Z. Phys. A - Atoms and Nuclei 300, 239–245 (1981)

Zeitschrift für Physik A Atoms and Nuclei

Density Matrix Approach to the Hartree-Fock Problem

S. Peltier* and A. Plastino**

Departamento de Fisica, Universidad Nacional, La Plata, Argentina

Received November 17, 1980; revised version February 16, 1981

The problem of determining the best one-body density matrix which minimizes the total energy of a many fermion system is studied, with the idea of providing an alternative approach to the method of Roothaan for solving the Hartree-Fock equation.

1. Introduction

The Hartree-Fock (HF) method constitutes the basic approach to the many-fermion problem. At the very least, it provides the best zero-order wave function upon which to construct a more involved variational or perturbative approach.

In applying the HF approach to nuclear structure problems the route usually followed is that of implementing the prescriptions given originally by Roothaan [1]. An alternative scheme has been employed for many years in atomic physics [2] and introduced recently in nuclear physics by Bonaccorso, Di Toro and Russo [3]. This scheme is based on the idea of determining the best one-body density matrix that minimizes the energy functional in the HF approach. Such a procedure may be quite convenient in many instances since it circumvents the need of solving iteratively a Schroedinger-like equation. Moreover, as "only" the search for a minimum is involved, inclusion of external constraints can be accomplished by recourse to standard, well-known techniques.

Quite a bit of physically relevant information is already determined, when one knows the one-body density matrix, that does not involve the explicit form of the selfconsistent single-particle (s.p.) wave functions.

Consequently, this alternative approach to the HF problem deserves careful scrutiny. In this spirit, we shall, in the present paper, discuss the HF density matrix approach, adopting a philosophy which is somewhat different from that of Bonaccorso et al. [3].

They consider an elegant (iterative) steepest descent approach, followed by a linearization approximation.

We shall reformulate the problem *ab initio* and discuss an *exact* solution in Sect. 2, and an approximate one in Sect. 3, which will be applied, in Sect. 4, to some simple situations in order to illustrate the procedure.

2. Formalism

The objective of the HF theory is to find that Slater determinant for A particles which minimizes the expectation value of the two-body hamiltonian

$$H=\sum_{i=1}^{A}\frac{p_i^2}{2m_i}+\frac{1}{2}\sum_{i\neq j}^{A}V(i,j), \tag{1}$$

in self-explanatory, usual notation.

This optimal Slater determinant is found by recourse to a linear expansion of the self-consistent orbitals $|\lambda\rangle$, in terms of a complete, orthonormal set $|i\rangle$

$$|\lambda\rangle=\sum_{i=1}^{N}C_i(\lambda)\,|i\rangle, \tag{2}$$

where, in practical calculations, N is a finite number.

The one-body HF density matrix is defined as [4]

$$\rho_{ij}=\sum_{\lambda=1}^{A}C_i(\lambda)\,C_j^*(\lambda). \tag{3}$$

* Member of CICBA, Argentina

** Member of CONICET, Argentina

0340-2193/81/0300/0239/$01.40

The HF energy is a functional of ρ [3, 4]

$$E(\rho)=\mathrm{Tr}(T\rho)+\tfrac{1}{2}\,\mathrm{Tr}\,\mathrm{Tr}\;\rho\;V\rho, \tag{4}$$

where T is the kinetic term and V is the antisymmetrized interaction.

To look for a minimum of (4) within the set of the self-adjoint one-body density matrices satisfying the conditions

$$\rho^2=\rho \tag{5}$$

and

$$\mathrm{Tr}(\rho)=A \tag{6}$$

is equivalent to solving the HF problem [2, 3].

The procedure of McWeeny [2] and Bonaccorso et al. [3] is to search for this minimum employing a steepest descent algorithm.

A proposal that is, conceptually, simpler would be that of attempting to minimize (4) with respect to ρ, subject to the constraints (5) and (6), which could be handled with Lagrange multipliers [5].

