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A NEW HARTREE-FOCK SCHEME

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ABSTRACT

A new algorithm for the solution of the Hartree-Fock equations is presented, which avoids matrix diagonalizations. The method is built around the variance of the Hartree-Fock hamiltonian, computed with respect to vectors arising from the Hartree-Fock transformation, and tries to make it vanish. The present approach is applied to the Lipkin model and to a simple numerical example

RESUMEN

Se presenta un nuevo algoritmo para la solución de las ecuaciones de Hartree-Foch, que evita diagonalizaciones de matrices. El método se construye alrededor de la varianza del Hamiltoniano de Hartree-Foch, calculada con respecto a vectores que aparecen en la transformación de Hartree-Foch, e intenta hacerla nula. Se aplica el método al modelo de Lipkin y a un ejemplo numérico simple.

1. INTRODUCTION

The Hartree-Fock (HF) approximation has had a long and distinguished history in atomic physics, and in the last 20 years it has been applied extensively in nuclear physics[1-5] where it has achieved a privileged status among the theoretical tools employed for the description of nuclear properties.

In view of its importance, the discussion of different aspects of the HF approach is always interesting, specially when it refers to the investigation of alternative procedures concerning numerical applications of the theory.

This is the purpose of the present work, in which a new algorithm for the solution of the HF equations will be proposed, which avoids the repeated diagonalizations involved in the usual approach. This will be briefly reviewed in Section 2. Section 3 will deal with our new scheme, which will be applied to two simple models in Section 4 and 5. Conclusions will be drawn in Section 6.

2. THE HARTREE-FOCK FORMALISM

Given A nucleons and a convenient, orthonormal set of single-particle (s.p.) wave functions $|j\rangle = a^{\dagger}|0\rangle$ it is the aim of the HF theory to determine that Slater determinant,

$$|\Psi\rangle = b^{\dagger}_{\lambda_1} b^{\dagger}_{\lambda_2} \cdots b^{\dagger}_{\lambda_A} |0\rangle \quad , \tag{1}$$

constructed with the so-called self-consistent s.p. orbitals $|\lambda\rangle = b_\lambda^\dagger |\, 0\rangle$ with

$$b_\lambda^\dagger = \sum_j c_j^\lambda a_j^\dagger \quad , \tag{2}$$

which minimizes the expectation value $\langle\Psi|H|\Psi\rangle$ of the Hamiltonian:

$$H = \sum_{ij} t_{ij} a_i^\dagger a_j + \frac{1}{4} \sum_{\substack{ij \\ mn}} V_{ijmn} a_i^\dagger a_j^\dagger a_n a_m \quad , \tag{3}$$

V_{ijmn} being an antisymmetrized matrix element[3].

The corresponding variational problem leads to the well-known HF equations[2], which have the form of an eigenvalue problem:

$$\sum_i h_{ji} c_i^\lambda = \varepsilon_\lambda \, c_j^\lambda \quad . \tag{4}$$

This possesses, however, a nonlinear character, in view of the fact that the HF hamiltonian h in Eq. (3) depends itself upon the c_j^λ:

$$h_{ji} = t_{ji} + \sum_{\lambda=1}^{A} \sum_{k\ell} c_k^{\lambda *} V_{jki\ell} c_\ell^\lambda = t_{ji} + \sum_{k\ell} V_{jki\ell} \rho_{\ell k} \quad , \tag{5}$$

ρ being the HF density matrix

$$\rho_{\ell k} = \sum_{\lambda=1}^{A} c_k^{\lambda *} c_\ell^\lambda \quad . \tag{6}$$

Eqs. (4) and (5) are customarily solved by recourse to the following iterative algorithm:

a) An initial set of coefficients $\{c_j^\lambda\}$ is guessed, together with information concerning which orbitals are occupied.

b) The HF hamiltonian is constructed.

c) Eq. (4) is solved by diagonalization of h, which yields a new set of coefficients $\{c_j^\lambda\}$.

d) One selects A orbitals (usually those for which the s.p. energy ε_λ is

lowest) to be occupied.

e) One returns to step b) unless convergence has been achieved.

