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Convergence Criteria for the Hartree Iterative Solution of the General Self-Consistent Field Equations

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Abstract

The traditional Hartree method of solving the Hartree–Fock equations, by repeated diagonalization and recalculation of the single-particle Hamiltonian, is expressed in terms of repeated unitary transformations and shown to be applicable to the general SCF (self-consistent field) equations. The necessary and sufficient conditions for convergence to a unique local SCF solution are derived and it is shown that only a small class of solutions are obtainable by this method.

1. *Introduction*

The HF (Hartree-Fock) SCF (self-consistent field) theory (Hartree, 1927–28; Fock, 1930) is perhaps the most fundamental of many-body theories in the sense that it is central to almost all other microscopic theories. But, in spite of its importance, we are not aware that the criteria for convergence of the standard Hartree iterative method for solving the HF equations have ever been established. The objective of this paper is to rectify this deficiency by determining convergence criteria for the general SCF equations, of which the HF equations are a particular case.

The general SCF theory (Rowe, 1968; Rowe and Wong, 1970; Rowe, 1972; Clement, 1969; Baranger, 1969; Agodi et al., 1971) can be stated compactly as follows: Let $|\Psi\rangle$ be a general many-particle state given uniquely in terms of a set of single-fermion states $|\psi_\nu\rangle$ with annihilation and creation operators a_ν, $a_\nu^\dagger$, respectively. These single-particle states, and hence the many-particle state $|\Psi\rangle$, are defined by the self-consistent field equation

$$\langle\Psi|\{a_\mu,[H,a_\nu^\dagger]\}|\Psi\rangle=\delta_{\mu\nu}\epsilon_\nu \qquad \text{for all } \mu,\nu \tag{1.1}$$

That equation (1.1) is indeed a self-consistent field equation is readily seen by expanding the Hamiltonian in the usual second quantized form

$$H = \sum_{\mu\nu} T_{\mu\nu} a_\mu^\dagger a_\nu + \frac{1}{4} \sum_{\mu\nu\mu'\nu'} V_{\mu\mu'\nu\nu'} a_\mu^\dagger a_{\mu'}^\dagger a_{\nu'} a_\nu \tag{1.2}$$

[See for example Appendix C of Rowe (1970) for clarification of notation.] Equation (1.1) then becomes

$$h_{\mu\nu} = T_{\mu\nu} + u_{\mu\nu}(\Psi) = \delta_{\mu\nu}\epsilon_\nu \tag{1.3}$$

where

$$u_{\mu\nu}(\Psi) = \sum_{\mu'\nu'} V_{\mu\mu'\nu\nu'} \langle \Psi | a_{\mu'}^\dagger a_{\nu'} | \Psi \rangle \tag{1.4}$$

Thus $u(\Psi)$ is a self-consistent field that depends on the single-particle states through the functional dependence of $|\Psi\rangle$ on those states.

In the event that Ψ is a slater determinant of the single-particle states ψ_ν, the above equations are those of the familiar HF approximation.

The simplest way to solve them is by the Hartree method, traditionally used to solve the HF equations, i.e., by repeated diagonalization and recalculation of the single-particle Hamiltonian (1.3), until successive iterations effect no change.

In Section 2, the Hartree method is expressed in a form convenient for a discussion of convergence, in terms of repeated unitary transformations. In Section 3, we derive convergence criteria and show that only a small class of solutions are attainable by this method. The HF approximation is examined in more detail in Section 4 and the convergence criteria are expressed in terms that explain a characteristic of the Hartree procedure that is well-known from practical experience, namely, that successive iterations invariably decrease the energy of the many-particle state. This characteristic of the Hartree method has long been a nuisance in the calculation of fission barriers in the constrained HF approximation. Thus it has only been by devious modifications (Giraud et al., 1970; Bassichis and Wilets, 1971) to the Hartree procedure that HF solutions could be obtained for which the energy is not a local minimum with respect to all possible variations. Section 5 contains some discussion and conclusions.

