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Multi-Configuration Hartree-Fock Theory in Nuclei*

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A variational method for the self-consistent solution of the nuclear many body problem with the inclusion of correlations is formulated. The trial function in this multi-configuration-Hartree-Fock (MCHF) theory is a linear combination of unrestricted Slater determinants. The MCHF equations are given and a simple procedure for solving them is outlined. A great advantage of this method is that it also yields the excited states. It is shown that the trial function is stable against particle-hole excitations. Therefore the Slater determinants differ from each other at least by two particle — two hole excitations. This method is applied to the Lipkin model. In the MCHF method the difference to the exact solution is reduced by a factor three to ten compared with the corresponding value in the HF approach.

1. Introduction

Within the last few years it became more and more obvious that even the doubly closed shell nuclei are not correctly described by the independent particle picture of the Hartree-Fock (HF) approach. This was established[1] notably for ^{40}Ca by transfer reactions like (d, p), $(^3\mathrm{He}, d)$, $(^3\mathrm{He}, \alpha)$, (d, t), (t, α). Hartree-Fock-Bogolyubov (HFB) calcu-

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1. BELOTE, T. A., A. SPERDUTO, and W. W. BUECHNER: Phys. Rev. **139**, B 80 (1965). — DORENBUSCH, W. E., T. A. BELOTE, and O. HANSEN: Phys. Rev. **146**, 734 (1966). — BELOTE, T. A., W. E. DORENBUSCH, and I. RAPAPORT: Phys. Rev. **156**, 1255 (1967). — LYNEN, U., R. BOCK, S. SANTO, and R. STOCK: Phys. Letters **25** B, 9 (1967).

lations[2] showed that pairing alone can not explain the large correlations detected in the ground states of ^{16}O and specially of ^{40}Ca. Two different methods have been tried to find these correlations in the ground state:

CELENZA, DREIZLER, KLEIN and DREISS[3] performed HF calculations in ^{16}O for the ground state, the states with two holes, and the states with four holes in the $1p$-shell. Afterwards, they diagonalized the neglected residual interaction H_{22} in the basis of the HF ground state, the lowest $2p-2h$ state, and the lowest $4p-4h$ state. On the other hand AGASSI, GILLET, and LUMBROSO[4] performed an RPA calculation on an oscillator basis and calculated the correlated ground state according to SANDERSON[5].

Neither method is completely self-consistent. The procedure of CELENZA *et al.*[3] finds the single particle states by minimizing the energies of the uncorrelated ground state, the $2p-2h$ states, and the $4p-4h$ states. AGASSI *et al.*[4] do not try at all to be self-consistent.

In this paper we want to propose a method to find the correlated ground state in a self-consistent way and which in addition yields also the excited states. We utilize a variational procedure, choosing as the trial function a linear combination of unrestricted Slater determinants. A similar ansatz but restricted to only two Slater determinants was proposed by BREMOND[6]. VEILLARD[7] formulated this two-configuration Hartree-Fock theory and HINZE and ROOTHAN[8] generalized it to a multi-configuration Hartree-Fock (MCHF) theory for atomic physics. But they imposed some limitations on the form of the allowed configurations (Slater determinants), which result in important mathematical simplifications. Here we are extending the MCHF theory to unrestricted configurations and adapting it to nuclear physics.

In Section 2 the general MCHF equations are derived and it is proved that the MCHF-function is stable against one particle-one hole excitations, while in Section 3 a simple procedure for solving the MCHF equations is outlined. Section 4 deals with the application of the theory to a simple model and, finally, conclusions are discussed in Section 5.