Condition (6) is a scalar one, involving just one such multiplier, which we shall call β. Condition (5) is a much more complicated one, in which *all* matrix elements (which are, in general, complex numbers) enter. We have then a set of Lagrange multipliers $\{\alpha\}$, which ensure that (5) is fullfilled for each *independent* matrix element ρ_{ij} (real and imaginary part must be handled separately). Because of hermiticity we have $\frac{N}{2}(N+1)$ independent matrix elements and the diagonal ones, of course, are real. Our variational problem adopts then the form [5]

$$\delta(E(\rho)-\beta\;\mathrm{Tr}(\rho)-\phi(\alpha))=0, \tag{7}$$

where

$$\begin{aligned}\phi(\alpha)=&\sum_{i=1}^{N}\alpha_{ii}\left(\sum_{j=1}^{N}\rho_{ij}\rho_{ji}-\rho_{ii}\right)\\&+\sum_{i>m}^{N}\alpha_{im}^{R}\left(\sum_{j=1}^{N}\mathrm{Re}(\rho_{ij}\rho_{jm})-\mathrm{Re}(\rho_{im})\right)\\&+\sum_{i>m}^{N}\alpha_{im}^{I}\left(\sum_{j=1}^{N}\mathrm{Im}(\rho_{ij}\rho_{jm})-\mathrm{Im}(\rho_{im})\right).\end{aligned} \tag{8a}$$

For the sake of the lighter notation it is convenient to rewrite (8) in abbreviated form

$$\phi(\alpha)=\sum_{i\geqq m}^{N}\alpha_{im}\left(\sum_{j=1}^{N}\rho_{ij}\rho_{jm}-\rho_{im}\right) \tag{8b}$$

and assume, consequently, that ρ is a real matrix. Our conclusions, of course, will remain valid in the general case.

This (in principle, exact) approach has been discussed by Russo and Di Toro [5]. Unfortunately, one faces in this case a non-linear problem, and a very complicated one, indeed, since the number of equations to be solved is enormous, of the order of N^2. Moreover, without a careful study of a given particular case, one would not even be able to ascertain whether the number of possible solutions is finite [6]. Here we find a clear indication of how difficult the many-body problem really is, even at the single-determinant stage.

3. An Approximate Treatment

We develop here an approximation to the problem of finding the HF density matrix, in the spirit of Sect. 2. There the main difficulty lies in the set of (idempotency) conditions (5) [5]. We propose to replace it by the *scalar* condition

$$\Omega=\mathrm{Tr}(\rho^2-\rho)^2=0, \tag{9}$$

introduced by McWeeny [2] in order to construct an idempotent matrix by the steepest descent method.

3.1. Building an Approximate Idempotent Matrix

Notice that if a given matrix ρ satisfies (9) *exactly*, then that matrix is an idempotent one, as is easily seen by inspection. Writing

$$\Omega=\sum_{i,m}((\rho^2)_{im}-\rho_{im})^2, \tag{10}$$

it is obvious that if for just one pair i,j is $\rho_{ij}\neq(\rho^2)_{i,j}$, then $\Omega\neq 0$.

Of course, both in McWeeny's approach [2] and in ours, one is just minimizing Ω, without necessarily attaining the (ideal) zero value. The question is, can one obtain an approximately idempotent matrix by minimizing Ω according to

$$\delta_\rho(\Omega[\rho]-\beta\;\mathrm{Tr}\;\rho)=0, \tag{11}$$

for a given (initial) matrix ρ (of fixed trace)?