In the last case, one evaluates with $|\Psi>$ those expectation values which are interest. In particular, the ground state energy is given by

$$E_{HF} = \sum_{\lambda=1}^{A} <\lambda|T|\lambda> + \frac{1}{2} \sum_{\lambda\mu=1}^{A} <\lambda\mu|V|\lambda\mu> = \frac{1}{2} \sum_{ij} (t_{ij} + h_{ij})\rho_{ji} \quad . \tag{7}$$

3. ALTERNATIVE APPROACH

The main idea of our approach is that of looking for a relationship between the expansion coefficients c_j^λ that are obtained in two successive iterations, say the k-th and the (k + 1)-th ones, of the above described algorithm. One may guess that this relationship must be of the general form

$$c_j^\lambda(k + 1) = \sum_{\mu i} G_{ji}^{\lambda\mu}(k) c_i^\mu(k) \quad , \tag{8}$$

where, eventually one must have, when convergence is achieved $G \equiv \delta_{\lambda\mu}\delta_{ij}$. Without loss of generality, one can give to G the structure

$$G_{ji}^{\lambda\mu}(k) = a_{\lambda\mu}(k) d_{ji}^{\lambda\mu}(k) + b_{\lambda\mu}(k) h_{ji}(k) \quad , \tag{9}$$

and the task to be confronted then would be to determine a, b and d from the HF equations.

We shall propose, instead, the following ansatz

$$G_{ji}^{\lambda\mu}(k) = \delta_{\lambda\mu}(a_\lambda \delta_{ij} + b_\lambda h_{ji}) \quad , \tag{10}$$

and will justify it in Subsection 3.3. In order to give and explicit interpretation to Eq. (10), which shall be done in Subsection 3.2, we review first a diagonalization method recently proposed.

3.1. *The 2 x 2 algorithm*

This is an iterative method which may under certain circumstances be an alternative to the Lanczos method for the diagonalization of Hermitian operators[6].

Let $\hat{A}$ be a linear, hermitian operator, defined everywhere in a finite dimensional vector space and $|k\rangle$ an arbitrary, normalized vector belonging to it. If A operates on $|k\rangle$ one obtains

$$\hat{A}|k\rangle = e_k|k\rangle + \nu_k|k'\rangle \quad , \tag{11}$$

with

$$\langle k|k'\rangle = 0; \qquad \langle k'|k'\rangle = 1 \quad . \tag{12}$$

The coefficient in the first term of the r.h.s. of Eq. (11) is

$$e_k = \langle k|\hat{A}|k\rangle \quad , \tag{13}$$

while in the second one we have the square root of the variance of $\hat{A}$ computed with vectors $|k\rangle$:

$$\nu_k^{\,2} = \langle k|\hat{A}^2|k\rangle - \langle k|\hat{A}|k\rangle^2 = \langle k|\hat{A}^2|k\rangle - e_k^{\,2} \quad . \tag{14}$$

The states $|k\rangle$ and $|k'\rangle$ define a 2 x 2 subspace in which $\hat{A}$ can be diagonalized. The corresponding matrix has the form

$$M = \begin{pmatrix} e_k & \nu_k \\ \nu_k & \alpha_k \end{pmatrix} \quad , \tag{15}$$

where

$$\alpha = \langle k'|\hat{A}|k'\rangle \quad . \tag{16}$$

Berger *et al.* have shown[6] that the eigenvalues (and eigenvectors)

of $\hat{A}$ can be obtained individually starting with the lowest one, via an iterative process in which the matrix M is repeatedly diagonalized. For every eigenvalue E of $\hat{A}$ there is a sequence of values e_k converging to it, while, at the same time ν_k tends to zero and $|k\rangle$ tends to the eigenvector belonging to E. The method has the advantage of drastically reducing the computer storage space, since, in any given iteration step, one deals with only two vectors.