2. FAESSLER, A., P. U. SAUER u. M. M. STINGL: Z. Physik **212**, 1 (1968). — WOLTER, H. H., A. FAESSLER, P. U. SAUER, and M. M. STINGL: Nuclear Phys. A **116**, 145 (1968). — SAUER, P. U., A. FAESSLER, H. H. WOLTER, and M. M. STINGL: To be published.
3. CELENZA, L. S., R. M. DREIZLER, A. KLEIN, and G. J. DREISS: Phys. Letters **23**, 241 (1966).
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5. SANDERSON, E. A.: Phys. Letters **19**, 141 (1965).
6. BREMOND, B.: Nuclear Phys. **58**, 687 (1964).
7. VEILLARD, A.: Theoret. chim. Acta (Berlin) **4**, 22 (1966).
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2. Theory

For the multi-configuration Hartree-Fock (MCHF) method we choose the trial-function

$$|\Psi\rangle = \sum_I C_I |I\rangle . \tag{1}$$

The Slater determinants $|I\rangle$ represent different configurations of self-consistent single particle states $|i\rangle$, $|k\rangle$, $|l\rangle$, $|m\rangle$, ...

$$|I\rangle = \prod_{i \subset I} a_i^\dagger |0\rangle$$

with:

$$|i\rangle = a_i^\dagger |0\rangle . \tag{2}$$

"$i \subset I$" indicates that the product goes over all A states belonging to the configuration $|I\rangle$. If one takes all possible configurations $|I\rangle$ the variation of the C_I alone already leads to the exact solution within this space. The number of configurations in a space with N single particle functions and A particles is $\binom{N}{A}$. Since this is a very large number for a reasonable Hilbert space, the sum in Eq. (1) is restricted to the configurations, which lie lowest in energy. We vary the single particle states $|i\rangle$ to compensate by part for this restriction. The coefficients C_I and the states $|i\rangle$, $|k\rangle$ ... in the trial function (1) are determined in the usual way by variation of the expectation value of the total Hamiltonian:

$$H = \sum_{ik} t_{ik} a_i^\dagger a_k + (1/4) \sum_{ikmn} V_{ik;\,mn} a_i^\dagger a_k^\dagger a_n a_m . \tag{3}$$

The expressions t_{ik} and $V_{ik;\,mn}$ represent the matrix elements of the kinetic energy and the antisymmetrized matrix elements of the nucleon-nucleon interaction respectively. In Eq. (3) one can subtract the operator for the total kinetic energy of the nucleus

$$\begin{aligned} T_{CM} = & \frac{1}{2mA} \sum_{ik} \langle i | p^2 | k \rangle a_i^\dagger a_k \\ & + \frac{1}{4mA} \sum_{ikmn} \langle ik | \boldsymbol{p}(1)\boldsymbol{p}(2) | mn \rangle a_i^\dagger a_k^\dagger a_n a_m \end{aligned} \tag{4}$$

to correct for the centre-of-mass motion. We assume that this correction is already included in the one- and two-body matrix elements of the Hamiltonian (3).

The expectation value of the total Hamiltonian (3) with the trial function (1) yields:

$$\langle \Psi | H | \Psi \rangle = \sum_{I,J} C_I \langle I | H | J \rangle C_J = \sum_{I,J} C_I \{ \delta_{I;J} \sum_{i \subset I} t_{ii} + 1/2\, \delta_{I;J} \cdot \sum_{ik \subset I} V_{ik;ik} + V_{i<k;r<s} \delta_{(I \cup J)-(I \cap J);rsik} \delta_{I \supset ik} \delta_{J \supset rs} \} C_J . \tag{5}$$

The single particle states are assumed to be ordered, so that the notation $i<k$ is meaningful. Symbols of the theory of sets are utilized to simplify the notation. "$i \subset I$" indicates that the sum (or product) runs only over single particle states which are occupied in the configuration I. The Kronecker Delta symbol $\delta_{I \supset ik}$ is zero if one of the states $|i\rangle$ or $|k\rangle$ is not occupied in the configuration $|I\rangle$ and it has the value 1 when both states are occupied. The symbol $\delta_{(I \cup J)-(I \cap J);ikrs}$ has the value 1 if the non-common states of the configurations $|I\rangle$ and $|J\rangle$ are $|i\rangle$, $|k\rangle$, $|r\rangle$, and $|s\rangle$, being zero otherwise.