The variational problem (11) leads to a relationship of the form

$$\rho_{l,m}=3(\rho^2)_{l,m}-2(\rho^3)_{l,m}+\frac{\beta}{2}\delta_{l,m}, \tag{12}$$

which, together with the condition on the trace (given by say, (6)) leads to

$$\begin{aligned}\rho_{l,m}=&3(\rho^2)_{l,m}-2(\rho^3)_{l,m}\\&-((3\,\mathrm{Tr}\;\rho^2-2\,\mathrm{Tr}\;\rho^3-A)/N)\;\delta_{l,m},\end{aligned} \tag{13}$$

where N is the size of the matrix. The set of Eq. (13) can be solved by iteration and we have found numerically that it converges if the norm of the "starting" matrix is smaller than unity. This norm can be expressed as the largest eigenvalue (in absolute value) of ρ_{initial} [7], which allows one to always fulfill the condition just by multiplying ρ_{initial} by the inverse of this particular eigenvalue. As a typical example, let us consider the (30×30) matrix

$$\rho_{ij} = i + (j-1)/30. \tag{14}$$

Its largest eigenvalue is of the order of 400. Division by this eigenvalue yields a matrix of norm smaller than unity. The initial value of Ω is 0.10. Just three iterations (13) suffice to obtain a new matrix ρ for which $(\rho^2)_{ij} - \rho_{ij}$ is smaller than 10^{-10} for all i,j with $\Omega = 0.14 \times 10^{-9}$.

3.2. Approximate Scheme

In the previous subsection we have seen that it makes sense to try to obtain an approximately idempotent matrix working with the (scalar) quantity Ω. The variational problem (7) can now be reduced to the much simpler one

$$\delta(E(\rho) - \alpha\Omega - \beta \text{ Tr } \rho) = 0 \tag{15}$$

involving two Lagrange multipliers. Variation yields

$$h - \alpha(4\rho^3 - 6\rho^2 + 2\rho) - \beta I = 0, \tag{16}$$

where I is the identity matrix and h the ordinary HF s.p. hamiltonian [4]

$$h_{lm} = T_{lm} + \sum_{nk}^{N} V_{ln,mk}\, \rho_{kn}. \tag{17}$$

Equation (16) is to be solved subject to the conditions

$$\text{Tr } \rho = A \tag{6}$$

and

$$\Omega = \text{Tr}(\rho^2 - \rho)^2 = 0 \tag{9}$$

The β Lagrange multiplier can be eliminated using Tr $\rho = A$ which leads to

$$N\beta = \text{Tr}(h - \alpha(4\rho^3 - 6\rho^2)) - 2\alpha A. \tag{18}$$

Analogously, one can proceed to eliminate the α Lagrange multiplier from $\Omega = 0$. This leads to a fourth order equation in α, whose solutions can thus be obtained analytically, and one should work with that value of α (selected among the four available ones) which minimizes the total energy.

In considering the non-linear problem posed by (16), and because of the lack of explicit formulae for the solution of non-linear systems, one usually is led to some iteration process to find an approximate solution of sufficient accuracy. One possibility is to reformulate the system (16) as a *fixed point problem*

$$\rho = \hat{F}(\rho) \tag{19}$$

for the iteration operator $\hat{F}$ defined as

$$\hat{F}(\rho) = h(\rho) - \frac{\beta}{2} I + \alpha(3\rho^2 - 2\rho^3). \tag{20}$$

Starting from some $\rho^{(0)}$ one generates the sequence $\rho^{(k)}$ by

$$\rho^{(k+1)} = F(\rho^{(k)}), \qquad k = 0, 1, 2, \ldots. \tag{21}$$

Theorems that characterize the convergence of methods of this kind may be classified as local, semi-local or global and are discussed, for example, in [8].

It may be convenient to remind the reader at this point that the hermitian condition [4]

$$\rho^{+} = \rho \tag{22}$$

has not been included as a constraint in the variational procedure. This omission is a permissible one because if one starts the iterative process (21) with a hermitian initial matrix $\rho^{(0)}$, this property will be automatically conserved by the operator $\hat{F}$.

We have thus found in (21) an alternative HF scheme which requires neither diagonalizations nor the numerical solution of any equation, and which could be considered as a *possible* alternative both to Roothaan's scheme and to McWeeny's.

Even if the convergence of this new procedure were slow, one might argue that a compensation for this can be found in its numerical simplicity. On the other hand, one could start the iterative process with a couple of Roothaan's iterations and thus establish a convenient starting $\rho^{(0)}$, and then proceed according to (21).

