matrix} 0 \\ \chi_i' \end{matrix} \right|, \qquad \text{for } i\,\epsilon\, d, \tag{A.3d}$$

$$|\varphi_i> \to |\varphi_i^{cs}> = \left| \begin{matrix} \varphi_i \\ \varphi_i \end{matrix} \right\rangle, \tag{A.3e}$$

$$< \varphi_i'| \to < \varphi_i'^{cs}| = \left\langle \begin{matrix} \varphi_i' \\ \varphi_i' \end{matrix} \right|. \tag{A.3f}$$

Therefore we consider the transformation

$$|\chi\} \to |\chi^{cs}\} = \left(\sqrt{N_a!}\mathcal{A}_a \prod_{i\epsilon a} \left| \begin{matrix} \chi_i \\ 0 \end{matrix} \right\rangle \right) \left(\sqrt{N_b!}\mathcal{A}_b \prod_{j\epsilon b} \left| \begin{matrix} 0 \\ \chi_j \end{matrix} \right\rangle \right), \tag{A.4a}$$

$$\{\chi'| \to \{\chi'^{cs}| = \left(\sqrt{N_c!} \prod_{i\epsilon c} \left\langle \begin{matrix} \chi_i' \\ 0 \end{matrix} \right| \mathcal{A}_c \right) \left(\sqrt{N_d!} \prod_{j\epsilon d} \left\langle \begin{matrix} 0 \\ \chi_j' \end{matrix} \right| \mathcal{A}_d \right). \tag{A.4b}$$

For χ a channel spin 'up' means that the orbital belongs to fragment a, and channel spin 'down' means that it belongs to fragment b. For χ' the distinction is between fragments c and d. Equal components in channel spin formalism, eqs. (A.3e) and (A.3f), are assigned to single-particle orbitals φ_i, φ_i' of trial functions Φ, Φ'. This assignment has no effect on total antisymmetrization,

$$|\Phi> \to |\Phi^{cs}> = \sqrt{N!}\mathcal{A} \prod_i \left| \begin{matrix} \varphi_i \\ \varphi_i \end{matrix} \right\rangle, \tag{A.4c}$$

$$< \Phi'| \to < \Phi'^{cs}| = \sqrt{N!} \prod_i \left\langle \begin{matrix} \varphi_i' \\ \varphi_i' \end{matrix} \right| \mathcal{A}. \tag{A.4d}$$

Now we introduce channel spin dependent potentials which replace V and V' but leave their matrix elements invariant. With the Pauli matrix σ_z^i acting on particle i in χ-channel spin representation and with $\sigma_z'^i$ acting on particle i in χ'-channel spin representation, the replacement of the interaction v_{ij} between particle i and j by

$$v_{ij}^{cs} = \frac{1}{2}(1 - \sigma_z^i \sigma_z^j) v_{ij} \text{ in } \chi\text{-channel spin representation}, \tag{A.5a}$$

$$v_{ij}'^{cs} = \frac{1}{2}(1 - \sigma_z'^i \sigma_z'^j) v_{ij} \text{ in } \chi'\text{-channel spin representation}, \tag{A.5b}$$

sets the interactions v_{ij}^{cs}, $v_{ij}'^{cs}$ to zero if acting within fragments and leaves them equal to v_{ij} otherwise. With the definition

$$V = \sum_{\substack{i\epsilon a \\ j\epsilon b}} v_{ij} \to V^{cs} = \sum_{i,j} \frac{1}{2}(1 - \sigma_z^i \sigma_z^j) v_{ij}, \tag{A.5c}$$

$$V' = \sum_{\substack{i\epsilon c \\ j\epsilon d}} v_{ij} \to V'^{cs} = \sum_{i,j} \frac{1}{2}(1 - \sigma_z'^i \sigma_z'^j) v_{ij}, \tag{A.5d}$$

it is easily seen that

$$< \Phi'|V|\chi\} =< \Phi'^{cs}|V^{cs}|\chi^{cs}\}, \tag{A.6a}$$

$$\{\chi'|V'|\Phi >= \{\chi'^{cs}|V'^{cs}|\Phi^{cs} > . \tag{A.6b}$$

In this enlarged channel spin space V^{cs} and V'^{cs} commute with $\mathcal{A}$,