If one restricts the trial function (1) to only one Slater determinant (one coefficient C_I equals unity and all other zero), expression (5) gives the total energy of the Hartree-Fock (HF) approximation.

In Eq. (5) we have employed a property of the wave function $|\Psi\rangle$ which is well known in the HF case. We justify this procedure by formulating the following theorem:

Theorem. The MCHF wave function $|\Psi\rangle$ is stable against one particle-one hole excitations.

This theorem will be proved by assuming that the trial function $|\Psi\rangle$ is a linear combination of configurations which are distinguished from each other by at least two particle-two hole excitations. The variation of the expectation value (5) is requested to be zero with respect to single particle states $|i\rangle$, $|k\rangle$, ... We are thus lead to the following equation.

$$0 = \langle \Psi | (\sum_{pq} \zeta_{pq} a_p^\dagger a_q)^\dagger H | \Psi \rangle = \sum_{I,J} C_I \langle I | \sum_{pq} \zeta_{pq}^* a_q^\dagger a_p H \cdot \{ \delta_{I;J} | I \rangle + a_{u \subset J}^\dagger a_{v \subset J}^\dagger a_{r \subset I} a_{s \subset I} | I \rangle \} C_J . \tag{6}$$

The configuration $|J\rangle \neq |I\rangle$

$$|J\rangle = a_{u \subset J}^\dagger a_{v \subset J}^\dagger a_{r \subset I} a_{s \subset I} | I \rangle \tag{7}$$

can be written in this way because a two-body operator connects at most a $2p-2h$ state with its reference state.

After introducing quasi-particles with $|I\rangle$ as the vacuum, the application of Wick's theorem and the independent variation of the coeffi-

cients ζ_{pq} results in the equation:

$$\zeta^*_{ps}\Big((t_{pq}\sum_{I\supset q}+\sum_k V_{pk;qk}\sum_{I\supset qk})\delta_{I\nmid p}C_I^2+\sum_{\substack{u>v\\ r(<s)}}V_{pr;uv}\sum_{\substack{I\supset rs\\ J\supset uv}}\cdot\delta_{p\nmid I}C_I C_J\delta_{(I\cup J)-(I\cap J);rsuv}\Big)=0. \tag{8}$$

The single particle states are assumed to be ordered so that the notation $u>v$ is meaningful. This restriction prevents double counting of a configuration.

Eq. (8) says that the wave function $|\Psi\rangle$ is stable against a particle-hole excitation (from q to p in the diagonal part and from s to p in the off-diagonal part).

Thus one can assume that the sum in the trial function (1) runs over configurations which are distinguished among themselves by a least a $2p-2h$ excitation. The variation

$$\langle\delta\Psi|H|\Psi\rangle-\sum_{ik}\varepsilon_{ki}\langle\delta i|k\rangle-E\sum_I\delta C_I C_I=0 \tag{9}$$

leads to two sets of equations:

One for the determination of the coefficient C_I

$$\sum_J\langle I|H|J\rangle C_J\equiv EC_I \tag{10}$$

with:

$$\langle I|H|J\rangle=\delta_{I;J}\Big\{\sum_{i\subset I}t_{ii}+1/2\sum_{ik\subset I}V_{ik;ik}\Big\}+V_{i<k;r<s}\cdot\delta_{(I\cup J)-(I\cap J);ikrs}\,\delta_{I\supset ik}\,\delta_{J\supset rs}$$

and a second for the determination of the single particle states $|i\rangle$. We expand the states $|i\rangle$

$$\begin{aligned}|i\rangle&=\sum_a A_{ai}|a\rangle\\ |a\rangle&=\sum_i A^*_{ai}|i\rangle\end{aligned} \tag{11}$$

into a complete basis system $|a\rangle, |b\rangle, |c\rangle, |d\rangle, \ldots$ to formulate the second set of equations.