2. *The Hartree Method*

Let $\{a_\nu^\dagger\}$ be a set of single-particle basis operators and

$$\Psi_0 = \Psi_0(\{\alpha_\nu^\dagger\}) \tag{2.1}$$

the corresponding many-particle wave function, defined uniquely by the basis. If X is an anti-Hermitian one-body operator, acting on the combined

Hilbert space of single- and many-particle states, we can define a new basis and a new many-particle state by the unitary transformation

$$\begin{aligned} \alpha_\nu^\dagger(X) &= e^X \alpha_\nu^\dagger e^{-X} \\ |\Psi(X)\rangle &= e^X |\Psi_0\rangle \end{aligned} \tag{2.2}$$

Thus the operator X serves to specify the basis $\{\alpha_\nu^\dagger(X)\}$. Our objective is therefore to find the particular X for which equation (1.1) is satisfied with

$$\begin{aligned} a_\nu^\dagger &= \alpha_\nu^\dagger(X) \\ |\Psi\rangle &= |\Psi(X)\rangle \end{aligned} \tag{2.3}$$

Let us suppose we start an iterative solution of the SCF equations with a many-particle state $|\Psi(T)\rangle$. Corresponding to this state we can define a single-particle Hamiltonian

$$h(T) = \sum_{\mu\nu} \langle \Psi(T) | \{\alpha_\mu(S), [H, \alpha_\nu^\dagger(S)]\} | \Psi(T)\rangle \alpha_\mu^\dagger(S)\alpha_\nu(S) \tag{2.4}$$

which operates on both the single- and many-particle state space. Note that $h(T)$ is here expressed in terms of some single-particle basis S, which need not be equal to T. It is therefore important to recognize that, whereas the matrix elements

$$h_{\mu\nu}(S, T) = \langle \Psi(T) | \{\alpha_\mu(S), [H, \alpha_\nu^\dagger(S)]\} | \Psi(T)\rangle \tag{2.5}$$

depend on both S and T, the Hamiltonian $h(T)$ depends only on T.

The Hartree procedure can now be expressed as follows: Given a many-particle state $|\Psi(T)\rangle$, a single-particle basis S is determined that diagonalizes $h(T)$, i.e.,

$$h_{\mu\nu}(S, T) = \delta_{\mu\nu}\epsilon_\nu(T) \tag{2.6}$$

$\Psi(T)$ is then replaced by $\Psi(S)$ and the process iterated until $S = T = X$, whence we have

$$\langle \Psi(X) | \{\alpha_\mu(X), [H, \alpha_\nu^\dagger(X)]\} | \Psi(X)\rangle = \delta_{\mu\nu}\epsilon_\nu(X) \tag{2.7}$$

and a solution to equation (1.1).

Our objective is now to determine what class of SCF solutions can be obtained by this procedure. To answer this question we consider a starting state arbitrarily close to a SCF solution and examine the criteria for convergence to that particular solution.

3. *Criteria for Convergence to a Unique Local Solution*

3.1. *A Special Case.* First we eliminate a special case for which it follows immediately that the Hartree procedure cannot converge to a unique local SCF solution.

Consider a particular solution Ψ for which there exists a subspace D of single-particle states spanned by a set of degenerate eigenstates of $h(\Psi)$, i.e.,

$$h_{\mu\nu}(\Psi) = \epsilon\delta_{\mu\nu}, \qquad \mu, \nu \in D$$

Since the matrix elements $h_{\mu\nu}$ are left invariant by an arbitrary unitary transformation e^S of the single-particle states in D, it follows that the Hartree method cannot define the single-particle basis states in D.

Therefore, if the many-particle state $e^S|\Psi\rangle$ differs from $|\Psi\rangle$ by more than a phase factor, it follows that $|\Psi\rangle$ cannot be defined uniquely by the Hartree procedure.

