Singularities of a Mean Field Green's Function

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A mean field approximation allows microscopic calculations of an N-body propagator \( G(z) = (z - H)^{-1} \). We investigate singularities of the resulting approximate Green's function, \( G_{mf}(z) \), by comparing them to the binding energies calculated by the Hartree-Fock approximation. We show that each Hartree-Fock energy induces a singularity of \( G_{mf} \).

§ 1. Introduction

Consider \( N \) non-relativistic fermions, either electrons or nucleons, with Hamiltonian

\[
H = \sum_i h_i + \sum_{i<j} v_{ij},
\]

where \( h_i \) may contain, besides the kinetic energy \( t_i \), a one body and often central potential \( u_i \). The potentials \( u_i \) and \( v_{ij} \) may be either Hermitian or non-Hermitian, indifferently. The singularities of the Green's function \( G(z) = (z - H)^{-1} \) are well known to be poles, corresponding to the bound states of all \( N \) particles, and cuts, corresponding to the bound states of the subsystems. This formal knowledge is of a limited numerical value, however, as soon as \( N \) exceeds 3, since then an accurate calculation of either the full \( G \) or most of the subsystem propagators is beyond the reach of modern computers.

For want of exact solutions, an approximate, practical knowledge of \( G \) is of major importance for the \( N \)-body problem, if only because of the central role of \( G \) in the theory of collisions. Any approximation leading easily to numerical estimates of \( G \) deserves some interest. Among other proposed methods, the time independent mean field (TIMF) method seems to have passed with success a few validation tests, corresponding to a few soluble models with \( N = 2, 3, 4 \), where it was found that the resulting approximate, \( G_{mf} \), was often quite close to \( G \). Hence the purpose of this paper is to investigate the analytical structure of \( G_{mf}(z) \), as a function of the complex energy \( z \), and compare it with the structure of \( G \). We will find that the (static) Hartree-Fock energies governed by \( H \) provide singularities of \( G_{mf} \).

This paper is organized as follows. Section 2 presents a very simple argument, with \( N = 2 \), which is a slight generalization of the traditional Hartree equations and, simultaneously, a reminder of the TIMF equations. A clear link will be established between Hartree energies and TIMF singularities. Then in § 3, the argument of § 2 is generalized for any value of \( N \), and one takes into account the Pauli principle and the partitions of \( N \). Section 4 deals with a special feature of mean field theories, namely, a slight compatibility problem between Galilean invariance and antisymmetr-
More generally, symmetry breakings by the mean field are briefly considered. Finally § 5 contains a discussion and a conclusion.

§ 2. Elementary example

We set $N=2$ with

$$H = h_1 + h_2 + v_{12} \quad (2\cdot1)$$

with a local potential $v_{12} = v(n - r_2)$. This corresponds, for instance, to the electrons of a neutral He atom. Opposite spins can spare the need for symmetrization of space coordinates $n$ and $r_2$, and we will temporarily consider Hartree equations rather than Hartree-Fock ones.

We consider the stationarity of the functional

$$E(\phi, \phi') = \frac{\langle \phi' [H] \phi \rangle}{\langle \phi'|\phi \rangle}, \quad (2\cdot2)$$

under the Hartree factorization restrictions of the trial functions $\phi$ and $\phi'$,

$$\langle r_1, r_2 | \phi \rangle = \phi_1(r_1) \phi_2(r_2), \quad (2\cdot3a)$$
$$\langle \phi'| r_1, r_2 \rangle = \phi_1^*(r_1) \phi_2^*(r_2). \quad (2\cdot3b)$$

It is clear that the functional $E$, Eq. (2·2), contains the usual Rayleigh-Ritz functional as a special case, when $|\phi\rangle = |\phi\rangle$. But now the two trial functions are independent, and the stationarity of $E$ corresponds in general to saddle points rather than minima or maxima. This generalization leaves for $|\phi\rangle$ and $|\phi\rangle$ the possibility of approximating wave packets of outgoing or ingoing waves, independently. Scattering Hartree solutions and stationary values $\bar{E}$ of $E$ in the continuum are thus possible, in principle at least.

A standard variation of $E$ then provides the generalized Hartree equations

$$(\varepsilon_1 - h_1 - U_1) \phi_1 = 0, \quad (2\cdot4a)$$
$$(\varepsilon_2 - h_2 - U_2) \phi_2 = 0, \quad (2\cdot4b)$$
$$\langle \phi_1 | (\varepsilon_1 - h_1 - U_1) \phi_1 \rangle = 0, \quad (2\cdot4c)$$
$$\langle \phi_2 | (\varepsilon_2 - h_2 - U_2) \phi_2 \rangle = 0, \quad (2\cdot4d)$$

where $\varepsilon_i$ is an eigenvalue of $h_i + U_i$, and

$$U_i(r_i) = \frac{\int dr_2 v(r_1 - r_2) \phi_2^*(r_2) \phi_2(r_2)}{\langle \phi_2^* | \phi_2 \rangle}, \quad (2\cdot5a)$$
$$U_2(r_2) = \frac{\int dr_1 v(r_1 - r_2) \phi_1^*(r_1) \phi_1(r_1)}{\langle \phi_1^* | \phi_1 \rangle}. \quad (2\cdot5b)$$

The independence of $\phi$ and $\phi'$ is expressed by the non-diagonal densities $\phi_i^* \phi_i$ present in Eqs.(2·5). In the following, any solution of Eqs. (2·4) will be denoted by
the resulting self-consistent orbitals $\bar{\phi}_1, \bar{\phi}_2, \phi'_1, \phi'_2$, potentials $\bar{U}_1, \bar{U}_2$, self-energies $\bar{\varepsilon}_1, \bar{\varepsilon}_2$ and extremum $\bar{E}$. It can be pointed out that the $\phi, \phi'$ have arbitrary norms and phases, while the $U, \varepsilon$ and $E$ are phase and norm independent.