Finally, we mention that an alternative approach for solving the system (16) may be that of defining $\hat{P}(\rho) = \hat{F}(\rho) - \rho$ and proceed then to apply Newton's method, which instead of $\hat{F}$ uses the iteration operator $\hat{Q}$ defined as

$$\hat{Q}(\rho) = \rho - \hat{P}(\rho)/\hat{P}'(\rho) \tag{20a}$$

and is characterized by a quadratic convergence.

4. Examples

4.1. The Lipkin Model

We shall illustrate our treatment of the HF density matrix problem by recourse to a simple model developed by Lipkin, Meshkov and Glick [9] in order to try new approximations to the quantum many-body problem.

The models deals with A particles distributed in two (A-fold) degenerate s.p. levels which are separated by the s.p. energy ε. We characterize the A lower states by $|p, \sigma=-1\rangle$ (for $p=1, \ldots, A$).

Introducing the quasi-spin operators

$$\hat{J}_z=\frac{1}{2}\sum_{p,\sigma}\sigma\, C^+_{p,\sigma}\, C_{p,\sigma}, \tag{23}$$

and

$$\hat{J}_+=\hat{J}^+_-=\sum_{\mathbf{p}} C^+_{p,+}\, C_{p,-}, \tag{24}$$

the hamiltonian reads

$$H=\varepsilon\,\hat{J}_z+\frac{v}{2}(\hat{J}^2_+ +\hat{J}^2_-). \tag{25}$$

The corresponding HF treatment has been given by Agassi et al. [10]. On account of the monopole character of the interaction in (25), the density matrix adopts a very simple form [10, 11]. It consists of A 2×2 blocks along the diagonal of the form

$$\tilde{\rho}=\begin{pmatrix}\tilde{\rho}_{++} & \tilde{\rho}_{+-}\\ \tilde{\rho}_{-+} & \tilde{\rho}_{--}\end{pmatrix}, \tag{26}$$

independent of the quantum number p, and satisfying the relationship $\mathrm{Tr}\,\tilde{\rho}=1$. For simplicity, we now write hereafter ρ instead of $\tilde{\rho}$.

The HF solution is obtained by performing a rotation around the J_x-axis in quasi-spin space [10, 11]. The corresponding angle, γ, is determined so as to minimize the HF energy.

Consequently, ρ adopts the form [10, 11].

$$\begin{aligned}\rho_{++}&=\sin^2\frac{\gamma}{2}\\ \rho_{--}&=\cos^2\frac{\gamma}{2}\\ \rho_{+-}&=\rho^*_{-+}=i\,\sin\frac{\gamma}{2}\cdot\cos\frac{\gamma}{2},\end{aligned} \tag{27}$$

with [8, 9]

$$\begin{aligned}\gamma&=\arccos(v(A-1))^{-1}, \quad v>v_c\\ \gamma&=0 \qquad\qquad\quad , \quad v\leqq v_c\end{aligned} \tag{28}$$

where $v_c=\dfrac{1}{A-1}$, [10, 11].

Our task is now to apply our approach and compare our solution to the HF result given by (27). Opposite to what happens in most treatments of the Lipkin model, we must deal here with the individual s.p. states $|p,\sigma\rangle$, and not with its $SU2$ group structure. In order to obtain the HF energy as a functional of ρ, the relevant matrix elements are

$$\langle p\mu|\hat{J}_z|q\tau\rangle=\tfrac{1}{2}\delta_{p,q}\delta_{\mu,\tau}(\delta_{\mu,+}-\delta_{\mu,-}), \tag{29}$$

and

$$\begin{aligned}&\langle p_1\mu_1 p_2\mu_2|\hat{J}^2_\pm|p_3\mu_3 p_4\mu_4\rangle\\ &\quad=2\delta_{p_1,p_3}\cdot\delta_{p_2,p_4}\cdot\delta_{\mu_3,\mu_4}\cdot\delta_{\mu_2,\mu_1}\\ &\qquad\cdot\delta_{\mu_1,\pm}\cdot\delta_{\mu_3,\mp}(1-\delta_{p_1,p_2}).\end{aligned} \tag{30}$$