3.2. *An interpretation of our Ansatz*

We propose, according to Eqs. (8) and (10), that the HF equations be solved by iteration of the relationship

$$c_j^{\lambda}(k+1) = a_{\lambda}(k)c_j^{\lambda}(k) + b_{\lambda}(k) \sum_i h_{ji}c_i^{\lambda}(k) \quad . \tag{17}$$

In order to get some insight concerning the meaning of Eq. (17) let us consider the HF Hamiltonian h(k) and a given orbital $|\lambda(k)\rangle$ after k iteration steps of the algorithm reviewed in Section 2. One could write in the spirit of Berger *et al.*[16].

$$\begin{aligned} h(k)|\lambda(k)\rangle &= e_{\lambda}(k)|\lambda(k)\rangle + \nu_{\lambda}(k)|\lambda'(k)\rangle \quad , \\ h(k)|\lambda'(k)\rangle &= \nu_{\lambda}(k)|\lambda(k)\rangle + \alpha_{\lambda}(k)|\lambda'(k)\rangle \quad , \\ \langle\lambda'(k)|\lambda'(k)\rangle &= 1 \quad , \quad \langle\lambda'(k)|\lambda(k)\rangle = 0 \quad , \end{aligned} \tag{18}$$

and consider e_{λ}, ν_{λ} to be the matrix elements of the projection of h onto a 2x2 subspace spanned by $|\lambda(k)\rangle$ and $|\lambda'(k)\rangle$. These states are given in terms of the basis $|j\rangle$, by the expansions

$$|\lambda(k)\rangle = \sum_j c_j^{\lambda}(k)|j\rangle \quad , \tag{19}$$

and

$$|\lambda'(k)\rangle = \sum_j P_j^{\lambda}(k)|j\rangle \quad , \tag{20}$$

where, according to the first of Eqs. (18), the P_j^λ are given by

$$P_j^\lambda(k) = \frac{1}{\nu_\lambda(k)} \left\{ \sum_i h_{ji}(k) c_i^\lambda(k) - e_\lambda(k) c_j^\lambda(k) \right\} \quad . \tag{21}$$

Furthermore, we have for ν_λ and α_λ the expressions

$$\nu_\lambda^2(k) = \langle \lambda(k) | h^2(k) | \lambda(k) \rangle - e_\lambda^2(k) \tag{22}$$

and

$$\alpha_\lambda(k) = \langle \lambda'(k) | h(k) | \lambda'(k) \rangle \quad . \tag{23}$$

If we were now to diagonalize the matrix

$$\begin{pmatrix} e_\lambda & \nu_\lambda \\ \nu_\lambda & \alpha_\lambda \end{pmatrix} \quad , \tag{24}$$

and focus our attention upon its lowest eigenvalue,

$$e'_\lambda = \frac{1}{2} \left[e_\lambda(k) + \alpha_\lambda(k) \right] - \left\{ \nu_\lambda^2(k) + \frac{1}{4} \left[\alpha_\lambda(k) - e_\lambda(k) \right]^2 \right\}^{\frac{1}{2}} \quad , \tag{25}$$

e'_λ would be smaller than $e_\lambda(k)$ [6] and generates a new vector $|\lambda''(k)\rangle$, with expansion coefficients

$$c_j^{\lambda''} = N_\lambda(k) \left\{ c_j^\lambda(k) + \left[e'_\lambda - e_\lambda(k) \right] P_j(k) / \nu_\lambda(k) \right\} \quad , \tag{26}$$

$N_\lambda(k)$ being a normalization constant given by

$$N_\lambda(k) = \left\{ 1 + \left[e'_\lambda - e_\lambda(k) \right]^2 / \nu_\lambda^2(k) \right\}^{-\frac{1}{2}} \tag{27}$$

Suppose now that we define

$$\begin{aligned} e_\lambda(k+1) &= e'_\lambda \quad , \\ c_j^\lambda(k+1) &= c_j^{\lambda''} \quad , \end{aligned} \tag{28}$$

and change the meaning of k, considering that it counts now the iteration steps performed with the relationship (17).

Eq. (26) adopts, explicitly, the form

$$c_j^{\lambda}(k+1) = N_{\lambda}(k)c_j^{\lambda}(k) + \frac{N_{\lambda}(k)}{\nu_{\lambda}^2(k)}\left\{e_{\lambda}(k+1) - e_{\lambda}(k)\right\}\cdot$$

$$\left\{\sum_i h_{ji}(k)c_i^{\lambda}(k) - e_{\lambda}(k)c_j^{\lambda}(k)\right\} \quad . \tag{29}$$

The set of Eqs. (29) present us with a nonlinear problem which will be showed to be equivalent to that posed by the HF Eqs. (4) and (5).