We now introduce the TIMF equations. The Green's function problem is stated in terms of two inversion problems,

\[
(z - H)|\phi \rangle = |\chi \rangle,
\]
\[
\langle \phi| (z - H) = \langle \chi' |.
\]

where $\chi$ and $\chi'$ are arbitrary source terms. For the sake of simplicity we assume that $\chi$ and $\chi'$ are square integrable wave packets rather than waves, if only because in collision theories the Green's function most often appears between prior and post potentials, which tend to truncate free or distorted waves. With an obvious notation $V'G V$, it is clear that the generic problem at stake is the calculation of matrix elements of $G$ between square integrable states. Again for the sake of simplicity, we can also assume that $\chi$ and $\chi'$ are products $\chi_1 \chi_2$ and $\chi'_1 \chi'_2$ of single particle states. Indeed such products make (over)complete bases in the Hilbert space.

Despite this factorization of $\chi$ and $\chi'$, the "Green's states" $\phi, \phi'$ defined by Eqs. (2.6) remain complicated states, containing strong correlations between particles 1 and 2. The TIMF method then consists in replacing $\phi, \phi'$, by products $\phi, \phi'$, as stated by the Hartree ansatz, Eqs. (2.3).

The Hartree ansatz is thus used now as an approximation for inversion rather than diagonalization. One must solve at best

\[
(z - H)|\phi_1 \phi_2 \rangle = |\chi \rangle,
\]
\[
\langle \phi| (z - H) = \langle \chi' |.
\]

The degree of freedom $r_3$ may be integrated out of Eqs. (2.7a, b) by projecting Eq. (2.7a) against $|\phi_3 \rangle$ and Eq. (2.7b) against $|\phi_2 \rangle$, respectively. We obtain

\[
(\eta_i - h_i - U_i)|\phi_i \rangle = \lambda_i |\chi_i \rangle,
\]
\[
\langle \phi_i| (\eta_i - h_i - U_i) = \lambda_i \langle \chi_i |.
\]

with

\[
\eta_i = z - \frac{\langle \phi_i | h_i | \phi_3 \rangle}{\langle \phi_3 | \phi_2 \rangle},
\]

and

\[
\lambda_i = \frac{\langle \phi_i | \phi_2 \rangle}{\langle \phi_3 | \phi_2 \rangle}, \quad \lambda_i = \frac{\langle \chi_i | \phi_2 \rangle}{\langle \phi_3 | \phi_2 \rangle}.
\]

In the same way $r_1$ can be integrated out, with the result

\[
(\eta_2 - h_2 - U_2)|\phi_2 \rangle = \lambda_2 |\chi_2 \rangle,
\]
\[
\langle \phi_2| (\eta_2 - h_2 - U_2) = \lambda_2 \langle \chi_2 |.
\]

with
and

\[ \lambda_0 = \frac{\langle \varphi_i | \chi_i \rangle}{\langle \varphi_i | \varphi_i \rangle}, \quad \lambda_0 = \frac{\langle \xi_i | \varphi_i \rangle}{\langle \varphi_i | \varphi_i \rangle}. \tag{2.9d} \]

It is straightforward to show that the four conditions, Eqs. (2.8), are stationarity conditions for the Schwinger-like functional

\[ F(\phi, \phi') = \frac{\langle \phi | \chi \rangle \langle \chi | \phi \rangle}{\langle \phi | (z - H) \phi \rangle} = \frac{\langle \phi | \chi \rangle \langle \chi | \phi \rangle}{\langle \phi | \phi \rangle [z - E(\phi, \phi')]} \tag{2.10} \]

which is insensitive to the norms and phases of \( \phi, \phi' \). It is thus possible to set \( \lambda_i = \lambda_i' = \lambda_0 = \lambda_0' = 1 \) in Eqs. (2.8). The stationary value \( \bar{F} \) of \( F \), if the trial functions are fully flexible, is the exact matrix element \( D(z) = \langle \chi | \phi \rangle = \langle \chi | G(z) | \chi \rangle \). We already know from a few soluble examples that the restrictions, Eqs. (2.3), can generate a reasonable approximation \( D_{m_f}(z) \approx D(z) \).

It must be stressed here that the potentials \( U_i, i = 1, 2 \), which appear in the TIMF equations, Eqs. (2.8), have exactly (see Eqs. (2.5)) the same functional dependence on the orbitals \( \varphi, \varphi' \), as those \( U_i \) found in the Hartree equations, Eqs. (2.4). This is one of the main reasons why the \textit{"static"} solutions \( \bar{\varphi}, \bar{\varphi}' \) of Eqs. (2.4) will turn out to be also TIMF solutions, namely, solutions of Eqs. (2.8), when \( z \to E \). This occurs for \textit{arbitrary} \( \chi \), and/or \( \chi' \), hence indicates singularities of the operator \( G_{mf} \).

To prove this feature, we first assume, for the sake of simplicity, that these static solutions (orbitals) describe a bound state rather than a scattering wave. These orbitals are then normalizable and \( \bar{E} \) is an isolated Hartree energy. Then we set \( z = \bar{E} + \delta z \), where \( \delta z \) is an infinitesimal, real or complex. Now we investigate the ansatz

\[ |\varphi_i\rangle = \frac{\langle \varphi_i | \chi_i \rangle}{\delta z \langle \varphi_i | \varphi_i \rangle} |\varphi_i\rangle + |\Delta \varphi_i\rangle, \tag{2.11a} \]

\[ \langle \varphi_i | \langle \varphi_i | \chi_i \rangle = \langle \varphi_i | \varphi_i \rangle \rangle + \langle \Delta \varphi_i \rangle \tag{2.11b} \]

with the constraints

\[ \langle \varphi_i | \Delta \varphi_i \rangle = \langle \Delta \varphi_i | \varphi_i \rangle = 0, \quad i = 1, 2. \tag{2.12} \]