Observe now, by inspection of equations (1.3) and (1.4) that $h(\Psi)$ depends on the state $|\Psi\rangle$ through its single-particle densities.

$$n_{\mu\nu} = \langle\Psi|a_\mu^\dagger a_\nu|\Psi\rangle$$

A necessary, but not sufficient, condition for a unique local solution is therefore that the density matrix elements $n_{\mu\nu}$ are also left invariant by the transformation e^S. Clearly the single-particle densities will be left invariant by a general unitary transformation in D if and only if

$$n_{\mu\nu} = n\delta_{\mu\nu} \qquad \text{for all} \qquad \mu, \nu \in D$$

Conversely then we see that the *Hartree procedure cannot converge to a unique local SCF solution unless the occupation numbers $n_{\nu\nu}$ are equal for all degenerate single-particle states ν.*

However, if only the single-particle densities but not other properties of the state $|\Psi\rangle$ are left invariant by an undefined transformation $e^S|\Psi\rangle$, the Hartree procedure can only converge to a unique local *subset* of SCF solutions, all of which have identical single-particle properties. The latter situation is undoubtedly extremely rare. It will nevertheless be included in the following analysis if we expand the definition of a "unique local solution" to mean the determination of any member of a unique local subset of many-particle states all of which are SCF solutions and have identical single-particle properties.

3.2. *The Remaining Cases.* With the exclusion of the above special case, it will be assumed for the following, although it is probably not essential, that the single-particle basis that diagonalizes the SCF Hamiltonian simultaneously diagonalizes the density matrix, i.e.,

$$\langle\Psi|a_\mu^\dagger a_\nu|\Psi\rangle = \delta_{\mu\nu}n_\nu \tag{3.1}$$

This is trivially true in the HF approximation and for all shell model generalizations of the SCF method that we invisage. Elimination of the special case then allows us to assume for the remainder that

$$n_\mu = n_\nu \qquad \text{if} \qquad \epsilon_\mu = \epsilon_\nu \tag{3.2}$$

To investigate the convergence of the Hartree procedure we suppose that $|\Psi\rangle$ is a self-consistent solutuion to equation (1.1) and consider a starting state

$$|\Psi_0\rangle = e^{-R}|\Psi\rangle \tag{3.3}$$

close to $|\Psi\rangle$ with

$$\alpha_\nu^\dagger = e^{-R} a_\nu^\dagger e^R$$

At the first iteration, S is given by requiring

$$h_{\mu\nu}(S, 0) = \langle\Psi_0|\{\alpha_\mu(S), [H, \alpha_\nu^\dagger(S)]\}|\Psi_0\rangle \tag{3.4}$$

to be diagonal, where

$$\alpha_\nu^\dagger(S) = e^S \alpha_\nu^\dagger e^{-S} = e^S e^{-R} a_\nu^\dagger e^R e^{-S} \tag{3.5}$$

Equation (3.4) can therefore be expressed as follows:

$$h_{\mu\nu}(S.\,0) = \langle\Psi|e^R e^S e^{-R}\{a_\mu, [e^R e^{-S} H e^S e^{-R}, a_\nu^\dagger]\}e^R e^{-S} e^{-R}|\Psi\rangle \tag{3.6}$$

Expanding to first order in R and S, we obtain

$$h_{\mu\nu}(S,0) = \delta_{\mu\nu}\epsilon_\nu + \langle\Psi|\{a_\mu, [[H, S-R], a_\nu^\dagger]\}|\Psi\rangle - \langle\Psi|[\{a_\mu, [H, a_\nu^\dagger]\}, S]|\Psi\rangle \tag{3.7}$$

It can easily be shown by expansion that

$$\langle\Psi|\{a_\mu, [[H, S], a_\nu^\dagger]\}|\Psi\rangle - \langle\Psi|[\{a_\mu, [H, a_\nu^\dagger]\}, S]|\Psi\rangle = (\epsilon_\mu - \epsilon_\nu)S_{\mu\nu} \tag{3.8}$$

Therefore $S_{\mu\nu}$ is given by

$$(\epsilon_\mu - \epsilon_\nu)S_{\mu\nu} = \sum_{\mu'\nu'} H_{\mu\nu,\mu'\nu'} R_{\mu'\nu'} \tag{3.9}$$

where

$$H_{\mu\nu,\mu'\nu'} = \langle\Psi|\{a_\mu, [[H, a_{\mu'}^\dagger a_{\nu'}], a_\nu^\dagger]\}|\Psi\rangle \tag{3.10}$$

$$= \delta_{\mu\mu'}\delta_{\nu\nu'}(\epsilon_\mu - \epsilon_\nu) + V_{\mu\nu'\nu\mu'}(n_{\nu'} - n_{\mu'}) \tag{3.11}$$