$$[V^{cs}, \mathcal{A}] = 0 = [V'^{cs}, \mathcal{A}], \tag{A.7}$$

and therefore

$$< \Phi'^{cs}|V^{cs}|\chi^{cs}\} =< \Phi'^{cs}|\mathcal{A}V^{cs}|\chi^{cs}\} =$$

$$\sqrt{N_a!N_b!} < \Phi'^{cs}|V^{cs}\mathcal{A}\mathcal{A}_a\mathcal{A}_b|\chi^{cs}) = \sqrt{\frac{N_a!N_b!}{N!}} < \Phi'^{cs}|V^{cs}|\chi^{cs} >, \tag{A.8a}$$

and correspondingly with (A.1b)

$$\{\chi'^{cs}|V'^{cs}|\Phi^{cs} >= \sqrt{\frac{N_c!N_d!}{N!}} < \chi'^{cs}|V'^{cs}|\Phi^{cs} > . \tag{A.8b}$$

We recall here that $\mathcal{A}\mathcal{A}_a = \mathcal{A}\mathcal{A}_b = \mathcal{A}$. It is thus possible to work with fully antisymmetrized wave functions only. The functional F of Eq.(2.5c) then reads in the channel spin formulation

$$F = \sqrt{\frac{N_a!N_b!}{N!}} < \Phi'^{cs}|V^{cs}|\chi^{cs} > + \sqrt{\frac{N_c!N_d!}{N!}} < \chi'^{cs}|V'^{cs}|\Phi^{cs} > - < \Phi'|(z - H)|\Phi >, \tag{A.9}$$

where the channel spin is not needed for the $<\Phi'|(z-H)|\Phi>$ matrix element. (An introduction of channel spin in this matrix element is nevertheless possible and would require a normalization factor $\frac{1}{\sqrt{2}}$ for every orbital φ_i, φ'_i, but has no further effect. Note that this normalization factor must be included inside $<\Phi'|(z-H)|\Phi>$ only.)

Within χ^{cs} and χ'^{cs} the orbitals can now be rearranged like those within Φ and Φ'. This leads to generalized channel spin orbitals

$$|\chi_i^{cs}>=\left|\begin{matrix}\chi_i^1\\ \chi_i^2\end{matrix}\right\rangle, \qquad (A.10a)$$

$$<\chi_i'^{cs}|=\left\langle\begin{matrix}\chi_i'^1\\ \chi_i'^2\end{matrix}\right|. \qquad (A.10b)$$

It is now possible to diagonalize the generalized overlap matrices $<\varphi_i'^{cs}|\chi_j^{cs}>$, $<\chi_i'^{cs}|\varphi_j^{cs}>$ and corresponding generalized cofactors M_{ij}^{cs}, $M_{ij}'^{cs}$ through linear rearrangement of the χ_i^{cs}, $\chi_i'^{cs}$ leaving the φ_i, φ'_i unchanged. This enables us to diagonalize $<\varphi'_i|\varphi_j>$ and $<\varphi'_i|h|\varphi_j>$ by linear rearrangement of the φ_i, φ'_i. In Eqs.(3.4a,b) the sum $\frac{1}{2}\sum_{\alpha\beta}$ has to be replaced by $\frac{1}{4}\sum_{kl}$ where the indices k, l run over all orbitals because of the totally antisymmetrized wave functions

$$<\Phi'^{cs}|V^{cs}|\chi^{cs}>=\frac{1}{4}\sum_{ijkl}<\varphi_i'^{cs}\varphi_j'^{cs}|v^{cs}|\chi_k^{cs}\chi_l^{cs}>M_{ijlk}^{cs}, \qquad (A.11a)$$

$$<\chi'^{cs}|V'^{cs}|\Phi^{cs}>=\frac{1}{4}\sum_{ijkl}<\chi_k'^{cs}\chi_l'^{cs}|v'^{cs}|\varphi_i^{cs}\varphi_j^{cs}>M_{klji}'^{cs}. \qquad (A.11b)$$

Here antisymmetrized matrix elements are used for v^{cs} and v'^{cs}.