$$\sum_b t_{ab}\,X(i)\,A_{bi}+\sum_{bcd;k}V_{ac;bd}\,X(ik)\,A_{bi}A^*_{ck}A_{dk}+\sum_{bcd}S(i\underline{k};\underline{r}\underline{s})\,V_{ac;bd}\,X(ik;rs)\,A_{br}A^*_{ck}A_{ds}-\sum_k\varepsilon_{ki}A_{ak}=0. \tag{12}$$

The configuration density matrices $X(ik; rs)$ are defined by the following expressions:

$$X(ik; rs) = \sum_{J \supset ik;\, I \supset rs} C_I C_J \delta_{(I \cup J)-(I \cap J);\, ikrs}$$

$$X(ik; ik) \equiv X(ik) = \sum_{I \supset ik} C_I^2 \tag{13}$$

$$X(i) \equiv X(ii) = \sum_{I \supset i} C_I^2.$$

In the symbol

$$S(ik; rs) = \delta_{i<k}\, \delta_{r<s} + \delta_{i>k}\, \delta_{r>s}$$

the bars in the Eq. (12) indicate a summation over the underlined single particle states. The Kronecker Delta $\delta_{i<k}$ is unity for $i<k$ and zero otherwise. This avoids double counting of configurations in the off-diagonal term of Eq. (5). ε_{ki} are the Lagrange multipliers for the orthogonality of the single particle states.

$$\langle i | k \rangle = \delta_{i;k}. \tag{14}$$

In the HF-approximation ε_{ki} can be diagonalized, since a Slater determinant is invariant under a unitary transformation between the occupied states. The MCHF wave function is a linear combination of different Slater determinants, so that a diagonalisation of the ε_{ki} is impossible. The physical interpretation of this result is obvious: Since $|\Psi\rangle$ contains correlations between the particles, the concept of single particle energies $\varepsilon_{ik} = \delta_{i;k}\, \varepsilon_i$ is lost.

The MCHF problem is now given by the coupled system of Eqs. (10), (12), and (14). A possible procedure for the solution of this problem will be suggested in the following section.

3. Solution of the Multi-Configuration-Hartree-Fock-Equations

In order to solve the multi-configuration Hartree-Fock equations (MCHF) (10), (12), and (14) we shall follow closely a quadratically convergent method proposed by HINZE and ROOTHAN[8]. The procedure can be summerized in the following steps.

α) A Hartree-Fock (HF) calculation allows one to find a zero order set for the coefficients $A \equiv A_{ai}$ defined in Eq. (11).

β) The single particle states

$$|i\rangle = \sum_a A_{ai}^{\nu} |a\rangle$$

defined by the A^ν corresponding to the ν^{th} iteration are utilized to build the configurations $|I\rangle$ and to calculate the elements $\langle I|H|J\rangle$ of Eq. (10). A diagonalisation of this matrix (10) yields the coefficients $C_I^{\nu,\sigma}$ ($\sigma=1$ for the ground state and $\sigma>1$ for excited states).

γ) The orthogonality relation of the A_{ai}^ν allows one to eliminate ε_{ki}^ν out of Eq. (12) as a function of the A^ν's and the coefficients $C_I^{\nu,1}$.

δ) One corrects now the coefficients A^ν by introducing into Eq. (12) and into the ε_{ki}^ν the expression $A^{\nu+1}=A^\nu+\delta A$. Linearizing the resulting expression a linear inhomogeneous equation for the δA obtained.

ε) The improved coefficients $A^{\nu+1}$ are orthogonalized by the Schmidt-method. The steps β to ε are repeated until convergence is attained ($\delta A\to 0$).