These expansions, Eqs. (2.11a, b) take advantage of the fact that all the functionals under consideration, \( F, E, U_i, \eta_i \), are independent of the norms and phases of the orbitals. Hence it makes sense to expand \( \varphi_i \) with a leading term of order \( (\delta z)^{-1} \), proportional to \( \varphi_i \), and a biorthogonal, \textit{finite} correction \( \Delta \varphi_i \), of order \( (\delta z)^0 \). The same holds for \( \varphi_i \) (see Eq. (2.11b)). All told, the ansatz, Eqs. (2.11), induces a first order correction, \( U_i = \bar{U}_i + \delta U_i \), for the mean fields. It also induces a second order correction for \( E \) as compared to \( \bar{E} \), and one can set \( z = E + \delta z \), with

\[ E = \frac{\langle \varphi_i | (h_i + U_j) | \varphi_i \rangle}{\langle \varphi_i | \varphi_i \rangle} + \frac{\langle \varphi_i | h_j | \varphi_i \rangle}{\langle \varphi_i | \varphi_i \rangle}, \quad j \neq i = 1, 2. \tag{2.13} \]
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(see the definition of $E$, Eq. (2.2)). We furthermore notice that the $(\varepsilon_i + \delta z - \varepsilon_i + \delta U_i - \delta U_i + \delta U_i - \delta U_i)$ contribution to the first term on the right-hand side of this form of $E$, Eq. (2.13), is stationary and can be replaced by $\varepsilon_i$, since we are investigating neighborhoods of right and left eigenstates of $\varepsilon_i + \delta U_i$. Taking into account the two terms involving $\delta U_i$, the TIMF equations can now be restated as

$$
\left( \varepsilon_i + \delta z - \varepsilon_i - \delta U_i - \delta U_i + \delta U_i - \delta U_i \right) \langle \varphi_i \rangle = \chi_i,
$$

(2.14a)

$$
\langle \varphi_i \rangle \left( \varepsilon_i + \delta z - \varepsilon_i - \delta U_i - \delta U_i + \delta U_i - \delta U_i \right) = \langle \chi_i \rangle,
$$

(2.14b)

where only second order corrections have been neglected. In particular the following first order terms,

$$
\frac{\langle \varphi_i \rangle \delta U_i}{\langle \varphi_i \rangle}, \frac{\langle \varphi_i \rangle \delta U_i}{\langle \varphi_i \rangle}, \frac{\langle \varphi_i \rangle \delta U_i}{\langle \varphi_i \rangle}, \frac{\langle \varphi_i \rangle \delta U_i}{\langle \varphi_i \rangle},
$$

(2.15)

differ from each other at second order only.

The ansatz, Eqs. (2.11) must now solve Eqs. (2.14) if the expansion hierarchy with respect to $\delta z$ is correct. Define the "projector" $\tilde{P}_i = \langle \varphi_i \rangle \langle \varphi_i \rangle / \langle \varphi_i \rangle \langle \varphi_i \rangle$ and its complement $\tilde{Q}_i = 1 - \tilde{P}_i$. It is clear that $\delta U_i$ appears in Eq. (2.14a) in a special form, which is denoted as $Q_i \delta U_i$, because it differs from $\tilde{Q}_i \delta U_i$ by a term of order $(\delta z)^2$ only. Similarly, Eq. (2.14b) contains a form $\delta U_i \tilde{Q}_i$ equal to $\delta U_i \tilde{Q}_i$, except for a second order term. Then in the limit $\delta z \to 0$ the "subspaces" defined by $\tilde{P}_i$ and $\tilde{Q}_i$ can be disentangled in Eqs. (2.14). Indeed, projecting Eq. (2.14a) against $\langle \varphi_i \rangle$ and Eq. (2.14b) against $\langle \varphi_i \rangle$, respectively, and inserting Eqs. (2.11), we obtain

$$
\langle \varphi_i \rangle \left( \varepsilon_i + \delta z - \varepsilon_i - \delta U_i - \delta U_i + \delta U_i - \delta U_i \right) = \langle \varphi_i \rangle \chi_i,
$$

(2.16a)

and

$$
\langle \varphi_i \rangle \left( \varepsilon_i + \delta z - \varepsilon_i - \delta U_i - \delta U_i + \delta U_i - \delta U_i \right) = \langle \chi_i \rangle \langle \varphi_i \rangle.
$$

(2.16b)

These are trivial identities, which justify the choice made in Eqs. (2.11) for the components $\tilde{P}_i \chi_i$ and $\tilde{Q}_i \chi_i$. Left multiplying Eq. (2.14a) and right multiplying Eq. (2.14b), respectively, by $\tilde{Q}_i$, then gives

$$
[\varepsilon_i + \delta z - \tilde{Q}_i (h_i + U_i + \delta U_i) \tilde{Q}_i] \Delta \varphi_i = \tilde{Q}_i \left( 1 + \frac{\delta U_i}{\delta z} \frac{\tilde{P}_i}{\tilde{Q}_i} \right) \chi_i,
$$

(2.17a)

and

$$
\Delta \varphi_i [\varepsilon_i + \delta z - \tilde{Q}_i (h_i + U_i + \delta U_i) \tilde{Q}_i] = \chi_i \left( 1 + \frac{\delta U_i}{\delta z} \frac{\tilde{P}_i}{\tilde{Q}_i} \right) \tilde{Q}_i.
$$

(2.17b)

If the $\varepsilon_i$ are isolated eigenvalues, these equations, Eqs. (2.17), are regular at the limit $\delta z \to 0$ and do define finite corrections $\Delta \varphi_i, \Delta \varphi_i$. For instance, Eq. (2.17a) reduces to

$$
|\Delta \varphi_i| = [\varepsilon_i - \tilde{Q}_i (h_i + U_i) \tilde{Q}_i]^{-1} \tilde{Q}_i \left( 1 + \frac{\delta U_i}{\delta z} \frac{\tilde{P}_i}{\tilde{Q}_i} \right) \chi_i.
$$

(2.18a)
The self-consistency of Eqs. (2·11) is thus established: Static Hartree solutions are also TIMF solutions, whatever the source terms $\chi, \chi'$ are.