Comparison with (17) allows one to write

$$a_{\lambda}(k) = N_{\lambda}(k)\left\{\nu_{\lambda}^2(k) - e_{\lambda}(k)\left[e_{\lambda}(k+1) - e_{\lambda}(k)\right]\right\}/\nu_{\lambda}^2(k) \quad ,$$

$$b_{\lambda}(k) = N_{\lambda}(k)\left\{e_{\lambda}(k+1) - e_{\lambda}(k)\right\}/\nu_{\lambda}^2(k) \quad . \tag{30}$$

The interpretation of the ansatz (23), with a_{λ} and b_{λ} given by Eq. (30), becomes now apparent. If we were to employ the standard algorithm for the solution of the HF Eqs., performing the corresponding diagonalizations according to Berger *et al.*[6], we would face a nest of two loops. For every orbital $|\lambda>$ one should iterate a relationship of the form (29) (internal, or 2 x 2 loop) until covergence is reached. The set of such internal loops should also, as a whole, be iterated (external, or HF loop), until convergence is attained.

Our proposal involves a different structure of the nest of loops. We interchange the order within the nest, performing, in succession, one internal loop followed immediately by an external one, i.e., given an orbital $|\lambda(k)>$ we obtain $|\lambda(k+1)>$ after just one 2 x 2 step and proceed to the next orbital. After we exhaust the list of orbitals, we have a sequence of values $e_{\lambda}(k+1)$. Selecting among these the $\hat{A}$ lowest ones, we construct h(k + 1) and restart the procedure, in order to get the $|\lambda(k+2)>$ set and so on. In the next subsection we shall try to justify this way of attacking the HF problem in which no actual diagonalizations need to be

performed, although a diagonalization method underlies the approach.

3.3. *Equivalence of the Algorithms*

The two algorithms we are concerned with in this work are obviously identical. Consequently, they will in general yield different intermediate results. We must require equivalence only in what refers to the final ones, when and if they converge. We shall endeavor now to prove that if a given set $\{c_j^\lambda\}$ is a solution of the HF Eqs. (4) and (5), it is also a solution of (29) and vice versa.

Let us assume first that a set of coefficients $\{g_j\}$ exists that satisfies selfconsistently the HF Eqs., *i.e.*

$$\sum_i \langle j|h\{g_j\}|i\rangle g_i^\lambda = \varepsilon_\lambda g_j^\lambda, \quad \text{for all} \quad \lambda\ ,\ j \qquad . \tag{31}$$

It should be proven now that, if after k iterations of the form (29) one finds that

$$c_j^\lambda(k) = g_j^\lambda;\ \text{for all } j \text{ and } \lambda \qquad , \tag{32}$$

then

$$c_j^\lambda(k+1) = c_j^\lambda(k)\ ;\quad \text{for all } j \text{ and } \lambda \qquad , \tag{33}$$

and

$$e_\lambda(k+1) = e_\lambda(k) = \varepsilon_\lambda;\ \text{for all } \lambda \qquad . \tag{34}$$

Proof: According to Eq. (18) we have

$$e_\lambda(k) = \sum_{ij} h_{ji}(k)\ c_j^{\lambda *}(k) c_i^\lambda(k) \qquad , \tag{35}$$

which together with (31) and (32) yields

$$e_\lambda(k) = \varepsilon_\lambda \tag{36}$$

Moreover, Eqs. (31), (32) and (36) allow one to rewrite (17) as

$$c_j^\lambda(k+1) = a_\lambda(k)c_j^\lambda(k) + e_\lambda(k)b_\lambda(k)c_j^\lambda(k) \quad , \tag{37}$$

so that, for (33) to hold it is necessary that

$$a_\lambda(k) + e_\lambda(k)b_\lambda(k) = 1 \quad . \tag{38}$$

But, in view of Eq. (30), this is verified if, (just sum the r.h.s. of the two Eqs. (30))

$$N_\lambda = 1 \; ; \quad \text{for all } \lambda. \tag{39}$$

In order to ascertain whether (39) holds, one must study the behavior of the variance $\nu_\lambda^2(k)$. From Eqs. (22), (32) and (34) one has

$$\begin{aligned} \nu_\lambda^2(k) &= \sum_{ij} c_j^{\lambda *}(k)h_{ji}^2(k)c_i^\lambda(k) - e_\lambda^2(k) \\ &= \sum_{ij\ell} c_j^{\lambda *}(k)h_{j\ell}(k)h_{\ell i}(k)c_i^\lambda(k) - e_\lambda^2(k) \\ &= e_\lambda(k) \sum_{j\ell} c_j^{\lambda *}(k)h_{j\ell}(k)c_\ell^\lambda(k) - e_\lambda^2(k) \\ &= e_\lambda^2(k) \sum_j c_j^{\lambda *}(k)c_j^\lambda(k) - e_\lambda^2(k) = 0 \quad . \end{aligned} \tag{40}$$