The Hartree-Fock method (HF), which is utilized to find the zero order approximation for the coefficients A, is well described in the literature (see for example the Ref.[9-11]). The selection of the different Slater determinants $|I\rangle$ is a straightforward procedure. In step γ one has to take into account, that the matrix ε_{ik} is hermitian. If the hermitian conjugate of the equation

$$\delta\langle\Psi|H|\Psi\rangle=\sum_{ik}\varepsilon_{ik}\,\delta\langle k|i\rangle+E\sum_I\delta C_I C_I \tag{15}$$

is subtracted from Eq. (15) one finds the equations:

$$\sum_{ik}(\varepsilon_{ik}-\varepsilon_{ki}^*)\,\delta\langle k|i\rangle=0,\qquad \varepsilon_{ik}=\varepsilon_{ki}^*. \tag{16}$$

It is well known, that the phases of the basis states $|a\rangle$, $|b\rangle$, ... can be chosen in such a way that the elements t_{ab} and $V_{ab;\,cd}$ are real. But it is not generally true that real coefficients A_{ai} will yield the deepest energy minimum of:

$$\langle\Psi|H|\Psi\rangle. \tag{17}$$

But from now on *we shall assume as usual that all the matrix elements and all coefficients A_{ai} are real.* Eq. (16) now requires that the matrix for the Lagrange multipliers ε_{ik} be symmetric. We guarantee this by eliminating ε_{ik} from the Eq. (12) with the help of the orthogonality relation

$$\sum_a A_{al}A_{ak}=\delta_{k;l} \tag{18}$$

9. RIPKA, C.: The Hartree-Fock theory und nuclear deformations. Lectures in theoretical physics 1965, vol. VIII C. University of Colorado Press.
10. DAVIES, K. T. R., S. J. KRIEGER, and M. BARANGER: Nuclear Phys. **84**, 545 (1966).
11. FAESSLER, A.: Hartree-Fock-Bogolyubov calculations in light nuclei. $T=0$ and $T=1$ proton-neutron correlations. Lectures on nuclear many body problems, Herceg Novi 1967.

in the following way:

$$\begin{aligned}
\tilde{\varepsilon}_{k\,i} &= 1/2(\varepsilon_{k\,i}+\varepsilon_{i\,k}) \\
&= 1/2\sum_{a}\left(A_{a\,k}\sum_{l}\varepsilon_{l\,i}\,A_{a\,l}+A_{a\,i}\sum_{l}\varepsilon_{l\,k}\,A_{a\,l}\right) \\
&= 1/2\,\Delta_{k\,i}\Big[\sum_{a\,b}t_{a\,b}\,A_{a\,k}\,A_{b\,i}\,X(i) \\
&\quad+\sum_{a\,b\,c\,d;\,l}V_{a\,c;\,b\,d}\,A_{a\,k}\,A_{b\,i}\,A_{c\,l}\,A_{d\,l}\,X(i\,l) \\
&\quad+\sum_{a\,b\,c\,d}S(i\,\underline{l};\underline{r}\,\underline{s})\,V_{a\,c;\,b\,d}\,A_{a\,k}\,A_{b\,r}\,A_{c\,l}\,A_{d\,s}\,X(i\,l;r\,s) \\
&\quad+\sum_{a\,b}t_{a\,b}\,A_{a\,i}\,A_{b\,k}\,X(k) \\
&\quad+\sum_{a\,b\,c\,d;\,l}V_{a\,c;\,b\,d}\,A_{a\,i}\,A_{b\,k}\,A_{c\,l}\,A_{d\,l}\,X(k\,l) \\
&\quad+\sum_{a\,b\,c\,d}S(k\,\underline{l};\underline{r}\,\underline{s})\,V_{a\,c;\,b\,d}\,A_{a\,i}\,A_{b\,r}\,A_{c\,l}\,A_{d\,s}\,X(k\,l;r\,s)\Big]
\end{aligned} \tag{19}$$

with:

$$\Delta_{i\,k}=\begin{cases}\delta_{i;\,k} & \text{for } i,k\subset\text{all } I\\ 1 & \text{for } i,k\not\subset\text{all } I\,.\end{cases} \tag{20}$$

Introducing the symbol $\Delta_{i\,k}$ we want to take advantage of the following degree of freedom: A determinant is unchanged by a orthonormal transformation among a part or all of the occupied states. If an inert core of states $|m_1\rangle$, $|m_2\rangle$, ... $|m_c\rangle$ is occupied in all the configurations $|I\rangle$, one can utilize the free orthonormal transformations among the $|m_1\rangle$ ... $|m_c\rangle$ to diagonalize $\varepsilon_{i,\,k}$ for $i,k\leqq m_c$.