If an $\varepsilon_i$ belongs to a continuum, the corresponding corrections $\Delta \varphi_i, \Delta \varphi'_i$ should be waves, as well as $\varphi_i, \varphi'_i$, incidentally. The normalizations assumed before Eqs. (2·11) should be modified accordingly. Standard precautions (on shell limits of off shell calculations, principal parts, etc.) might validate the consistency of Eqs. (2·11), but their discussion is beyond the scope of the present paper.

Little is changed to the arguments of this section if we accept as source terms non-factorized $\chi, \chi'$. Indeed one can define a posteriori, with partial integrations, $|\chi_i\rangle = \langle \varphi_i|\chi \rangle$ and $|\chi'_i\rangle = \langle \varphi'_i|\chi' \rangle$.

In summary of the present section, it has been shown that the solutions of this elementary two particle Hartree problem automatically generate singularities of the corresponding Green's function problem, when the latter is treated in the TIMF approximation. In particular the form of Eqs. (2·11), with their $(\delta z)^{-1}$ terms, shows that Hartree bound states induce poles for the TIMF orbitals. One might then think that the $F$ functional, which is insensitive to the divergence of the orbitals, could retain a finite value. It is clear, however, that one may renormalize $\phi, \phi'$ into finite states, with $\langle \phi'|\phi \rangle = 1$ for instance. Then the denominator $(z-E)$ of $F$ vanishes linearly as a function of $\delta z$, hence the stationary value $F$ shows a simple pole. One may conjecture that the singularity becomes a cut if the Hartree solutions describe a continuum rather than isolated states.

§ 3. Generalization

With an arbitrary (but finite) $N$, we again consider functionals $E$, Eq. (2·2) and $F$, Eq. (2·10), with the most general form of the Hamiltonian, Eq. (1·1). The trial functions $\phi, \phi'$ are now Slater determinants made of $N$ orbitals $\varphi_i, \varphi'_i$, respectively, and it is possible to linearly rearrange these orbitals within each determinant in such a way that a biorthogonality rule,

$$\langle \varphi_i|\varphi_j \rangle = 0, \quad i \neq j, \quad (3·1)$$

is kept. The matrix elements of the two body force $v$ are antisymmetrized, and there is no need to label the mean fields with a particle index. A unique $U$, valid for all orbitals, replaces the Hartree potentials $U_i$. Its matrix elements between two arbitrary test functions $\tau, \tau'$ read

$$\langle \tau'|U|\tau \rangle = \sum_{i=1}^{N} \frac{\langle \tau'|\varphi'_i|v|\varphi_i \rangle}{\langle \varphi'_i|\varphi_i \rangle}. \quad (3·2)$$

The variation of

$$E = \sum_{i=1}^{N} \frac{\langle \varphi_i|h|\varphi_i \rangle}{\langle \varphi_i|\varphi_i \rangle} + \sum_{i>j=1}^{N} \frac{\langle \varphi'_i|v|\varphi_j \rangle}{\langle \varphi'_i|\varphi_i \rangle \langle \varphi'_j|\varphi_j \rangle} \quad (3·2)$$

generates the Hartree-Fock equations,

$$(\varepsilon_i - h - U)|\varphi_i \rangle = 0, \quad (3·3a)$$
and the familiar, dual equations for $\langle \varphi \rangle$,

$$
\langle \varphi \rangle (\varepsilon - h - U) = 0.
$$

(3.3b)

We will now study the neighborhood of a solution $\bar{\varphi}, \bar{\varphi}'$, of Eqs. (3.3). Namely, our orbitals and self-energies read \{ $\bar{\varphi}_i + \delta \varphi_i, \bar{\varphi}_i' + \delta \varphi_i', \varepsilon_i, i = 1, \cdots N$\}, and the orbitals can be multiplied by arbitrary, complex coefficients. For the sake of elegance, one should even ensure that the variations $\delta \varphi_i, \delta \varphi_i'$ are orthogonal to the Fermi sea, but this technical precaution can be spared. Spurious variations inside the Fermi sea will just generate vanishing components of the gradients of the functionals $E, F,$ and $U$ and can be easily discarded later. The corresponding Hartree-Fock energy is denoted by $\bar{E}$. In such a neighborhood, $\bar{E}$ differs from $E$ by a second order term only, naturally. The self-energies are also stationary, except for a contribution of the deviation $\delta U$ away from $\bar{U}$. The value of $\varepsilon$ driving the TIMF equations will be $\varepsilon = \bar{E} + \delta \varepsilon$, or, equivalently, $\varepsilon = E + \delta \varepsilon$.

The detailed derivation of the antisymmetrized TIMF equations has been published elsewhere. With arbitrary $N$-body source terms $\chi, \chi'$, we attempt to solve Eqs. (2.6) at best, by means of Slater determinants only. The TIMF equations derive from the stationarity of the functional $F$ with respect to variations of the single particle orbitals contained in the trial determinants. We just recall the result, whose structure is intuitive, since it is similar to Hartree-Fock equations, but now with source terms as right-hand sides. These TIMF equations read

$$
(\eta_i - h - U) |\varphi_i\rangle = \frac{\delta \langle \varphi'_i | \chi \rangle}{\delta \langle \varphi_d | \varphi_i \rangle},
$$

(3.4a)

$$
\langle \varphi'_d | (\eta_i - h - U) = \frac{\delta \langle \chi | \varphi_i \rangle}{\delta \langle \varphi'_d | \varphi_i \rangle},
$$

(3.4b)

with

$$
\eta_i = \varepsilon - E + \frac{\langle \varphi'_d | (h + U) | \varphi_i \rangle}{\langle \varphi'_d | \varphi_i \rangle}.
$$

(3.4c)

The right-hand sides of Eqs. (3.4a,b) can be normalized arbitrarily.