Before proceeding it is important to note some important characteristics of the operators R and S and their relationship. The operator R effects a transformation only of the many-particle state, equation (3.3), whereas S effects a transformation of single-particle states, equation (3.5). Now since the matrix element $h_{\mu\nu}(S, 0)$ of the single-particle Hamiltonian that determines S is the expectation of a one-body operator $\{\alpha_\mu(S), [H, \alpha_\nu^\dagger(S)]\}$ [cf. equation (3.4)], it is clear that S is left invariant by any transformation of $|\Psi_0\rangle$ that leaves its single-particle density invariant. To first order in R

$$\langle\Psi_0|a_\alpha^\dagger a_\beta|\Psi_0\rangle = \langle\Psi|a_\alpha^\dagger a_\beta|\Psi\rangle - R_{\beta\alpha}(n_\alpha - n_\beta) \tag{3.12}$$

Thus S cannot depend on any elements $R_{\beta\alpha}$ for which $n_\alpha = n_\beta$. In solving equation (3.9) for S we may therefore set all such elements of R equal to zero.

The corresponding elements of S cannot be set directly equal to zero, since they are needed in transforming $h_{\mu\nu}(S, 0)$ to diagonal form. However, at each Hartree iteration we can diagonalize $h_{\mu\nu}(S, T)$ in two successive stages:

$$e^S = e^{S_1} e^{S_2} \tag{3.13}$$

where S_2 only ensures the partial diagonalization

$$h_{\mu\nu}(S_2, T) = 0 \qquad \text{for } n_\nu \neq n_\mu \tag{3.14}$$

and S_1 completes the diagonalization between states of equal occupancy. Now a unitary transformation among states of equal occupancy leaves the single-particle density invariant to all orders. The transformation $\exp(S_1)$ can therefore be neglected at each iteration except the last since it cannot influence the calculation of S at any subsequent iteration. In considering the convergence of the Hartree procedure it is therefore sufficient to consider only the calculation of S_2. This is a generalization of the well-known characteristic of the Hartree–Fock approximation in which diagonalization of the single-particle Hamiltonian within the space of occupied, or unoccupied states, can be left until convergence is already achieved.

We therefore proceed to solve equation (3.9) within the subspace of states for which $n_\nu \neq n_\mu$ and $n_{\nu'} \neq n_{\mu'}$. Combining this restriction with equation (3.2), we see that the indices in equation (3.9) can be restricted to those for which

$$\begin{aligned} \epsilon_\mu - \epsilon_\nu \neq 0, \qquad & n_\mu - n_\nu \neq 0 \\ \epsilon_{\mu'} - \epsilon_{\nu'} \neq 0, \qquad & n_{\mu'} - n_{\nu'} \neq 0 \end{aligned} \tag{3.15}$$

It is now convenient to multiply both sides of equation (3.9) by $(n_\nu - n_\mu)$:

$$(n_\nu - n_\mu)(\epsilon_\mu - \epsilon_\nu)S_{\mu\nu} = \sum_{\mu'\nu'} \mathscr{H}_{\mu\nu,\mu'\nu'} R_{\mu'\nu'} \tag{3.16}$$

where $\mathscr{H}$ is the Hermitian matrix

$$\mathscr{H}_{\mu\nu,\mu'\nu'} = \delta_{\mu\mu'}\delta_{\nu\nu'}(n_\nu - n_\mu)(\epsilon_\mu - \epsilon_\nu) + (n_\nu - n_\mu)V_{\mu\nu'\nu\mu'}(n_{\nu'} - n_{\mu'}) \tag{3.17}$$

Now let us order the indices such that

$$\mu > \nu \qquad \text{if} \qquad (n_\nu - n_\mu)(\epsilon_\mu - \epsilon_\nu) > 0 \tag{3.18}$$