We see in the limit $\{c_j^\lambda(k)\} \to \{g_j^\lambda\}$ which for the sake of brevity shall be abbreviated as the "g-limit", *i.e.*, in the limit in which the $c_j^\lambda(k)$ become the self-consistent eigenvectors of the HF hamiltonian, *the variance* $\nu_\lambda^2(k)$ *vanishes*. In this same limit $p_j^\lambda(k)$ also tends to zero (the numerator goes to zero as $\nu_\lambda^2(k)$, the denominator only as $\nu_\lambda(k)$) and, consequently, $\alpha_\lambda(k)$ also vanishes, as rapidly as $\nu_\lambda^2(k)$ (see Eq. (23)). If we focus our attention now on Eq. (25), taking into account the definition (28) one can establish, after a Taylor expansion of the square root, that

$$\{e_\lambda(k+1) - e_\lambda(k)\} \to 0 \quad \text{as} \quad \nu_\lambda^2(k) \to 0 \quad , \tag{41}$$

proving (34) and implying that, in the g-limit,

$$\{e_\lambda(k+1) - e_\lambda(k)\}\, \nu_\lambda^{-1}(k) \to 0 \quad , \tag{42}$$

and, as a consequence, $N_\lambda \to 1$, which completes the proof.

Conversely, it ought to be proven now that, if after k iterations of the new algorithm, Eqs. (33) and (34) hold, then the $c_j^\lambda(k)$ are the self-consistent eigenvectors of h, *i.e.*, Eqs. (31) and (32) are true.

Proof: We know that Eqs. (33) and (34) imply both that (24) is diagonal and that $\alpha_\lambda(k)$ vanishes. The fact that $\nu_\lambda^2(k) = 0$ implies, in view of Eq. (22), that

$$\sum_{ij\ell} c_j^{\lambda *}(k) h_{j\ell}(k) h_{\ell i}(k) c_i^\lambda(k) = e_\lambda(k) \sum_{nm} c_n^{\lambda *}(k) h_{nm}(k) c_m^\lambda(k) \quad . \tag{43}$$

Define

$$Q_\ell^\lambda(k) = \sum_j h_{j\ell}(k) c_j^{\lambda *}(k) \quad . \tag{44}$$

Introduction of this into Eq. (43) yields

$$\sum_{i\ell} Q_\ell^\lambda(k) h_{\ell i}(k) c_i^\lambda(k) = e_\lambda(k) \sum_m Q_m^\lambda(k) c_m^\lambda(k) \quad , \tag{45}$$

which, after equating the coefficients of $Q_\ell^\lambda(k)$ on both sides gives the desired result:

$$\sum_i h_{\ell i}(k) c_i^\lambda(k) = e_\lambda(k) c_\ell^\lambda(k) \tag{46}$$

and thus completes the proof.

3.4. *Practical considerations*

From the practical point of view of numerical applications, an unpleasant feature of the present algorithm is that, in order to evaluate $\nu_\lambda^2(k)$ (Eq. (22)) and α_λ (Eq. (23)), one needs h^2 and h^3, respectively.

This difficulty can be overcome as follows. Replace the first of Eqs. (18) by

$$h(k)|\lambda(k)> = e_\lambda(k)|\lambda(k)> + |P> \quad , \tag{47}$$

and expand $|P>$ in terms of the known basis $|j>$:

$$|P> = \sum_j B_j^\lambda(k)|j> \quad . \tag{48}$$

Since we know the coefficients $c_j^\lambda(k)$ of the expansion (19), we obtain for B_j^λ the expression

$$B_j^\lambda(k) = \sum_i h_{ji}(k)c_i^\lambda(k) - e_\lambda(k)c_j^\lambda(k) \quad , \tag{49}$$

and, considering that $<\lambda'(k)|\lambda'(k)> = 1$,

$$\nu_\lambda^2(k) = <P|P> = \sum_j |B_j^\lambda(k)|^2 \quad . \tag{50}$$

Moreover, $|\lambda'(k)> = |P>/\nu_\lambda(k)$ implies

$$\alpha_\lambda(k) = \nu_\lambda^{-2}(k)<P|h(k)|P> = \nu_\lambda^{-2}(k) \sum_{ij} B_i^{\lambda *}(k)h_{ij}(k)B_j^\lambda(k) \quad . \tag{51}$$