Since variations with respect to $\varphi_i, \varphi'_i$ are independent, we can study Eqs. (3.4a) and (3.4b) separately. For the former, we freeze $\varphi_i = \bar{\varphi}_i$ temporarily and define

$$
|\bar{\chi}_i\rangle = \frac{\delta \langle \varphi'_i | \chi \rangle}{\delta \langle \varphi_d | \varphi_i \rangle} |\varphi_i\rangle.
$$

(3.5a)

Notice that $\langle \varphi'_d | \bar{\chi}_i \rangle = 0, i \neq j$, since $\bar{\varphi}'$ is a determinant. Then Eq. (3.4a) reads

$$
\left[ \delta \varepsilon + \frac{\langle \varphi'_d | (h + U + \delta U) | \varphi_i \rangle}{\langle \varphi'_d | \varphi_i \rangle} - h - U - \delta U \right] |\varphi_i\rangle = |\bar{\chi}_i\rangle.
$$

(3.6a)

Because of the stationarity of the normalized matrix element of $(h + U)$ contained on its left-hand side, Eq. (3.6a) becomes

$$
\left( \varepsilon_i - h - U + \delta \varepsilon + \frac{\langle \varphi'_d | \delta U | \varphi_i \rangle}{\langle \varphi'_d | \varphi_i \rangle} - \delta U \right) |\varphi_i\rangle = |\bar{\chi}_i\rangle.
$$

(3.7a)
We then define the “projectors”

\[ P_i = \frac{|\phi_i\rangle\langle\phi_i|}{\langle\phi_i|\phi_i\rangle}, \quad Q_i = 1 - P_i, \quad (3.8) \]

and solve Eq. (3.7a) by

\[ |\varphi_i\rangle = \frac{P_i}{\delta z} \mathcal{P}_i + \left[ \bar{\varepsilon}_i + \delta z - \bar{Q}_i(h + \bar{U} + \delta U)\bar{Q}_i \right]^{-1} \bar{Q}_i \left( 1 + \frac{\delta U}{\delta z} P_i \right) \mathcal{P}_i. \quad (3.9a) \]

This is the same result as Eq. (2.11a) and Eq. (2.18a), as expected. The TIMF solution is thus shown to be trapped in the neighborhood of the static solution.

It is now trivial to derive dual partners of Eqs. (3.5a–7a) by freezing \( \varphi_i = \varphi_i \) and freeing \( \varphi'_i \). We can notice that Eq. (3.9a) and its obvious dual result for \( \varphi_i' \)

\[ \langle\varphi_i'\rangle = \frac{P_i}{\delta z} \mathcal{P}_i + \left[ \bar{\varepsilon}_i + \delta z - \bar{Q}_i(h + \bar{U} + \delta U)\bar{Q}_i \right]^{-1} \bar{Q}_i \left( 1 + \frac{\delta U}{\delta z} P_i \right) \mathcal{P}_i. \quad (3.9b) \]

are compatible with the constraints, Eq. (3.1). Indeed, since \( \langle\varphi_i'|\varphi_i\rangle \) satisfies Eq. (3.1), the same is true for \( \langle\varphi_i'|\mathcal{P}_i\mathcal{P}_i|\varphi_i\rangle \), hence for the \( (\delta z)^{-2} \) term of \( \langle\varphi_i'|\varphi_i\rangle \).

As was noticed at the end of § 2, the \( \varphi_i, \varphi_i' \) given by Eqs. (3.9) can be multiplied by \( \delta z \), for instance, hence renormalized into finite vectors. The factor \( \langle\varphi'|\chi|\varphi\rangle /\langle\varphi|\varphi\rangle \) in \( F \) reaches \( \langle\tilde{\varphi}|\chi|\tilde{\varphi}\rangle /\langle\tilde{\varphi}|\tilde{\varphi}\rangle \), a non-vanishing limit except for exceptional choices of \( \chi \) and/or \( \chi' \). Simultaneously the factor \( (z - E) \) in the denominator vanishes and induces the predicted singularity.

A comment on partitions of \( N \) is now in order. If the exact Schroedinger equation has factorized eigenstates \( \varphi = \varphi_A \varphi_B \), corresponding to far separated eigenstates of parts of \( H \) into clusters A and B, then the static Hartree-Fock equations are expected to generate corresponding approximations \( \tilde{\varphi} = \tilde{\varphi}_A \tilde{\varphi}_B \). The large separation in coordinate representation makes it irrelevant whether the Pauli principle is imposed upon the full \( \varphi \) and \( \tilde{\varphi} \), or whether only the clusters experience internal antisymmetrization. In any case, exchange matrix elements being cancelled by the separation, energies can be additive, \( E = E_A + E_B \). The same is obviously true if there are more than two clusters. Thus, in the same way as the exact \( G \) shows a (threshold) singularity at that energy sum of the cluster eigenenergies, the TIMF \( G_{mf} \) shows a singularity at that energy sum of the cluster Hartree-Fock energies. (Notice, however, that one should also keep track of zero point energies for relative motions between clusters, if necessary.) It is tempting to suspect that this singularity of \( G_{mf} \) is also the threshold of a branch cut, but the non-linearity of TIMF demands additional investigations before a complete understanding of its analytic structure is reached.

To summarize this section, we have found that Hartree-Fock solutions are also solutions of the antisymmetrized TIMF approximation for the inversion problems described by Eqs. (2.6). This occurs for any value of \( N \) and any source terms \( \chi \) and \( \chi' \). Threshold energies for cluster separation, when calculated in the Hartree-Fock approximation, are also singularities for the TIMF Green's function.
§ 4. Symmetries and degeneracies

In this section we briefly discuss the possibility that symmetries of $H$ may lead to non-unique TIMF solutions. The occurrence of such a multiplicity of solutions could create difficulties in the identification of the singularities of TIMF. Additional steps in the theory may become necessary, in the same way as the discovery of deformed nuclear Hartree-Fock solutions demanded angular momentum projection in order to describe rotation bands correctly.