With (29) and (30) one easily specializes (4) to the present case and writes down

$$E(\rho)=\frac{A}{2}(\rho_{++}-\rho_{--})+\frac{A}{2}(A-1)\,v(\rho^2_{-+}+\rho^2_{+-}). \tag{31}$$

a) Exact Treatment. It is easy to see that, for a 2×2 matrix of unit trace like (26), one always has

$$(\rho^2)_{+-}=\rho_{+-}, \quad \text{and} \quad (\rho^2)_{-+}=\rho_{-+}.$$

The idempotency requirements for ρ_{++} and ρ_{--} read

$$\begin{aligned}\rho_{++}&=\rho^2_{++}+|\rho_{+-}|^2\\ \rho_{--}&=\rho^2_{--}+|\rho_{+-}|^2.\end{aligned} \tag{32}$$

Now, since

$$\mathrm{Tr}\,\rho=1, \tag{33}$$

We have

$$\rho^2_{++}+\rho^2_{--}+2|\rho_{+-}|^2=1. \tag{34}$$

It is of advantage to introduce the constraints explicitly into the expression for $E(\rho)$. Setting

$$\rho_{+-}=R+i\,I, \tag{35}$$

We rewrite (31) as

$$E=\frac{A}{2}(2\rho_{++}-1)+v\,A(A-1)\,(R^2-I^2). \tag{36}$$

We can work with just one constraint, after explicit use of (33) in (34), writing (8) as

$$\phi(\rho)=\rho^2_{++}+(1-\rho_{++})^2+2(R^2+I^2)-1=0 \tag{37}$$

so that our variational equation reads

$$\delta(E(\rho)-\alpha\,\phi(\rho))=0. \tag{38}$$

We obtain then, after variation of (38) with respect to, respectively, ρ_{++}, R, I, the set of equations

$$\begin{aligned} &A-4\alpha\rho_{++}+2\alpha=0\\ &(vA(A-1)-4\alpha)R=0\\ &-(vA(A-1)+4\alpha)I=0. \end{aligned} \tag{39}$$

We see that it is not possible to have simultaneously both $R\neq 0$ and $I\neq 0$. Choosing $R=0$ yields a lower energy than opting for $I=0$. Then

$$\alpha=-\frac{v}{4}A(A-1), \tag{40}$$

$$\rho_{++}=\frac{1}{2}\left(1-\frac{1}{v(A-1)}\right), \tag{41}$$

and from $\phi(\rho)=0$, if we set $\cos\gamma=1/v(A-1)$

$$\rho_{+-}=i\cos\frac{\gamma}{2}\sin\frac{\gamma}{2}. \tag{42}$$

Notice that $v=v_c$ implies $\rho_{++}=0$ (all particles "downstairs"). For $v<v_c$, ρ_{++} would be negative, which is impossible, so that the solution (41) breaks down and a "phase transition" ensues.
Our theory thus reproduces the HF results of Agassi et al. [10]. The Lipkin model is simple enough so as to allow one to apply the exact treatment of Sect. 2.

b) Approximate Treatment. In this case it reduces trivially to the exact one, since for a 2×2 matrix of unit trace, the condition $\Omega=0$ leads to exactly the same relationship as does the idempotency condition $\rho^2=\rho$.