The alternative HF scheme can then be set forth thus

a) An initial set $\{c_j^\lambda\}$ is guessed, together with information concerning the occupied states. $h(1)$ is evaluated and $e_\lambda(1)$ given the value $<\lambda(1)|h|\lambda(1)>$.

b) B_j^λ is evaluated for all j using Eq. (49).

c) Employ (50) and (51) to obtain $\nu_\lambda(k)$ and $\alpha_\lambda(k)$.

d) With Eq. (25) obtain $e_\lambda(k+1)$ and with Eq. (27) $N_\lambda(k)$. Then, via Eq. (30), compute $a_\lambda(k)$ and $b_\lambda(k)$.

e) By recourse to Eq. (29) get the $c_j^\lambda(k+1)$ for all j.

f) Steps b) to e) should be performed for all λ. Having the complete set

of values $e_\lambda(k+1)$ for all λ, select the $\hat{A}$ lowest ones and construct $h(k+1)$.

g) Return to b) until convergence is achieved.

4. APPLICATION TO A SIMPLE MODEL

Let us consider 4 identical fermions of spin $\frac{1}{2}$ and 3 s.p. levels, of degeneracy 2, characterized by a quantum number p (p = 1, 2, 3), with s.p. energies ε_p given (in arbitrary units) by -1, 0 and +1 respectively. Our s.p. states are of the form $|p,\sigma\rangle$ where $\sigma(=\pm 1)$ indicates the spin projection. In the perturbed ground state one occupies the s.p. states $|1, +1\rangle$, $|1, -1\rangle$, $|2, +1\rangle$ and $|2, -1\rangle$. Assume a two-body interaction with antisymmetrized matrix elements given by

$$V_{p_1\sigma_1 p_2\sigma_2;p_3\sigma_3 p_4\sigma_4} = -|G| \frac{(\sigma_1 - \sigma_2)(\sigma_3 - \sigma_4)}{(\sigma_1 + \sigma_2)(\sigma_3 + \sigma_4)} \tag{52}$$

$$\delta_{\sigma_1, -\sigma_2}\, \delta_{\sigma_3, -\sigma_4}\, \delta_{p_1 p_2}\, \delta_{p_3 p_4}\, F(p_1,p_2,p_3,p_4)$$

with

$$F(p_1,p_2,p_3,p_4) = \delta_{p_1,p_3} + \delta_{p_1,p_3+1} + \delta_{p_1,p_3-1} . \tag{53}$$

The last two terms in Eq. (52) indicate that the interaction is able, say, to take two particles from p = 1 to p = 2 or from p = 2 to p = 3, but not from p = 1 to p = 3.

We shall look for an axially symmetric HF solution[3], which is tantamount to say that the HF transformation (Eq. (2)) is independent from σ,

$$|\lambda,\sigma_\lambda\rangle = \delta_{\sigma_\lambda\sigma_p} \sum_{p=1} c_p^\lambda |p, \sigma_p\rangle . \tag{54}$$

If we write

$$h_{ij} = t_{ij} + \Gamma_{ij} \quad , \tag{55}$$

thus defining the so-called HF potential Γ (Cf. Eq. (5))[3], we have in our case

$$t_{p\sigma,q\mu} = \delta_{pq}\delta_{\sigma\mu}\varepsilon_p \quad , \tag{56}$$

and Γ becomes a 6x6 matrix, that, since axial symmetry is required, is built out of two 3x3 submatrices, placed along the diagonal. The usual HF treatment involves thus the repeated diagonalization of a 3x3 matrix, as indicated by the transformation (54).