4.1. Galilean invariance

In atomic physics the microscopic coordinates $r_i$ which must be antisymmetrized refer to the nuclear center, there exist one body potentials $u_i$, and there is thus no Galilean invariance of $H$. In molecular physics also, the electronic coordinates refer to a skeleton of nuclei which moves slowly enough to define a valid instantaneous frame, excluding Galilean invariance. In both atomic and molecular cases, remote electrons, after ionization, can be reasonably well described by Hartree-Fock orbitals $\Psi, \Psi'$ lying at positive self-energies. There should be no specially difficult problem in recognizing the nature of TIMF singularities in connection with the Hartree-Fock spectrum, despite the approximate validity of this spectrum when compared to more precise calculations of the exact one.

The situation is much different for nuclear physics. An $N$ nucleon problem should be formulated, in principle at least, in terms of $(N-1)$ Jacobi coordinates $(\rho)$, which makes antisymmetrization painful for small values of $N$ and impossible for larger values of $N$. Efficient antisymmetrized manipulations of the Schroedinger equation, and the Hartree-Fock approach in the first place, demand a representation in terms of $N$ microscopic single nucleon coordinates, referring to an abstract origin. This origin is understood as the shell model center, distinct from the center of mass. The spurious degree of freedom represented by the center of mass thus creeps into the dynamics. At best the center of mass remains localized in a (factorized?) wave packet centered around the abstract origin.

Two cases may happen, namely, i) either the energy $P^2/(2Nm)$ of the center of mass has been removed from $H$ or ii) there is a center of mass energy in $H$. This energy may be independent of the internal dynamics, or in some cases such as phenomenological shell models, the center of mass and the internal dynamics may even be dynamically, spuriously coupled.

There is a rich literature on center of mass spurious effects in nuclear physics. It deals mainly with precautions for shell model configuration mixing, but also corrects Hartree-Fock spuriousness. Nothing has been published about the center of mass effects on TIMF. For the sake of simplicity, this section discusses only the rigor oriented case i) where the Hamiltonian is the strict internal Hamiltonian, $H_{\text{int}} = H - P^2/(2Nm)$.

In such a case, it is trivially known that, for each static Hartree-Fock solution $\Psi$, there exists a completely degenerate set of equivalent, translated solutions $\Psi_a = \exp(-ia \cdot \rho) \Psi$, with $a$ an arbitrary vector. This happens, obviously, because the
technical space \( \{ \mathbf{r}_i, i=1, \cdots N \} \), in which the Hartree-Fock calculations are performed, is the tensor product of the dynamical space (the Jacobi coordinate space \( \{ \mathbf{p} \} \) with dimension \( 3N-3 \)) and the center of mass, inert spectator space. Since \( \mathcal{H} \) can be described as an eigenstate of the Hartree-Fock Hamiltonian in \( N \) body space, \( \mathcal{H}(\mathcal{H}, \mathcal{F}')=\sum_{i=1}^{N}(h_i+U_i) \), the “displaced” formula

\[
[(\sum_{i=1}^{N} \mathcal{E}_i)-\exp(-ia\cdot P)]\exp(ia\cdot P)]\exp(-ia\cdot P)\mathcal{F}=0,
\]

also describes a stationarity of the functional \( E \).

We now turn to the non-homogeneous equations, Eqs. (2.6), and their TIMF formulation, Eqs. (3.4a, b). In general, the source terms \( \chi, \chi' \), when written in the shell model representation \( \{ \mathbf{r}_i \} \), are not translation invariant. With \( \mathbf{R} \) the center of mass position, it is even advantageous, whenever possible, to choose a factorization of the center of mass, of the form

\[
\chi(\{ \mathbf{r} \}, \mathbf{R})=\chi_{\text{int}}(\{ \mathbf{r} \})\exp(-R^2)
\]

for instance, and the same for \( \chi' \), in order to induce a similar factorization of the states \( \phi, \phi' \) with their center of mass motion in a wave packet around the shell model center. There is no need for the factorization, Eq. (4.2), to be strict if a removal of the degeneracy, Eq. (4.1), is requested. What is important is that, while the homogeneous Schrödinger problem and its Hartree-Fock approximation have degenerate solutions, the non-homogeneous problems, Eqs. (2.6), should have unique solutions. We then expect to find in TIMF a corresponding removal of degeneracy.

This can be seen as follows. Consider the source terms in Eqs. (3.4), and for instance,

\[
|\chi\rangle=\frac{\delta\langle\phi'|\chi\rangle}{\delta\langle\phi|}
\]

Assume that, for each TIMF solution \( \phi, \phi' \) there exists a family of translated solutions \( \phi_a, \phi'_a \), with \( a \) arbitrary. Then the whole consistency of the TIMF equations demands that \( \chi_a \) experiences the same translation, namely, with \( \mathbf{p} \) the one body momentum operator,

\[
\exp(-ia\cdot \mathbf{p})\frac{\delta\langle\phi'|\chi\rangle}{\delta\langle\phi|}\cdot
\exp(ia\cdot \mathbf{p})\frac{\delta\langle\phi'|\chi\rangle}{\delta\langle\phi|}\cdot
\]

This is contradictory, since \( \chi \) is not invariant,

\[
|\chi\rangle\neq\exp(ia\cdot \mathbf{p})|\chi\rangle.
\]

Then we must face a paradox. On one hand, all the degenerate Hartree-Fock solutions create singularities of TIMF, and on the other hand the exact Green's states \( \phi, \phi' \) are unique and we expect a unique set of diverging orbitals \( \phi_1/\delta z, \phi'_1/\delta z \). The paradox is solved if we notice that, because of the degeneracy, the singularity \( z=E \) is the same, whichever the degenerate static solution which drives that singularity. We can conclude that, for each pair of source terms \( \chi, \chi' \), just one special Hartree-Fock solution \( \phi_{sp}, \phi'_{sp} \), fitted to \( \chi, \chi' \), will be selected, among all the degenerate ones,
and it will drive the singularity under study.