4.2. A Simple Numerical Application

We can illustrate our approximate treatment of Sect. 3, (21), by means of a very simple numerical example. We consider four fermions distributed among three doubly-degenerate single-particle levels, which will be labelled by a quantum number $p(p=1, 2$ or $3)$, with s.p. energies $\varepsilon_p=-1,0,1$, respectively, in arbitrary units. A given s.p. states is characterized then by two quantum numbers, i.e. p, σ with $\sigma=\pm 1$. Consider a simple schematic interaction, related to the pairing force, of the form

$$-2|G|\sum_{p,q,\sigma} f(p,q)\, b^+_{q,-\sigma} b^+_{q,\sigma} b_{p,\sigma} b_{p,-\sigma}, \tag{43}$$

where we choose $f(p,q)=1$ except for the case $p=1$, $q=3$ (or viceversa) for which we take $f(p,q)=0$.
We perform a HF transformation which preserves "axial symmetry", of the type

$$\left|\lambda,\sigma_\lambda\right\rangle=\delta_{\sigma_\lambda,\sigma_\mathbf{p}}\sum_{p=1}^{3} C^\lambda_p\left|\, p,\sigma_p\right\rangle, \tag{44}$$

and solve the corresponding HF problem both using the conventional Roothaan's approach and the scheme given in Sect. 3.
We have varied $|G|$ between 0.1 and 100, and found that, up to six digits, the scheme of (21) yields, for total energies, self-consistent s.p. energies and density matrix identical results as those provided by the orthodox HF approach.

4.3. $SU_2\times SU_2$ Model

As a last illustration we shall study the validity of the condition $\Omega=0$ in the case of an exactly soluble model [12] whose structure is a bit more complicated than that of Lipkin's.
In the model of [12] we also deal with A particles distributed in two s.p. levels, each A-fold degenerate, as in Lipkin's case. In addition to the quasi-spin operators (23), (24), we introduce, after setting for convenience $P=A-p+1$, the new operators

$$\begin{aligned} &\hat S_+=\hat S_-^+=\sum_p C^+_{p+}C_{P-}\\ &\hat S_z=\hat J_z \end{aligned} \tag{45}$$

The operators $\hat S_+$, $\hat S_-$, $\hat S_z$ commute among themselves like angular momentum ones, i.e., they are quasi-spin operators. If we define further

$$\hat U=\tfrac{1}{2}\sum_{p,\mu}\mu\, C^+_{p,\mu}C_{P,\mu}, \tag{46}$$

and

$$\begin{aligned} \hat V_+&=\hat V_-^+=\tfrac{1}{2}(\hat J_+ +\hat S_+),\\ \hat W_+&=\hat W_-^+=\tfrac{1}{2}(\hat J_+ -\hat S_+),\\ \hat V_z&=\tfrac{1}{2}(\hat J_z+\hat U),\\ \hat W_z&=\tfrac{1}{2}(\hat J_z-\hat U), \end{aligned} \tag{47}$$

We obtain two additional quasi-spin sets: $\hat V_+$, $\hat V_-$, $\hat V_z$ and $\hat W_+$, $\hat W_-$, $\hat W_z$. Moreover, any given $\hat V$ operator commutes with all $\hat W$ ones and viceversa ($SU_2\times SU_2$). In terms of the operators (47) the hamiltonian reads [12]

$$\hat H=\hat J_z+\tfrac{1}{2}v(2\hat V_z\hat W_z+\hat W_+\hat V_-+\hat W_-\hat V_+). \tag{48}$$

The exact solution is obtained by diagonalization of $\hat H$ in an $SU_2\times SU_2$ basis. Since $\hat H$ commutes both with $\hat V^2$ and $\hat W^2$, it suffices to restrict one's attention to a given multiplet $|V,W,V_z,W_z\rangle$ with V, W fixed. The HF approach looks for the zero particle-zero hole $(0p-0h)$ wave function in the selfconsistent or "b" representation, which is a suitable linear com-

bination of the original, or "c", one. The corresponding coefficients are chosen so as to minimize the expectation value of the hamiltonian in the new $0p-0h$ state. It can be shown [13] that for the given hamiltonian the most general HF transformation can be viewed as consisting of two successive rotations [11, 13]

$$\begin{pmatrix} C_{p,-} \\ C_{p,+} \end{pmatrix} = \begin{pmatrix} \cos\frac{\beta}{2} & -i\sin\frac{\beta}{2} \\ -i\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} \begin{pmatrix} a_{P,-} \\ a_{p,+} \end{pmatrix}, \tag{49}$$

and

$$\begin{pmatrix} a_{p,-} \\ a_{p,+} \end{pmatrix} = \begin{pmatrix} \cos\frac{\alpha}{2} & -i\sin\frac{\alpha}{2} \\ -i\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{pmatrix} \begin{pmatrix} b_{p,-} \\ b_{p,+} \end{pmatrix}. \tag{50}$$