Fig. 1 depicts the HF binding energy, for the case $|G| = 0.2$ obtained both with the standard algorithm and with the present one, as a function of the iteration number k. We compare also in Fig. 1 the "Fermi level" as given by the two methods, $\varepsilon_2(k)$ and $e_2(k)$, respectively. It is clearly seen that intermediate results are different, although the two approaches converge to identical final results. Similar curves can be drawn for other values of the coupling constant G. Several different configurations were tried as zero order guesses, without noticeable effects in the final results.

5. LIPKIN MODEL

The study made in Subsection 3.3 makes it clear that the variance $\nu_\lambda^2(k)$ (Eq. (22)) is the protagonist of the new algorithm, that converges when it vanishes. We illustrate this central role in the case of a simple model that enjoys a high degree of esteem among nuclear theorists[7].

We have two A-fold degenerate s.p. levels, separated by the s.p. energy ε, and A identical fermions. Two quantum numbers characterize a s.p. state $|j>$. One of them adopts the value -1 (lower level) and +1 (upper level). The other, which may be called the p-spin, singles out a state within the A-fold degeneracy, and runs from 1 to A. The s.p. basis is then

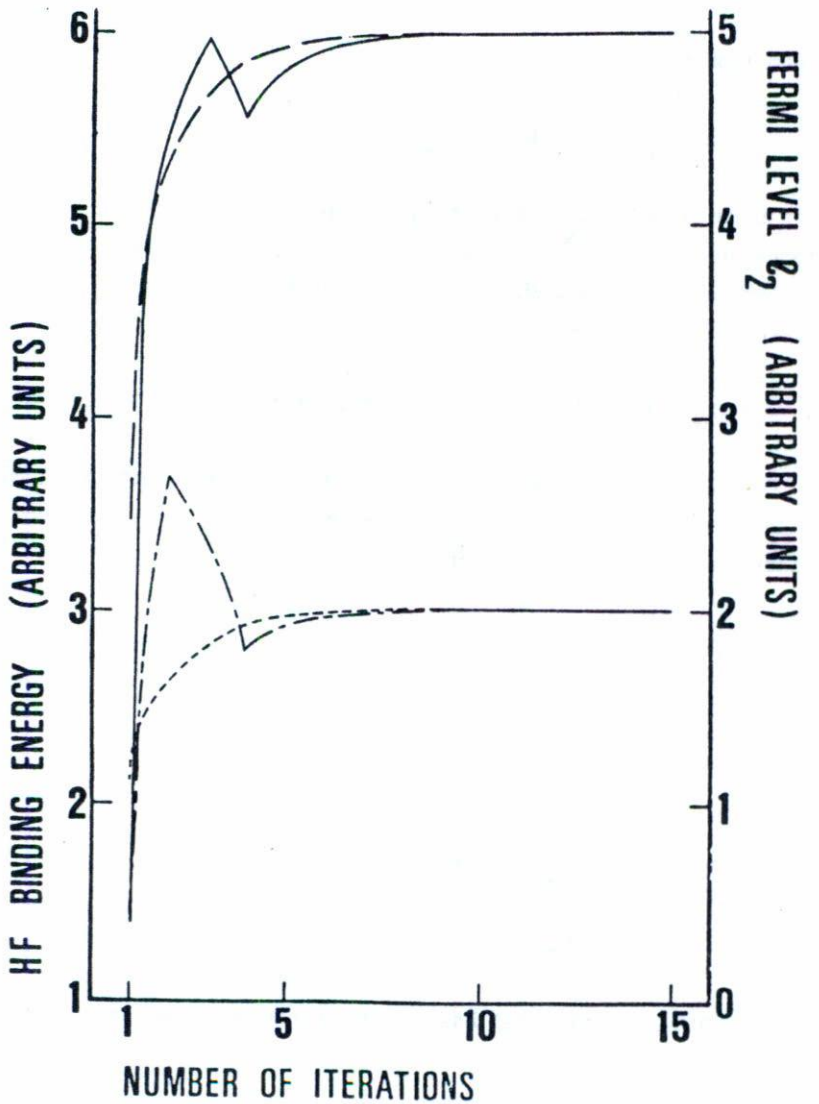

Fig. 1. With reference to the model in Section 4, the HF binding energy computed both with our approach (solid line), and with the standard one (dashed line) are plotted as a function of the corresponding number of iterations. Also shown (see scale on the righ side) are the self-consistent Fermi levels e_2 (dashed-point) and ε_2 (short dashes). After about ten iterations both methods yield undistinguishable results.