Then S can be expressed

$$S = \sum_{\mu > \nu} (S_{\mu\nu} a_\mu^\dagger a_\nu - S_{\mu\nu}^* a_\nu^\dagger a_\mu) \tag{3.19}$$

and R likewise. This enables us to write the solutions to equation (3.16) in matrix form

$$\begin{pmatrix} S \\ S^* \end{pmatrix} = \begin{pmatrix} (n\epsilon)^{-1} & 0 \\ 0 & (n\epsilon)^{-1} \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} R \\ R^* \end{pmatrix} \tag{3.20}$$

where $(n\epsilon)$ is the diagonal positive definite matrix with elements

$$(n\epsilon)_{\mu\nu} = (n_\nu - n_\mu)(\epsilon_\mu - \epsilon_\nu), \qquad \mu > \nu \tag{3.21}$$

and

$$A_{\mu\nu\mu'\nu'} = \mathscr{H}_{\mu\nu\mu'\nu'}, \qquad B_{\mu\nu\mu'\nu'} = -\mathscr{H}_{\mu\nu\nu'\mu'}, \qquad \mu > \nu, \mu' > \nu' \tag{3.22}$$

The submatrices A and B are simple generalizations of the standard RPA (random phase approximation) (Rowe, 1970; Thouless, 1961) matrices to which they reduce in the HF approximation.

To see if the Hartree procedure is convergent it is convenient to expand R and S in terms of the solutions to the equation

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X_\lambda \\ Y_\lambda \end{pmatrix} = \omega_\lambda \begin{pmatrix} n\epsilon & 0 \\ 0 & n\epsilon \end{pmatrix} \begin{pmatrix} X_\lambda \\ Y_\lambda \end{pmatrix} \tag{3.23}$$

This is an eigenvalue equation for a Hermitian matrix with a positive definite metric. Its eigenvalues are therefore real. Now if $\binom{X_\lambda}{Y_\lambda}$ is an eigenvector with eigenvalue ω_λ, it follows from symmetry that $\binom{Y_\lambda^*}{X_\lambda^*}$ is also an eigenvector of eigenvalue ω_λ. Thus we can express all solutions in the form $\binom{X_\lambda}{X_\lambda^*}$. These solutions can be obtained from

$$X = (n\epsilon)^{-1/2} Z_\lambda \tag{3.24}$$

where Z_λ is a solution of the eigenvector equation

$$\begin{pmatrix} \bar{A} & \bar{B} \\ \bar{B}^* & \bar{A}^* \end{pmatrix} \begin{pmatrix} Z_\lambda \\ Z_\lambda^* \end{pmatrix} = \omega_\lambda \begin{pmatrix} Z_\lambda \\ Z_\lambda^* \end{pmatrix} \tag{3.25}$$

with unit metric and

$$\begin{aligned} \bar{A} &= (n\epsilon)^{-1/2} A (n\epsilon)^{-1/2} \\ \bar{B} &= (n\epsilon)^{-1/2} B (n\epsilon)^{-1/2} \end{aligned} \tag{3.26}$$

We assume that the eigenvectors are normalized in the conventional way, so that

$$\begin{aligned} Z_\kappa^\dagger Z_\lambda + \text{c.c.} &= \delta_{\kappa\lambda} \\ X_\kappa^\dagger (n\epsilon) X_\lambda + \text{c.c.} &= \delta_{\kappa\lambda} \end{aligned} \tag{3.27}$$

We may therefore expand

$$R = \sum_\lambda C_\lambda X_\lambda \tag{3.28}$$

with C_λ real and given by

$$C_\lambda = X_\lambda^\dagger (n\epsilon) R + \text{c.c.} \tag{3.29}$$

Substituting the above expansion for R into equation (3.20) we obtain the solution

$$S = \sum_{\lambda} \omega_\lambda C_\lambda X_\lambda \tag{3.30}$$

Thus comparing equations (3.28) and (3.30) we see that the Hartree method diverges with respect to any mode λ if $\omega_\lambda < 0$ or $\omega_\lambda > 2$.