4.2. Rotations

The situation is partly similar to that of the previous subsection. The question of atomic deformations seldom arises, since the central $u_i = -Z/r_i$ is very strong and the resulting sphericity of the atomic shell model is not much modified by the mean field corrections $U_i$ induced by electronic repulsions. Conversely, in molecular physics, the geometry of the skeleton imposes such a deformation of outer electron orbitals, either a priori or via hybridization processes, that rotational degeneracies of Hartree-Fock solutions in the presence of a fixed skeleton are exceptional. Difficulties arise mainly again in nuclear physics only.

Consider, for instance, a collision $p + ^{19}$F, obviously described by the Hamiltonian of $^{20}$Ne. One may select for $x$, respectively $x'$, spherically symmetric states, where an eigenstate of the target is coupled to a proton partial wave and its spin into an initial, respectively final state with well-defined angular momentum labels. The total angular momentum may be chosen as $J=0$, a perfect case for the sphericity of $x, x'$. It is likely, nonetheless, that the well-known deformations of the static mean fields of both $^{20}$Ne and $^{19}$F will induce a degenerate set of TIMF solutions $\phi, \phi'$.

If such "rotationally degenerate" TIMF solutions occur, there is no elementary separation of the nuclear degrees of freedom between collective Euler angles $\alpha, \beta, \gamma$, conjugate to the total angular momentum $J$, and an intrinsic set of scalar coordinates $\{\sigma\}$. Furthermore, while the separation $\langle R, P \rangle, \{\rho\}$ for the center of mass resulted in a decoupling of the collective motion from the intrinsic motion, Coriolis forces prevent such a dynamical decoupling in a separation $\langle \alpha, \beta, \gamma, J \rangle, \{\sigma\}$. One may attempt to remove the TIMF degeneracy by polarizing $x, x'$, namely, by freezing specific orientations of the $^{19}$F target or the $^{20}$Ne composite system, as was done in Eq. (4.2) for a specific center of mass "polarization" (factorization, actually). But Coriolis forces are still active anyhow, and moreover the interpretation of $x, x'$ as partial waves with precise angular momentum labels is lost. It may be more relevant to select for $x, x'$ those labels which are most suitable for the description of channel waves. In particular, initial and final momentum labels $k, k'$ indicate privileged directions, which should normally prevent angular degeneracy of TIMF.

Nonetheless one can linearly mix the degenerate TIMF solutions if they occur. More explicitly, when degenerate TIMF solutions $\phi_\alpha, \phi'_\alpha$ depending on angular labels $\Omega, \Omega'$ are found, a new trial function

$$\phi_{\text{mix}} = \int d\Omega f(\Omega) \phi_\alpha , \quad (4.7a)$$

may be inserted in the variational functional, Eq. (2.10). A similar prescription obviously holds for a trial function

$$\phi_{\text{mix}}' = \int d\Omega' f'(\Omega') \phi'_\alpha . \quad (4.7b)$$

The special case where a generator coordinate amplitude $f, f'$ becomes a rotation matrix $D_{kk'}$ corresponds obviously to angular momentum projection.
4.3. **Discrete symmetries**

Assume that $\chi, \chi'$ describe an elastic $a+a$ collision, with the usual spin up-spin down symmetry and also, in the absence of Coulomb forces, proton-neutron symmetry. With the addition of forward-backward symmetry, it is clear that a self-consistent ansatz consists in deriving all 8 orbitals of the trial $\phi$ from just one of them, $\varphi_i$ for instance. However, when a “non-symmetric” threshold such as $^7\text{Li} + p$ is crossed, a second solution, made of a symmetry breaking set of orbitals $\varphi_i^{ab}$, must also be found. A linear admixture of all the competing solutions will then induce a projection of the symmetry.

To summarize this section, it is found that the problems raised in TIMF by broken symmetries are very similar to those found in static Hartree-Fock calculations. The same techniques of *a posteriori* symmetry projection are available. One may even use trial functions which are symmetry projected Slater determinants and optimize the projected determinant rather than the determinant alone. There is a significant, and convenient reduction of solution degeneracies for TIMF, however, because suitably non-symmetric source terms $\chi, \chi'$ may remove ambiguities linked to that homogeneous problem, the diagonalization of $H$.

§ 5. **Discussion and conclusion**

The link between i) solutions of a homogeneous linear problem $(E-H)\phi=0$ and ii) singularities of the related, inhomogeneous linear problem $(z-H)\phi=\chi$ belongs to common wisdom. This paper claims that a similar relation exists between non-linear approximations to the former and the latter. This is less obvious. Indeed, while Hartree-Fock equations are still a diagonalization problem

$$[(\sum_{i=1}^{N}\varepsilon_i)-\mathcal{H}]|\phi\rangle=0,$$

(5·1)

there is no simple analog for TIMF. At best, if $\chi$ is a Slater determinant made of orbitals $\chi_i$, one may take advantage of Eqs. (3·4) to obtain

$$[(\sum_{i=1}^{N}\eta_i)-\mathcal{H}]|\phi\rangle=\sum_{i=1}^{N}|\phi_i\rangle,$$

(5·2)

where $\phi_i$ is a particle-hole state obtained from $\phi$ by the replacement of $\varphi_i$ by $\chi_i$. This cannot be recognized as a canonical, non-homogeneous equation associated to Hartree-Fock and tells little about singularities of TIMF. We will show that the basic reason for a link between Hartree-Fock and TIMF is rather contained in the behaviors of the functionals $E$ and $F$, Eqs. (2·2) and (2·10).

Consider a manifold of “density matrices”

$$\mathcal{D}=\frac{|\phi\langle \phi'\rangle|}{\langle \phi'|\phi \rangle},$$

(5·3)

where $\phi, \phi'$ may be Slater determinants, or BCS states, or any more general states as long as they are suitable for practical calculations. The sum of two $\mathcal{D}$'s does not
need to be a third $\mathcal{D}$ in general, hence the manifold under consideration is a curved space in general. We notice that, because of the denominator in Eq. (5.3), there is no phase or norm ambiguity in the $\mathcal{D}$'s. Since $\text{Tr} \mathcal{D}=1$, the manifold can be viewed as a subset of the sphere of normalized "densities".

