

Application of the Multi-Configuration Hartree-Fock Theory to a Simple Model*

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Received October 10, 1968

The Lipkin model is extended to yield a non-trivial Hartree-Fock (HF) solution for any coupling constant of the two-body force. In this model the multi-configuration Hartree-Fock (MCHF) approach is compared with the exact solution and with the HF solution. The results show a strong superiority of the MCHF method over the HF approximation.

1. Introduction

Recently a variational method for the solution of the nuclear many-body problem was proposed¹ taking, as a trial wave function, a linear combination of Slater determinants. In this multi-configuration Hartree-Fock (MCHF) method one simultaneously varies both the coefficients of the expansion and the single-particle states. The method yields the excited states apart from giving selfconsistently the correlated ground state. It was tested by the simple Lipkin model^{2,3} for which the exact solution is known². This model has the drawback of producing only two particle-two hole excitations. The unperturbed ground state therefore is already the Hartree-Fock (HF) state and only for not too small values of the interaction constant the unperturbed solution becomes unstable. It is desirable to have a model which yields for all values of the coupling

* Work done under the auspices of the Fund for Overseas Research Grant and Education, Inc., USA, the Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina, and the Deutsches Bundesforschungs-Ministerium, Germany.

** Member of the Scientific Research Career of the Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina.

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¹ FAESSLER, A., and A. PLASTINO: To be published.

² LIPKIN, H. J., N. MESHKOV, and A. J. GLICK: Nuclear Phys. **62**, 188 (1965).

³ AGASSI, D., H. J. LIPKIN, and N. MESHKOV: Nuclear Phys. **86**, 321 (1966).

constant a non-trivial HF solution in order to compare the MCHF approach with the exact and with the competing HF solution. Here we are proposing a model which has the same merit of being accessible to an exact group theoretical solution as the Lipkin model. But in contrast with this model it produces one particle-one hole excitation and therefore always has a non-trivial HF solution.

In Section 2 the model is introduced and reformulated in the language of quasi-spin operators. The exact, the HF, and the MCHF solutions are given in Section 3. Finally the results are summarized in Section 4.

2. The Model

The model has two Ω -fold degenerate single-particle levels which are separated by the single-particle energy ε . We characterize the Ω lower levels by $|p\sigma = -1\rangle$ and the upper levels by $|p\sigma = +1\rangle$ (for $p=1, \dots, \Omega$) as LIPKIN *et al.*^{2,3} does. The nucleons interact via a two-body monopole force with the strength V

$$\hat{H} = \frac{1}{2} \varepsilon \sum_{\mu p} c_{p\mu}^\dagger \mu c_{p\mu} + \frac{1}{2} V \sum_{\mu \nu p} c_{p\mu}^\dagger \nu c_{p\nu} \sum_{\sigma \tau q} \sigma c_{q\sigma}^\dagger c_{q\tau}. \quad (1)$$

Opposite to the Lipkin model the interaction can also produce forward scattering of one or both particles.

Introducing the quasi-spin operators

$$\begin{aligned} J_z &= \frac{1}{2} \sum_p c_{p\sigma}^\dagger \sigma c_{p\sigma}, \\ J_+ &= J_-^\dagger = \sum_p c_{p+}^\dagger c_{p-}, \end{aligned} \quad (2)$$

which fulfill the angular-momentum commutation relations, one can write the Hamiltonian (1) into the following form:

$$\hat{H} = J_z + \frac{1}{2} v [2J^2 + 2J_z^2 + 2J_z(J_+ - J_-) + 2(-J_+ + J_-)J_z - J_-^2 - J_+^2], \quad (3)$$

where the energy is given in units of $\varepsilon (v \equiv V/\varepsilon)$.

It is now straightforward to construct N -particle eigenfunctions of the total quasi-spin operator and of the z -component of the quasi-spin operators. The problem becomes especially simple if we consider $N = \Omega$ particles in the two levels. The unperturbed ground state for $N = \Omega$ is the stretched configuration with the largest negative z -component of the quasi-spin:

$$|n=0, c\rangle \equiv |J = \frac{1}{2} N; J_z = -\frac{1}{2} N; c\rangle = \prod_{p=1}^N c_{p-}^\dagger |0\rangle, \quad (4)$$

where the number of particle-hole states is indicated by n .