$$|j> \equiv |p, \sigma>; \quad p = 1, \ldots, A; \quad \sigma = \pm 1, \tag{57}$$

and the Hamiltonian reads

$$H = \varepsilon \sum_{p\sigma} \sigma a^{\dagger}_{p\sigma} a_{p\sigma} + \frac{V}{2} \sum_{pq\mu} a^{\dagger}_{p\mu} a^{\dagger}_{q\mu} a_{q-\mu} a_{q-\mu} \quad , \tag{58}$$

where ε is usually set equal to unit and we choose $V > 0$. The HF solution can be found analitically[8] employing the so-called quasi-spin algebra[7]. We shall here find it, instead, by recourse to the condition $\nu^2_\lambda = 0$. The HF transformation (2) is here[8].

$$|\lambda, \tau> = \delta_{\lambda p} \{\cos(\alpha/2)|p, \sigma = \tau> - i \sin(\alpha/2)|p, \sigma = -\tau>\} \quad . \tag{59}$$

On account of the monopole character of the interaction in Eq. (58) the density matrix (6) adopts a very simple form[9]. It consists of A 2 x 2 blocks along the diagonal, of the form

$$\begin{pmatrix} \rho_{--} & \rho_{-+} \\ \rho_{+-} & \rho_{++} \end{pmatrix} \quad , \tag{60}$$

with

$$\rho_{--} = \cos^2(\alpha/2) \; ; \quad \rho_{++} = \sin^2(\alpha/2) \quad , \qquad \rho_{+-} = \rho^{*}_{-+} = i \sin(\alpha/2)\cos(\alpha/2) \quad . \tag{61}$$

The HF hamiltonian (5) has, as a consequence, the same structure, and one easily finds that

$$h_{--} = -\tfrac{1}{2} \; ; \quad h_{++} = \tfrac{1}{2} \quad , \qquad h_{+-} = \frac{i}{2} V(A-1)\sin(\alpha/2)\cos(\alpha/2) \quad . \tag{62}$$

We determine the angle so as to make the variance to vanish, *i.e.*,

$$\langle\lambda|h^2|\lambda\rangle = e_\lambda^2 \quad , \tag{63}$$

and use the expansion (35) and that given in (40) for e_λ and $\nu_\lambda^2(k)$, respectively. The results

$$e_\lambda = \frac{1}{2}(h_{++} + h_{--}) + \frac{1}{2}(h_{--} - h_{++})\cos(\alpha) - |h_{+-}|\sin(\alpha) \quad , \tag{64}$$

and

$$\langle\lambda|h^2|\lambda\rangle = \frac{1}{2}(h_{++}^2 + h_{--}^2) + \frac{1}{2}(h_{--}^2 + -h_{++}^2)\cos(\alpha) + |h_{+-}|^2 - (h_{++} + h_{--})|h_{+-}|\sin(\alpha) \quad , \tag{65}$$

allow one to rewrite Eq. (63), utilizing first Eq. (62), as

$$tg(\alpha) = V(A - 1)\sin(\alpha) \quad , \tag{66}$$

which yields two solutions

$$\alpha = 0 \quad ,$$
$$\cos(\alpha) = \{V(A - 1)\}^{-1} \quad , \tag{67}$$

with the second one, of course, restricted to the situation for which

$$V > (A - 1)^{-1} \quad . \tag{68}$$

These are indeed the HF solutions found by Agassi *et al.* [8]. When (67) is replaced into (61) and (62), and the HF energy (7) is then evaluated, one finds that the second solution (67) prevails energetically over the first one, when (68) is satisfied.

6. CONCLUSIONS

We have presented a new scheme for the solution of the HF equations, which in principle does not involve diagonalizations, although it is founded on a diagonalization algorithm. The method is based on the idea that the variance of the HF hamiltonian, computed with linear combinations of a convenient s.p. basis, must vanish. Since the HF hamiltonian itself depends upon such linear combinations, a nonlinear problem arises, expressed by the set of equations (29). These equations have been numerically solved in Section 4 for a very simple model, while the central idea has been illustrated with reference to the Lipkin model.

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