The functional $E$ is nothing but $\text{Tr}(H \mathcal{D})$, and Hartree-Fock solutions $\mathcal{D}$ are found when the gradient of $E$ vanishes, $\nabla E=0$. In a neighborhood of $\mathcal{D}$, the functional variations of $E$ are driven by the symmetric matrix $\mathcal{M}$ of second order derivatives of $E$. Let us denote a variation of $\mathcal{D}$ by its components $d \mathcal{D}$, on any suitable basis of the tangent plane of the manifold. (For Slater determinants, such a basis is known to be the particle-hole basis.) Then in the neighborhood of $\mathcal{D}$ we obtain

$$ E = \bar{E} + \frac{1}{2} \sum_{n,l} \mathcal{M}_{kl} d \mathcal{D}_k d \mathcal{D}_l, \quad (5.4) $$

and the corresponding components of the gradient,

$$ (\nabla E)_k = \sum_l \mathcal{M}_{lk} d \mathcal{D}_l. \quad (5.5) $$

Consider now the "projector" $C = |\chi \rangle \langle \chi'|$ and the functional $C=\text{Tr}(C \mathcal{D})$. In the neighborhood of $\mathcal{D}$ the gradient $\nabla C$ has finite components $(\nabla C)_k$. These can be calculated at the point $\mathcal{D}$, and can then be considered as constants $(\nabla C)_k$ up to first order. Accordingly, the variation of $C$ in the neighborhood under consideration is a first order variation,

$$ C = \overline{C} + \sum_k (\nabla C)_k d \mathcal{D}_k, \quad (5.6) $$

where $\overline{C}=\text{Tr}(C \mathcal{D})$.

We will now take advantage of the relation $F=C/(z-E)$. Consider an infinitesimal $d\zeta$ and solve for the components $d \mathcal{D}$, the conditions

$$ (\nabla E)_k = -d\zeta (\nabla C)_k. \quad (5.7) $$

According to Eqs. (5.5), this is straightforward if the matrix $\mathcal{M}$ is not singular. The regularity of this matrix is indeed a generic case, with the exception of the symmetry peculiarities studied in § 4. Except when such peculiarities demand special precautions, the solution of Eqs. (5.7) thus defines a vector $T$ in the tangent plane of the manifold, with components $T_i=d \mathcal{D}_i/d\zeta$. By its very definition, $T$ defines a line, issued from $\mathcal{D}$, along which the vectors $\nabla E$ and $\nabla C$ are parallel.

At any point $\mathcal{D}+T d\zeta$ on that line the gradient of $F$ is given by

$$ \nabla F = \frac{\nabla C + F \nabla E}{(z-E)} = \frac{(1-F d\zeta) \nabla C}{(z-E)}. \quad (5.8) $$

We notice that, since $F$ is a ratio, it plays the role of a Lagrange multiplier relating the gradients of its numerator and denominator. The gradient of $F$ vanishes, and thus defines a TIMF solution, if $F=(d\zeta)^{-1}$. Simultaneously, this value of $F$ is actually the stationary value $\bar{F}$. The singular behavior of $\bar{F}$ when $d\zeta \to 0$ is transparent. Finally the corresponding value of $dz=(z-E)C/F$ is thus $dz=C/\bar{F} = \bar{C} d\zeta$. 

This argument completely recovers the proofs found in §§ 2 and 3.

One problem, of some importance, has been left open in the present paper. In exact scattering theories, thresholds induce cuts along the real axis of the complex plane for $z$. We do not know whether the same is true for TIMF, and actually the numerical evidence of soluble models\(^3\) may point to a different conclusion. More precisely, for any real or slightly complex value of $z$ above threshold, we always found numerically one pair, at least, of distinct complex solutions. The two solutions of a pair are strictly complex conjugate with respect to each other when $z$ is real. One of the solutions approximates the retarded Green’s function, while the other solution approximates the advanced Green’s function. Nothing special occurs when $z$ approaches the real axis with the usual infinitesimal part, $z=\Re z + i\varepsilon$, both solutions being continuous when $\varepsilon$ changes its sign. It is very likely that the solution which approximates the retarded Green’s function when $\varepsilon>0$ will approximate its continuation in the second Riemann sheet when $\varepsilon<0$.

The conjugate self-energies $\eta$ of both TIMF solutions in such a conjugate pair merge into real values when $z$ reaches the threshold energy. Hence this singularity is confirmed locally. But the existence of pairs of TIMF solutions for $z$ complex, and their unexpected smooth evolution when $z$ becomes real, may indicate that some singularities of TIMF might occur for some complex values of $z$ as well as real ones. Indeed, there are more than just one pair of TIMF solutions for each $z$, and little is known about the crossing of different solution branches. The same question arises for the static Hartree-Fock equations, incidentally, in particular with independent bra and ket trial functions $\phi, \phi'$. Little is known about the whole multiplicity of solutions of these static equations. This question of branch crossing in TIMF and its possible link with static Hartree-Fock solutions far from traditional energy minima deserves further investigation.

In any case, as a summary of this paper, we may point out that the derivation, found in this section, of the existence of a line of TIMF solutions in the neighborhood of Hartree-Fock solutions, is based on purely geometrical considerations. The exact nature of the variational manifold is not restricted to Slater determinants. Only minor assumptions concerning the existence of a tangent plane, and properties of first or second order derivatives of functionals, are used in the proof. It can be concluded that TIMF, which uses Slater determinants, is just one among many possible approximate scattering theories, either linear (generator coordinate\(^6\) theories for instance) or non-linear. Every simultaneous use of functionals $E$ and $F$ with an extended class of trial densities defines a scattering theory, and the same theorem, the subject of this paper, will apply. Namely, any “eigenvalue” $\bar{E}$ of the approximation to the spectrum generates a singularity of the corresponding approximation for the Green’s function. This theorem shows the internal coherence of such approximate collision theories, and of TIMF in particular.

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