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A RAPIDLY CONVERGENT METHOD FOR SOLVING THE STATIC HARTREE-FOCK PROBLEM

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ABSTRACT : An improved version of the direct density method for solving the static Hartree-Fock equations is presented. A simple relation with the imaginary time method is exhibited.

The aim of this note is two fold : to present a rapidly convergent method for the solution of the Hartree-Fock (HF) equations and to establish a connection between the imaginary time [1] and the direct density (DD) [2] methods with each other and also with the conventional [3] HF method.

In the DD method, the HF density matrix ρ is obtained by the following iteration procedure [2]

$$\rho_{n+1} = e^{i\chi_n}\, \rho_n\, e^{-i\chi_n} \tag{1}$$

$$\text{with } \chi_n = -\lambda[i[h_F(\rho_n), \rho_n]]^+ \tag{2}$$

where n is the iteration number and h_F is the HF Hamiltonian [4]. Let us note that when the density changes from ρ_n to ρ_{n+1}, the energy decrease, up to third order, may be shown to be

$$\Delta E = \text{Trace}[h_F(\rho_n) + \frac{1}{2} h'_F(\rho_n)\Delta\rho + \frac{1}{6} h''_F(\rho_n)(\Delta\rho)^2 + \ldots]\ \Delta\rho \tag{3}$$

Or

$$\Delta E = \text{Trace}\ h_{eff}\ \Delta\rho \tag{4}$$

with

$$h_{eff}(\rho_n) = h_F(\rho_n) + \frac{1}{2} h'_F(\rho_n)\Delta\rho + \frac{1}{6} h''_F(\rho_n)(\Delta\rho)^2 + \ldots \tag{5}$$

Where h'_F and h''_F are the first and second derivatives of the HF hamiltonian with respect to the density matrix . From eqs. (3-5) it seems natural to try to improve the convergence of the iteration scheme of eq.(1) by replacing eq.(2) by

$$\chi_n = -\lambda[\,i[h_{eff}(\rho_n),\rho_n]\,]^+ \qquad (6)$$

with h_{eff} as in eq.(5).

The higher order terms in eq.(5) that contain derivatives of h_F have a simple relation to the conventional HF method and also to the imaginary time method. The conventional HF iteration scheme uses the HF Hamiltonian $h_F(\rho_n)$ at the n^{th} iteration. However, it has been found [4] in practice that an average Hamiltonian $\frac{1}{2}\{h_F(\rho_n)+h_F(\rho_{n-1})\}$ leads to faster convergence. It is easy to see that this prescription is identical to eq.(5) up to second order. In the imaginary time method the iteration scheme at the n^{th} operation uses [1]

$$h_F^{(n+\frac{1}{2})} = \frac{1}{2}\{h_F(\rho_n)+h_F(\rho_{n+1})\}+\frac{t_3}{32}(\rho_{n+1}-\rho_n)^2 \qquad (7)$$

where t_3 is a constant of the Skyrme interaction. It can easily be seen that eq.(7) is identical to eq.(5) up to third order.

Computationally the DD iteration scheme of eq.(1) and (2) is simple. However as previously observed [2] the convergence rate of this method is much slower than the HF method, but this is not a serious drawback because the DD method is much faster. Nevertheless, as shown here, the convergence rate of the DD method may be significantly improved by the use of the operator h_{eff}. Such a procedure requires a careful linearization of eq.(5) since h_{eff} is dependent on $\Delta\rho$. To calculate $\Delta\rho=\rho_{n+1}-\rho_n$ we use the predictor corrector method in which $\Delta\rho$ is estimated by successively introducing the higher order terms of eq.(5) to obtain a progressively better approximation for $\Delta\rho$ during each iteration.

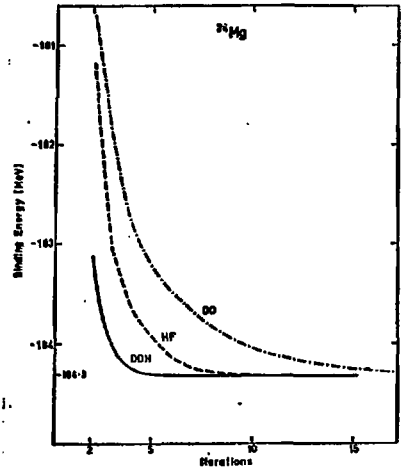

Fig.1 Convergence rate for total binding energy

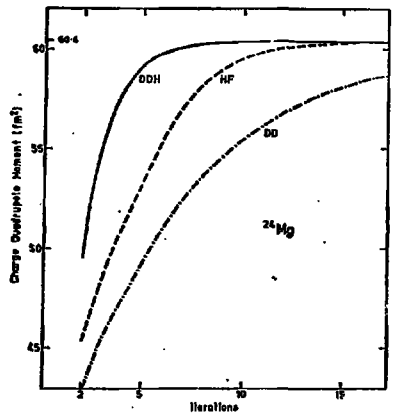

Fig.2 Convergence rate for charge quadrupole moment

Now we compare the convergence rates in Figs.1 and 2 for the total binding energy and charge quadrupole moment for the three cases : (i) the conventional HF method [4] (ii) the DD method, which uses the iteration scheme given by eq.(1) and eq.(2) (iii) the DDH scheme, which uses the iteration procedure of eq.(1) and eq.(6). In all cases the full Skyrme Hamiltonian for the SII force [4] is used. It can be seen that the DDH scheme has the fastest convergence rate. Also in contrast to the HF and DD cases, the binding energy and charge quadrupole moment converge simultaneously in the DDH method.

In this note we have shown that the DD method may be improved by including higher order terms in its iteration procedure, but without any loss of its computational simplicity. We find that the convergence rate is faster than the conventional HF method.

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