The derivatives with respect to the single-particle orbitals φ_i, φ'_i must take into account the fact that φ_i resp. φ'_i appear twice inside the channel spin trial functions. With the relations for generalized channel spin wave functions

$$<\varphi_m'^{cs}\varphi_n'^{cs}|v^{cs}|\chi_k^{cs}\chi_l^{cs}>=<\varphi'_m\varphi'_n|v|\chi_k^1\chi_l^2+\chi_k^2\chi_l^1>, \qquad (A.12a)$$

$$<\chi_m'^{cs}\chi_n'^{cs}|v'^{cs}|\varphi_k^{cs}\varphi_l^{cs}>=<\chi_m'^1\chi_n'^2+\chi_m'^2\chi_n'^1|v|\varphi_k\varphi_l> \qquad (A.12b)$$

for the antisymmetrized matrix elements, Eqs.(3.5a,b) become:

$$\frac{\delta C}{\delta<\varphi'_i|}=\sqrt{\frac{N_a!N_b!}{N!}}\Bigg(\frac{1}{2}\sum_{jkl}<\cdot\varphi'_j|v|\chi_k^1\chi_l^2+\chi_k^2\chi_l^1>M_{ijlk}^{cs} \qquad (A.13a)$$

$$+\frac{1}{4}\sum_{jmnkl}<\varphi'_m\varphi'_n|v|\chi_k^1\chi_l^2+\chi_k^2\chi_l^1>M_{mnijlk}^{cs}|\chi_j^1+\chi_j^2>\Bigg),$$

$$\frac{\delta C'}{\delta|\varphi_i>} = \sqrt{\frac{N_c!N_d!}{N!}}\Bigg(\frac{1}{2}\sum_{jkl} < \chi_k'^1\chi_l'^2 + \chi_k'^2\chi_l'^1|v|\cdot\varphi_j > M_{klji}'^{cs} \tag{A.13b}$$

$$+\frac{1}{4}\sum_{jmnkl} < \chi_k'^1\chi_l'^2 + \chi_k'^2\chi_l'^1|v|\varphi_m\varphi_n > M_{kljinm}'^{cs} < \chi_j'^1 + \chi_j'^2|\Bigg).$$

Now the self consistent channel potentials can be defined by

$$< \cdot|S_1|\chi_l^1 > = \frac{1}{< \Phi'^{cs}|\chi^{cs} >}\sum_{nk} < \cdot\varphi_n'|v|\chi_l^1\chi_k^2 > M_{nk}^{cs}, \tag{A.14a}$$

$$< \cdot|S_2|\chi_l^2 > = \frac{1}{< \Phi'^{cs}|\chi^{cs} >}\sum_{nk} < \cdot\varphi_n'|v|\chi_l^2\chi_k^1 > M_{nk}^{cs}, \tag{A.14b}$$

$$< \chi_l'^1|S_1'|\cdot > = \frac{1}{< \chi'^{cs}|\Phi^{cs} >}\sum_{kn} < \chi_l'^1\chi_k'^2|v|\cdot\varphi_n > M_{kn}'^{cs}, \tag{A.14c}$$

$$< \chi_l'^2|S_2'|\cdot > = \frac{1}{< \chi'^{cs}|\Phi^{cs} >}\sum_{kn} < \chi_l'^2\chi_k'^1|v|\cdot\varphi_n > M_{kn}'^{cs}. \tag{A.14d}$$

Then Eqs.(3.5c,d) and (3.6e,f) do not change because there are no χ, χ' involved, but Eqs.(3.7a,b) now read

$$\frac{\delta C}{\delta < \varphi_i'|} = \sqrt{\frac{N_a!N_b!}{N!}} < \Phi'^{cs}|\chi^{cs} > \Bigg[\sum_j A_{ji}^{cs}(S_1|\chi_j^1 > +S_2|\chi_j^2 >)$$

$$+\frac{1}{2}\sum_{jml}\left(< \varphi_m'|S_1|\chi_l^1 > + < \varphi_m'|S_2|\chi_l^2 >\right)A_{ji}^{cs}A_{lm}^{cs}|\chi_j^1 + \chi_j^2 >$$

$$-\sum_{jml}\left(< \varphi_m'|S_1|\chi_l^1 > + < \varphi_m'|S_2|\chi_l^2 >\right)A_{jm}^{cs}A_{li}^{cs}|\chi_j^1 + \chi_j^2 >\Bigg], \tag{A.15a}$$