It should be noted that convergence can sometimes be achieved even if one of the ω_λ is outside the range for convergence provided the coefficient C_λ for the offending mode can be maintained precisely equal to zero throughout the calculation by the imposition of some symmetry.

Now $\omega_\lambda > 0$, for all λ, if and only if the matrix

$$\begin{pmatrix} \bar{A} & \bar{B} \\ \bar{B}^* & \bar{A}^* \end{pmatrix} \tag{3.31}$$

is positive definite. Equivalently, since $(n\epsilon)$ is positive definite, $\omega_\lambda > 0$, for all λ, if and only if the matrix

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \tag{3.32}$$

is positive definite.

It is interesting to note that, in the HF approximation, this convergence condition reduces to Thouless' stability condition for real RPA roots (Thouless, 1961).

The condition that $\omega_\lambda < 2$, for all λ, is that the matrix

$$2\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} - \begin{pmatrix} \bar{A} & \bar{B} \\ \bar{B}^* & \bar{A}^* \end{pmatrix} \tag{3.33}$$

should be positive definite. Again, since $(n\epsilon)$ is positive definite, this is equivalent to the condition that

$$2\begin{pmatrix} n\epsilon & 0 \\ 0 & n\epsilon \end{pmatrix} - \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \tag{3.34}$$

is positive definite.

The above two convergence conditions can be put into a symmetric form by defining the two Hamiltonians

$$H_\pm = h \pm V_{\text{res}} \tag{3.35}$$

where h is the single-particle SCF Hamiltonian and V_{res} the residual interaction; i.e., the original Hamiltonian H is equal to H_+. We can then define the matrices

$$\begin{aligned} A_\pm &= A(H_\pm) \\ B_\pm &= B(H_\pm) \end{aligned} \tag{3.36}$$

Furthermore we note from equation (3.17) that

$$A(h) = n\epsilon \tag{3.37}$$

Thus the conditions for convergence, with respect to all modes λ, are that the matrices

$$\begin{pmatrix} A_\pm & B_\pm \\ B_\pm^* & A_\pm^* \end{pmatrix} \tag{3.38}$$

should both be positive definite.

Comparison of equations (3.28) and (3.30) shows that the rate of convergence of the Hartree procedure is maximum when $\omega_\lambda = 1$, for all λ. Now $\omega_\lambda = 1$, for all λ, only if V_{res} is zero, in which case the whole Hamiltonian is one-body and the problem is trivial. In typical nuclear situations, for example, one or two values of ω_λ are ~ 0.5 and the others ~ 1.0. The low values correspond to low-lying collective excitations in the many-particle spectrum. Thus the effect of such collective excitations is to substantially reduce the rate of convergence of the Hartree iterative solution.

4. *The Hartree-Fock Approximation*

It is instructive to pursue the significance of the above convergence conditions for the standard HF approximation. In the HF approximation $|\Psi\rangle$ is a Slater determinant and the matrices $A_\pm$ and $B_\pm$ can be written in the alternative form

$$\begin{aligned} A^\pm_{ph,p'h'} &= \langle\Psi|[a_h^\dagger a_p,[(h \pm :V:), a_{p'}^\dagger a_{h'}]\,]\,|\Psi\rangle \\ B^\pm_{ph,p'h'} &= -\langle\Psi|\,[a_h^\dagger a_p,[(h \pm :V:), a_{h'}^\dagger a_{p'}]\,]\,|\Psi\rangle \end{aligned} \tag{4.1}$$

where $:V:$ is the two-body interaction arranged in normal order with respect to $|\Psi\rangle$ as particle-hole vacuum, i.e.,

$$:V: = \frac{1}{4} \sum_{\mu\nu\mu'\nu'} V_{\mu\nu\mu'\nu'} :a_\mu^\dagger a_\nu^\dagger a_{\nu'} a_{\mu'}:$$

It is then easily shown that the convergence conditions become

$$\langle\Psi|\,[[H_\pm, S], S]\,|\Psi\rangle > 0 \tag{4.2}$$

for *all* particle-hole operators S (Rowe, 1970; Thouless, 1961).