In step δ we introduce the symmetrized $\varepsilon_{k\,i}$ of Eq. (19) into Eq. (12) and replace $A^{\nu}_{a\,i}$ by $A^{\nu+1}_{a\,i}=A^{\nu}_{a\,i}+\delta A_{a\,i}$. The linearisation of the resulting expression yields:

$$\sum_{b,\,k}M^{\nu}_{a\,i;\,b\,k}\,\delta A_{b\,k}=D^{\nu}_{a\,i}\,. \tag{21}$$

The superscript ν indicates that the matrices M and D are constructed using the coefficients A of the ν^{th} iteration.

The Schmidt orthogonalisation required in step ε is also a well known method:

$$\tilde{A}_{a\,i}=A_{a\,i}-\sum_{k=1}^{i-1}A^{N}_{a\,k}\sum_{b}A^{N}_{b\,k}\,A_{b\,i}\,, \tag{22}$$

$$A^{N}_{a\,i}=\tilde{A}_{a\,i}\Big(\sum_{b}\tilde{A}^{2}_{b\,i}\Big)^{-1/2}. \tag{23}$$

For this procedure it is of advantage to order the states $|i\rangle$ so, that in the overlap matrix

$$o_{ik}=\sum_a A_{ai}\,A_{ak} \tag{24}$$

the smallest off diagonal elements lie in the upper left corner and the largest in the lower right one. In this way one gets the least possible rearrangement of the single particle states. The main difficulty of the whole procedure is the size of the matrix $M_{ai;\,bk}$. Without making use of symmetries it exceeds already for ^{16}O (with a basis including all states up to the $2s-1d$ shell) the numerical possibilities of standard calculating facilities. Time reversal and isospin invariances suffice to reduce already the problem to managable dimensions. The size of the matrix M can be furthermore reduced, if one requests for additional symmetries:

Rotational invariance around the intrinsic z-axis and parity invariance restrict the summation in Eq. (11) to states of the same angular momentum projection K and parity π:

$$|i;K\pi\rangle=\sum_a A_{ai}^{K\pi}\,|a;K\pi\rangle. \tag{25}$$

These symmetry requirements also allow for reduction of the remaining matrix $M_{a\,i\,K_i\pi_i;\,b\,k\,K_k\pi_k}$ into smaller unconnected matrices:

$$M_{a\,i\,K_i\pi_i;\,b\,k\,K_k\pi_k}=\delta_{K_i;\,K_k}\,\delta_{\pi_i;\,\pi_k}\,M_{a\,i;\,b\,k}^{K_i\pi_i}. \tag{26}$$

This entails that we neglect in each cycle of the iteration the effect on the matrices $M^{\pi,K}$ caused by the changes in the coefficients $A_{ai}^{\pi K}$ which belong to different symmetries. Although this slows down the convergence of the iteration, it reduces drastically the size of the irreducible matrices.

4. Applications to a Simple Model

The above developed multi-configuration Hartree-Fock (MCHF) theory will now be applied to the LIPKIN[12] model. This simple model is suggested by LIPKIN and coworkers[12,13] for testing new approaches to the solution of the many body problem. The Hamiltonian is of such a form that it allows for such an exact group theoretical solution.