The letter “ c ” recalls one that the basis or “ c ” representation is employed. The other states with the same total quasi-spin are constructed by the raising operator J_+ . Since the Hamiltonian (3) is not changing the total quasi-spin, the exact solution is found by diagonalizing (3) in the $2J+1=N+1$ space of the total quasi-spin. The energy matrix can be calculated utilising the following results of angular-momentum algebra:

$$\begin{aligned} J_z |n\rangle &= (n-J) |n\rangle, \\ J_+ |n\rangle &= [(2J-n)(n+1)]^{\frac{1}{2}} |n+1\rangle, \\ J_- |n\rangle &= [(2J-n+1)n]^{\frac{1}{2}} |n-1\rangle. \end{aligned} \quad (5)$$

3. The Solutions

The *exact solution* is found by diagonalization of the matrix:

$$\begin{aligned} \langle n' | H | n \rangle &= (n-J) + \frac{1}{2} v \{ \delta_{n',n} 2(2J^2 + J + n^2 - 2Jn) \\ &\quad + \delta_{n',n+1} 2[(2J-n)(n+1)]^{\frac{1}{2}} + \delta_{n',n-1} 2[(2J-n+1)n]^{\frac{1}{2}} \\ &\quad - \delta_{n',n+2} [(2J-n-1)(n+2)(2J-n)(n+1)]^{\frac{1}{2}} \\ &\quad - \delta_{n',n-2} [(2J-n+2)(n-1)(2J-n+1)n]^{\frac{1}{2}} \}. \end{aligned} \quad (6)$$

The number of particle-hole states is indicated by n ,

$$|n\rangle \equiv |J; J_z = n - J\rangle.$$

In the *HF approach* we are looking for the selfconsistent single-particle states:

$$\begin{pmatrix} a_{p-}^\dagger \\ a_{p+}^\dagger \end{pmatrix} = \begin{pmatrix} \cos \frac{\beta}{2} & \sin \frac{\beta}{2} \\ -\sin \frac{\beta}{2} & \cos \frac{\beta}{2} \end{pmatrix} \begin{pmatrix} c_{p-}^\dagger \\ c_{p+}^\dagger \end{pmatrix}. \quad (7)$$

Here we are allowing for only an orthogonal transformation. This is the restriction which is customarily imposed on HF calculations in actual nuclei. The single-particle transformation (7) corresponds in quasi-spin space, to the following rotation:

$$\begin{aligned} J_x(c) &= \cos \beta J_x(a) + \sin \beta J_z(a), \\ J_y(c) &= J_y(a), \\ J_z(c) &= \cos \beta J_z(a) - \sin \beta J_x(a). \end{aligned} \quad (8)$$

Since the operators J_i are the generators of a rotational group, we can write

$$\begin{aligned} |J; J_z = n - J; c\rangle &= \sum_{n'=0}^N |J; n' - J; a\rangle \langle a; J; n' - J | R(\beta) | J; n - J; a\rangle \\ &= \sum_{n'=0}^N d_{n'-J; n-J}^J(-\beta) |J; n' - J; a\rangle. \end{aligned} \quad (9)$$

The operator $R(\beta)$ indicates a positive rotation around the y -axis. The rotational matrices $d_{M', M}^J(\beta)$ are defined, for example, by EDMONDS⁴ (Eq. (4.1.15)).

The angle β is found by minimising the ground state expectation value of the total Hamiltonian in the a -representation,

$$\langle 0, a | H(a) | 0, a \rangle = -J \cos \beta + v J [2J \cos^2 \beta + 1 + \sin^2 \beta + 2 \sin \beta]. \quad (10)$$

The letter “ a ” in $H(a)$ denotes the transformation of the Hamiltonian (3) into the a -representation with the help of Eq. (8)

$$\begin{aligned} H(a) &= \cos \beta J_z(a) + \sin \beta J_x(a) + 2v [\cos^2 \beta J_z(a) + \sin \beta J_x^2(a) \\ &\quad + \cos \beta \sin \beta [J_z(a) J_x(a) + J_x(a) J_z(a)] \\ &\quad + J_y^2(a) + \cos \beta J_x(a) - \sin \beta J_z(a)]. \end{aligned} \quad (11)$$

The HF function can be expanded into the wave functions of the basis representation by employing the inverse transformation of Eq. (9),

$$|0, a\rangle \equiv |J \equiv \frac{1}{2} N; J_z = -J, a\rangle = \sum_n d_{-J; n-J}^J(-\beta) |n; c\rangle \quad (12)$$

with

$$d_{-J; n-J}^J(\beta) = (-)^n \left[\frac{N!}{n!(N-n)!} \right]^{\frac{1}{2}} \left(\cos \frac{\beta}{2} \right)^{N-n} \left(\sin \frac{\beta}{2} \right)^n.$$

To find the *MCHF solution* one has only to take a linear combination of the configurations which are different by at least two particle-two hole excitations, as proved in ref.¹. Here the trial function is restricted to the $0p-0h$ and to the $2p-2h$ configuration:

$$\psi = \cos \phi |0, a\rangle + \sin \phi |2, a\rangle. \quad (13)$$

The two angles ϕ and β are found by numerically minimising the expectation value of the total Hamiltonian:

$$\begin{aligned} \langle \psi | H | \psi \rangle &= \cos^2 \phi \langle 0; a | H | 0; a \rangle + 2 \sin \phi \cos \phi \langle 2; a | H | 0; a \rangle \\ &\quad + \sin^2 \phi \langle 2; a | H | 2; a \rangle. \end{aligned} \quad (14)$$

⁴ EDMONDS, A. R.: Angular momentum in quantum mechanics. Princeton, New Jersey: University Press 1960.