Now suppose that $|\Psi_0\rangle$ is a determinant close to $|\Psi\rangle$ and that diagonalization of $h_{\mu\nu}(S, 0)$ for this state yields an operator S. We may then expand the Hamiltonian in normal order with respect to the state $|\Psi_0\rangle$ as particle-hole vacuum, i.e.,

$$H = \text{const} + h(0) + :V: \tag{4.3}$$

We wish to compare the energy expectation of the state

$$|\Psi(S)\rangle = e^S\,|\Psi_0\rangle \tag{4.4}$$

with that of $|\Psi_0\rangle$. Since $h(0)$ is diagonal in the S representation

$$h(0) = \Sigma \epsilon_\nu(S)\alpha_\nu^\dagger(S)\alpha_\nu(S) \tag{4.5}$$

there are no linear terms in S in the expansion

$$\langle\Psi_0|h(0)|\Psi_0\rangle = \langle\Psi(S)|h(0)|\Psi(S)\rangle + \tfrac{1}{2}\langle\Psi(S)|[[h(0), S], S]|\Psi(S)\rangle + \cdots \tag{4.6}$$

And since $:V:$ is normal ordered with respect to $|\Psi_0\rangle$ there are no zero or first order terms in S in the expansion

$$\langle\Psi(S)|:V:|\Psi(S)\rangle = \tfrac{1}{2}\langle\Psi_0|[[:V:, S], S]|\Psi_0\rangle + \cdots \tag{4.7}$$

Therefore

$$\langle\Psi(S)|H|\Psi(S)\rangle = \langle\Psi_0|H|\Psi_0\rangle - \tfrac{1}{2}\langle\Psi_0|[[(h(0) - :V:), S], S]|\Psi_0\rangle + \cdots \tag{4.8}$$

which to second order in S can be written

$$\langle\Psi(S)|H|\Psi(S)\rangle = \langle\Psi_0|H|\Psi_0\rangle - \tfrac{1}{2}\langle\Psi|[[H_-, S], S]|\Psi\rangle \tag{4.9}$$

Thus, if the convergence condition for H_- is satisfied, we find that the energy expectation must decrease at each Hartree iteration. But the convergence condition for H_+ is that the energy expectation $\langle\Psi|H|\Psi\rangle$ for the HF solution is a minimum with respect to all infinitesimal variations. Thus we can understand the necessity for both conditions to be satisfied for the Hartree method to converge.

5. *Discussion*

In this paper we have derived necessary and sufficient conditions for convergence of the Hartree method of solving the general SCF equations. By considering the HF approximation in some detail, we were able to interpret the physical significance of the conditions. We also learned that the Hartree procedure can only converge to a very restricted class of SCF solutions. In particular, in the HF approximation, it can only converge to those solutions for which the energy is a local minimum with respect to all possible allowed infinitesimal variations. This is the condition

$$\langle\Psi|[[H_+, S], S]|\Psi\rangle > 0 \qquad \text{for all } S \tag{5.1}$$

corresponding to Thouless' stability condition for real RPA roots (Thouless, 1961).

Now, in nuclear physics, the residual interaction, V_{res}, is predominantly attractive. Given that the condition (5.1) is satisfied, it is unlikely therefore that the other condition for convergence, i.e.,

$$\langle\Psi|[[H_-, S], S]|\Psi\rangle > 0 \qquad \text{for all } S \tag{5.2}$$

would not also be satisfied. Thus we expect that, for the ground-state HF solution (the minimum minimorum), the Hartree procedure would normally converge, although the rate of convergence might be slow, if low-lying RPA collective roots occur.

For systems in which the residual interaction is strong and repulsive, on the other hand, it is possible that even the ground-state solution is unobtainable by the Hartree procedure. However it is possible that such systems are of no practical interest.

In a following paper we shall consider the Newton-Kantorovic method for solving both the SCF and the generalized variational equations. We shall show that it converges in all cases of practical interest and that, even when the Hartree procedure does converge, the former converges much faster.

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