$$\frac{\delta C'}{\delta|\varphi_i>} = \sqrt{\frac{N_c!N_d!}{N!}} < \chi'^{cs}|\Phi^{cs} > \Bigg[\sum_j A_{ij}'^{cs}(< \chi_j'^1|S_1' + < \chi_j'^2|S_2')$$

$$+\frac{1}{2}\sum_{jml}\left(< \chi_l'^1|S_1'|\varphi_m > + < \chi_l'^2|S_2'|\varphi_m >\right)A_{ij}'^{cs}A_{ml}'^{cs} < \chi_j'^1 + \chi_j'^2|$$

$$-\sum_{jml}\left(< \chi_l'^1|S_1'|\varphi_m > + < \chi_l'^2|S_2'|\varphi_m >\right)A_{mj}'^{cs}A_{il}'^{cs} < \chi_j'^1 + \chi_j'^2|\Bigg] \tag{A.15b}$$

These equations are invariant under linear rearrangement of the orbitals χ_i^{cs}, $\chi_i'^{cs}$, and they reduce to Eqs.(3.7a,b) when the wave functions (A.3a,b,c,d) are used. In a representation where both overlap matrices $< \varphi_i'^{cs}|\chi_j^{cs} >$ and $< \chi_i'^{cs}|\varphi_j^{cs} >$ are diagonal, equations

(A.15a,b) reduce to

$$\frac{\delta C}{\delta < \varphi_i'|} = \sqrt{\frac{N_a!N_b!}{N!}} \frac{< \Phi'^{cs}|\chi^{cs} >}{< \varphi_i'|\chi_i^1 + \chi_i^2 >} \Bigg[(S_1|\chi_i^1 > + S_2|\chi_i^2 >)$$

$$+ \frac{1}{2}\left(\sum_l \frac{< \varphi_l'|S_1|\chi_l^1 > + < \varphi_l'|S_2|\chi_l^2 >}{< \varphi_l'|\chi_l^1 + \chi_l^2 >} \right) |\chi_i^1 + \chi_i^2 >$$

$$- \sum_j \frac{< \varphi_j'|S_1|\chi_i^1 > + < \varphi_j'|S_2|\chi_i^2 >}{< \varphi_j'|\chi_j^1 + \chi_j^2 >} |\chi_j^1 + \chi_j^2 > \Bigg], \qquad (A.16a)$$

$$\frac{\delta C'}{\delta|\varphi_i >} = \sqrt{\frac{N_c!N_d!}{N!}} \frac{< \chi'^{cs}|\Phi^{cs} >}{< \chi_i'^1 + \chi_i'^2|\varphi_i >} \Bigg[(< \chi_i'^1|S_1' + < \chi_i'^2|S_2')$$

$$+ \frac{1}{2}\left(\sum_l \frac{< \chi_l'^1|S_1'|\varphi_l > + < \chi_l'^2|S_2'|\varphi_l >}{< \chi_l'^1 + \chi_l'^2|\varphi_l >} \right) < \chi_i'^1 + \chi_i'^2|$$

$$- \sum_j \frac{< \chi_i'^1|S_1'|\varphi_j > + < \chi_i'^2|S_2'|\varphi_j >}{< \chi_j'^1 + \chi_j'^2|\varphi_j >} < \chi_j'^1 + \chi_j'^2| \Bigg]. \qquad (A.16b)$$

Note that

$$< \Phi'^{cs}|\chi^{cs} >= \prod_i < \varphi_i'|\chi_i^1 + \chi_i^2 > \text{ and } < \chi'^{cs}|\Phi^{cs} >= \prod_i < \chi_i'^1 + \chi_i'^2|\varphi_i > . \qquad (A.17)$$

These equations can now be combined with Eqs.(3.8c,d) where $< \varphi_i'|\varphi_j >$ and $< \varphi_i'|h|\varphi_j >$ are diagonal. Because all the cofactors are simultaneously diagonalized when the three overlap matrices are chosen diagonal, the enormous number of cofactors, like N^6 for M_{mnijlk} with six indices, is reduced to the number of diagonal elements only. The price to be paid for this simplification is that one has to deal with two component wave functions. They give rise to additional terms in the inhomogenous parts of (A.16a,b) as compared to (3.7a,b). A generalization of this two-component channel spin formalism is possible for more than two fragments in one or both channels. For n fragments in a channel, n-component channel spin wave functions can be introduced in the corresponding matrix elements and give again a possibility of using full antisymmetrization.