The former is a rotation in quasi-spin S-space, while the latter is a rotation in quasi-spin J-space. As a result of (49) and (50) both the V-quasi-spin and the W-one rotate around the x-axis the corresponding angles being $(\alpha+\beta)$ and $(\alpha-\beta)$, respectively. The eigenvalues of both $\hat{V}^2$ and $\hat{W}^2$ are preserved in this rotations.

On account of the character of the interaction and of the symmetries of the problem, it is easy to see that the density matrix adopts a very simple form. It consist of $A/2$ identical blocks, of dimension 4×4, placed along the main diagonal. Defining

$$\begin{aligned} a &= \tfrac{1}{2}(1+\cos\alpha\cos\beta) \\ b &= \tfrac{1}{2}\cos\beta\sin\alpha \\ c &= \tfrac{1}{2}\sin\alpha\sin\alpha \\ d &= \tfrac{1}{2}\cos\alpha\sin\beta, \end{aligned} \tag{51}$$

the blocks adopt the form indicated in Table 1. The trace of each of this blocks equals 2. The matrix representation of the HF hamiltonian possesses, of course, the same structure. The general form of the corresponding blocks is given in Table 2, where use has been made of the abbreviation

$$g = v\,A/4. \tag{52}$$

Using now (4), one finds that the HF energy can be written as

$$\begin{aligned} E_{\mathrm{HF}} &= 2a^2 - 2(1+g)\,a + (1+g/2) \\ &\quad + 2g(b^2 - d^2 - c^2). \end{aligned} \tag{53}$$

Table 1. The density matrix for the $SU_2\times SU_2$ model consists of $A/2$ identical 4×4 blocks placed along the main diagonal. The form of these blocks is given in the table (see (51))

	p_+	p_-	P_+	P_-
p_+	$(1-a)$	$-ib$	c	$-id$
p_-	ib	a	id	$-c$
P_+	c	d	$(1-a)$	$-ib$
P_-	id	$-c$	ib	a

Table 2. The HF hamiltonian matrix consists of $A/2$ identical 4×4 blocks placed along the main diagonal. The form of these blocks is given in the table (see (51) and (52))

h	p_+	p_-	P_+	P_-
p_+	$g(1-2a)/2$	$-igb$	$-gc$	igd
p_-	igb	$-g(1-2a)/2$	$-igd$	gc
P_+	$-gc$	igd	$g(1-2a)/2$	igb
P_-	$-igd$	gc	igb	$-g(1-2a)/2$

Minimization of (53) with respect to α, β yields, of course, the HF solutions found in [12]. What we wish to emphasize, however, is that the (approximate) idempotency requirement $\Omega=0$ obtains exactly for those solutions. As a matter of fact, each of the five pairs of (α,β) values that extremalize the HF energy (see Table 1 of [12]) gives $\Omega=0$. Let us consider some examples. In the present case we have for the expression

$$\begin{aligned} \Omega/2 &= ((1-a)^2+b^2+c^2+d^2+a-1)^2 \\ &\quad + (a^2+b^2+c^2+d^2-a^2)^2 \\ &\quad + (c(1-2a)+bd)^2 + (c(2a-1)+bd)^2, \end{aligned} \tag{54}$$

If we consider the (trivial) solution $\alpha=\beta=0$, then $a=1$, $b=c=d=0$, so that (54) immediately yields $\Omega=0$. When $v>W/2$, the lowest lying HF solution is that corresponding to [12]

$$\alpha=0, \qquad \beta=\arccos\left(\frac{1}{2\,v\mathrm{W}}\right). \tag{55}$$

Now one has

$$\begin{aligned} a &= \left(1+\frac{1}{2v\mathrm{W}}\right)\Big/2 \\ b &= c = 0 \\ d^2 &= a(1-a), \end{aligned} \tag{56}$$

which substituted in (54) yields again $\Omega=0$.