The model consists of two N-fold degenerate single particle levels ($|p\sigma\rangle$; $\sigma=\pm1$, $p=1,\ldots N$). They are separated by an energy gap ε. The number of nucleons is N. The interaction is a monopole force

12. LIPKIN, H. J., N. MESKOV, and A. J. GLICK: Nuclear Phys. **62**, 188 (1965).
13. AGASSI, D., H. J. LIPKIN, and N. MESHKOV: Nuclear Phys. **86**, 321 (1966).

scattering two particles from one level into the other.

$$\hat{H}=(1/2)\,\varepsilon \sum_{\sigma=\pm 1,\, p=1,\ldots N} \sigma\, c^{\dagger}_{p\sigma}\, c_{p\sigma}+1/2\, V \sum_{pq\sigma} c^{\dagger}_{p\sigma}\, c^{\dagger}_{q\sigma}\, c_{q-\sigma}\, c_{p-\sigma}. \quad (27)$$

With the help of the quasi-spin operators

$$\begin{aligned} J_Z(c)&=1/2 \sum_{p\sigma} \sigma\, c^{\dagger}_{p\sigma}\, c_{p\sigma} \\ J_+(c)&=J^+_-(c)=\sum_p c^{\dagger}_{p+}\, c_{p-}\,, \end{aligned} \quad (28)$$

which fulfill the angular momentum commutation rules, one writes the Hamiltonian into the form[12]:

$$H=J_Z(c)+1/2\, v\left[J^2_+(c)+J^2_-(c)\right]. \quad (29)$$

The energy is now given in units of the single particle energy ε ($v=v/\varepsilon$). The unperturbed ground state $|n=0, c\rangle$ (an $n=0$ particle-$n=0$ hole state in the basis or "c" representation) is the member with the lowest quasi-spin projection in the following representation:

$$|J=(1/2)\,N;\, J_Z=n-J;\, c\rangle \equiv |n;\, c\rangle. \quad (30)$$

Since the Hamiltonian (29) is not changing the total quasi-spin the finding of the *exact solution* implies that one has to diagonalize a $2J+1=N+1$ matrix. These solutions have been tabulated by LIPKIN *et al.*[12].

The *HF approach* looks for the $0p-0h$ wave function $|n=0, a\rangle$ in the self-consistent or "a" representation. The basis and the single particle states are connected by the unitary transformation:

$$\begin{pmatrix} a^{\dagger}_{p-} \\ a^{\dagger}_{p+} \end{pmatrix} = \begin{pmatrix} \cos\frac{\beta}{2} & -i\sin\frac{\beta}{2} \\ -i\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} \begin{pmatrix} c^{\dagger}_{p-} \\ c^{\dagger}_{p+} \end{pmatrix}. \quad (31)$$

In quasi-spin space this corresponds to[13]:

$$\begin{aligned} J_x(c)&=1/2\left[J_+(c)+J_-(c)\right]=J_x(a) \\ J_y(c)&=i/2\left[-J_+(c)+J_-(c)\right]=\cos\beta\, J_y(a)-\sin\beta\, J_z(a) \\ J_z(c)&=\cos\beta\, J_z(a)+\sin\beta\, J_z(a) \end{aligned} \quad (32)$$

or:

$$\begin{aligned} |c\rangle &= R(-\beta)\,|a\rangle \\ |a\rangle &= R(\beta)\,|c\rangle. \end{aligned}$$

β is the second Euler angle representing a rotation around the x-axis.

The HF-solution

$$\delta\langle 0, a|H(a)|0, a\rangle = 0 \tag{33}$$

can easily be found[13]:

For: $1 \geqq v(2J-1)$

$$\beta = 0$$

$$E_{\mathrm{HF}} = -J \equiv -(1/2)N .$$

For: $1 < v(2J-1)$

$$\cos\beta = [v(2J-1)]^{-1} \equiv b^{-1}$$

$$E_{\mathrm{HF}} = -J/b - 1/2\, J b(1-b^{-2}) . \tag{34}$$

Although it is not explicitly stated in Ref.[13] one can easily show that the HF ground state has the form:

$$\begin{aligned} |0, a\rangle &\equiv |J, -J, a\rangle \\ &= \sum_n |n, c\rangle \langle n, c|R(-\beta)|0, a\rangle \\ &= \sum_{n=0}^{N} d^J_{-J;\, n-J}(-\beta)\,|n, c\rangle . \end{aligned} \tag{35}$$