We see then that minimizing the HF energy as a functional of ρ with the restriction $\Omega=0$ will reproduce the (exact) HF solutions obtained in Ref. [12].

5. Conclusion

We have in this work endeavoured to show that an alternative to Roothaan's HF scheme can be obtained by minimizing the functional $E_{HF}(\rho)$ with the restriction $\Omega=0$. The resulting scheme, given by (21), (6) and (9) can be solved iteratively. Opposite to Roothaan's case, no equation needs to be solved *numerically*. Our approach differs from that of McWeeny [2] in that we insert this condition via a Lagrange multiplier, without recourse to the steepest-descent method.

The condition $\Omega=0$ can be used as a numerical device in order to build an idempotent matrix from a given initial one, as illustrated in Sect. 3.1.

Application to two exactly soluble models has shown that the condition $\Omega=0$ leads to the (previously) known HF solutions. A simple numerical example (Sect. 4.2) that actually iterates (21), (6) and (9) leads to the same conclusion.

Of course, only the possibility of attaining an alternative scheme to Roothaan's has been established here. Extensive numerical work is still needed in order to test the reliability of the new approach.

The authors acknowledge fruitful discussions with Profs. J. Zabolitzky and C. Cambell, Dr. G. Dussel and Lic. M.T. Martin Helpful comments on the manuscript by Prof. M. Di Toro are also very much appreciated.

References

1. Roothaan, C.C.J.: Rev. Mod. Phys. **23**, 69 (1951)
2. McWeeny, R.: Proc. R. Soc. London, Ser. A**235**, 496 (1957); Rev. Mod. Phys. **32**, 335 (1960)
3. Bonaccorso, A., Di Toro, M., Russo, G.: Phys. Lett. **72**B, 27 (1977)
4. Ripka, G.: Advances in Nuclear Physics. Baranger, M., Vogt, E. (eds.). New York: Plenum Press 1968
5. Russo, G., Di Toro, M.: Nuovo Cimento **54**A, 371 (1979)
6. Walker, R.: Algebraic curves. Princeton, New Yersey: Princeton Univeristy Press 1950
7. Isaacson, E., Keller, H.B.: Analysis of Numerical Methods. New York: John Wiley 1966
8. Tapia, R.A.: Am. Math. Mon. **78**, 389 (1971)
   Rall, L.B.: Nonlinear Functional Analysis and Applications. New York: Academic Press 1971
   Rall, L.B.: Computational solution of Nonlinear operator Equations. New York: John Wiley 1969
   Ortega, J.M., Rheinboldt, W.C.: Iterative Solution of Nonlinear Equations in several variables. New York: Academic Press 1970
9. Lipkin, H.J., Meshcov, N., Glick, A.J.: Nucl. Phys. **62**, 188 (1965)
10. Agassi, D., Lipkin, H.J., Meshcov, N.: Nucl. Phys. **86**, 321 (1966)
11. Faessler, A., Plastino, A.: Z. Phys. **220**, 88 (1969)
12. Cambiaggio, M.C., Plastino, A.: Z. Phys. A - Atoms and Nuclei **291**, 277 (1979)
13. Cambiaggio, M.C., Plastino, A., Szybisz, L.: Nucl. Phys. A**344**, 233 (1980)
14. Abecasis, S.M., Faessler, A., Plastino, A.: Z. Phys. **218**, 394 (1969)

S. Peltier
A. Plastino
Universidad Nacional de La Plata
Facultad de Ciencias Exactas
Departamento de Fisica
Casilla de correo 67
RA-1900 La Plata
Argentina