The function $d^J_{M',M}(\beta)$ is defined by EDMONDS[14] in Eq. (4.1.15). But our phase convention (31) requires the replacement of $\sin\frac{\beta}{2}$ by $i\sin\frac{\beta}{2}$. The expressions needed in Eq. (35) are:

$$d^{1/2N}_{-1/2N;\, n-1/2N}(\beta) = (-)^n \left(\frac{N!}{n!(N-n)!}\right)^{1/2} \left(\cos\frac{\beta}{2}\right)^{N-n} \left(i\sin\frac{\beta}{2}\right)^n . \tag{36}$$

The absolut squares of these amplitudes represent a binomial distribution as found by AGASSI *et al.*[13].

The *MCHF approach* takes

$$|\Psi\rangle = \sum_{n=0,\,2\,\ldots\,n\,(\max)} b_n |n, a\rangle$$

as the trial wave function. We restrict ourselves to the two configurations $|0, a\rangle$ and $|2, a\rangle$.

$$\begin{aligned} |\Psi\rangle &= \cos\phi\,|0, a\rangle + \sin\phi\,|2, a\rangle \\ \langle\Psi|H|\Psi\rangle &= \cos^2\phi\,\langle 0, a|H|0, a\rangle \\ &\quad + 2\cos\phi\sin\phi\,\langle 2, a|H|0, a\rangle + \sin^2\phi\,\langle 2, a|H|2, a\rangle . \end{aligned} \tag{37}$$

14. EDMONDS, A. R.: Angular momentum in quantum mechanics. Princeton: University Press 1960.

Table. *Total binding energies of the exact, the HF, and the MCHF solution in the Lipkin*[12] *model*

The first column gives the number of nucleons, the second the coupling constant v in energy units of ε. The next column lists the exact total binding energy. The two last columns represent the difference between the HF and the exact energy and between the HF and the exact energy and between the MCHF and the exact energy, respectively. All the energies are in units of the level splitting ε.

N	$N \times v$	E (exact)	ΔE (HF)	ΔE (MCHF)
14	0.4	− 7.038	0.038	0.002
	0.6	− 7.088	0.088	0.007
	0.8	− 7.163	0.163	0.024
	1.0	− 7.270	0.270	0.060
	2.0	− 8.636	0.251	0.087
	5.0	−17.268	0.264	0.017
30	0.4	−15.040	0.040	0.002
	0.6	−15.094	0.094	0.008
	0.8	−15.179	0.179	0.035
	1.0	−15.314	0.314	0.096
	2.0	−18.547	0.168	0.019
	5.0	−38.049	0.247	0.013
50	0.4	−25.041	0.041	0.003
	0.6	−25.096	0.096	0.011
	0.8	−25.186	0.186	0.040
	1.0	−25.340	0.340	0.119
	2.0	−31.039	0.161	0.017
	5.0	−64.043	0.242	0.012

The matrix elements are easily calculated with the help of angular momentum algebra. The total energy is minimized as a function of the two angles β and ϕ.

The table shows the exact total binding energy of the model nucleus[12]. Furthermore the difference between the HF and the exact binding energy and the difference between the MCHF and the exact binding energy are listed. The last numbers are by a factor three to ten smaller than those corresponding to the HF case.

5. Conclusion

A linear combination of Slater determinants has been used as a trial function in the nuclear many body problem. Both the single particle states and the coefficients of the different configurations are varied at the same time. One thus obtains the energy minimum of the expectation value of the total Hamiltonian. This multi-configuration Hartree-Fock

(MCHF) approach yields a relatively simple system of equations for the determination of the coefficients and single particle states. The method not only gives self-consistently the ground state with the inclusion of correlations of any type but also the excited states. Due to the inclusion of correlations it is impossible to speak in this approach of single particle energies: The matrix of the Lagrange multipliers for the orthogonality of the single particle states yield the single particle energies as eigenvalues in the HF-approach. In the MCHF-approach such a diagonalisation is impossible. This is the price one has to pay to include correlations.

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