Table 1. The total binding energies of the exact, of the HF, and of the MCHF solutions. The first column lists the number of particles N , the second contains the coupling constant v , and the third gives the exact value of the total binding energy. The two last columns denote the differences between the MCHF and the exact and between the HF and the exact solutions. All the energies are given in units of ϵ , the energy gap between the two unperturbed single particle levels

N	v	Exact	$E_{\text{MCHF}} - E_{\text{Exact}} \times 10^5$	$E_{\text{HF}} - E_{\text{Exact}} \times 10^4$
4	10^{-3}	-1.9900069	0.0	0.1
	2×10^{-3}	-1.9800281	0.0	0.1
	5×10^{-3}	-1.9501787	0.0	0.8
	10^{-2}	-1.9007311	0.0	3.1
	2×10^{-2}	-1.8030601	0.0	12.4
	5×10^{-2}	-1.5220968	2.2	79.1
	10^{-1}	-1.1138018	70.0	247.5
10	10^{-3}	-4.9450324	0.0	0.2
	2×10^{-3}	-4.8901323	0.0	1.0
	5×10^{-3}	-4.7258598	0.0	5.9
	10^{-2}	-4.4536631	0.4	24.4
	2×10^{-2}	-3.9168961	11.9	106.6
	5×10^{-2}	-2.4505702	665.6	548.0
	10^{-1}	-1.2499972	58.8	86.9
20	10^{-3}	-9.7901161	0.0	1.0
	2×10^{-3}	-9.5804790	0.0	3.9
	5×10^{-3}	-8.9532287	0.6	26.1
	10^{-2}	-7.9148866	19.0	116.7
	2×10^{-2}	-5.8911480	572.0	587.0
	5×10^{-2}	-2.4999985	32.3	88.3
	10^{-1}	-1.2500000	0.7	10.0
40	10^{-3}	-19.180445	0.0	4.0
	2×10^{-3}	-18.361875	0.2	16.8
	5×10^{-3}	-15.913814	23.5	121.8
	10^{-2}	-11.885143	853.0	671.3
	2×10^{-2}	-6.2499934	85.9	189.4
	5×10^{-2}	-2.5000003	0.5	10.1
	10^{-1}	-1.2500124	1.2	1.5

The first matrix element is given in Eq. (10). The remaining ones can be calculated utilising Eqs. (5) and (11),

$$\begin{aligned}
 \langle 2; a | H | 0; a \rangle &= -v \cos^2 \beta [J(2J-1)]^{\frac{1}{2}} \\
 \langle 2, a | H | 2, a \rangle &= (2-J) \cos \beta + v [2 \cos^2 \beta (2-J)^2 \\
 &\quad + (1 + \sin^2 \beta)(J(J+1) - (2-J)^2) - 2(2-J) \sin \beta].
 \end{aligned}
 \tag{15}$$

Table 2. *Overlap of the wave functions corresponding to the exact solutions with those of the HF and MCHF methods for four values of the number of particles N and two values of the coupling constant v in units of e*

N	v	$\langle \text{Exact} \text{HF} \rangle$	$\langle \text{Exact} \text{MCHF} \rangle$
4	0.01	0.999922	1.000000
4	0.05	0.997826	0.999997
10	0.01	0.000335	0.999999
10	0.05	0.973252	0.997758
20	0.01	0.996401	0.999969
20	0.05	0.998558	0.999955
40	0.01	0.969568	0.997368
40	0.05	0.999932	0.999999

Table 3. *Mixing coefficients of the exact solution, of the HF approach, and of the MCHF method for the number of particles N=10 and the coupling constants v=0.01 and v=0.05. The entry n indicates the number of particle-hole states into which the total wave function is expanded*

n	v=0.01			v=0.05		
	Exact	HF	MCHF	Exact	HF	MCHF
0	0.9986	0.9993	0.9986	0.8467	0.7573	0.8435
1	-0.0365	-0.0387	-0.0367	-0.3765	-0.5726	-0.4105
2	0.0373	0.0010	0.0372	0.3289	0.2905	0.2804
3	-0.0020	-0.0000	-0.0022	-0.1519	-0.1134	-0.1811
4	0.0013	0.0000	0.0001	0.0918	0.0359	0.0869
5	-0.0001	-0.0000	-0.0000	-0.0363	-0.0094	-0.0311
6	0.0000	0.0000	0.0000	0.0162	0.0021	0.0086
7	-0.0000	-0.0000	-0.0000	-0.0051	-0.0004	-0.0018
8	0.0000	0.0000	0.0000	0.0016	0.0001	0.0003
9	-0.0000	-0.0000	-0.0000	-0.0003	-0.0000	-0.0000
10	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000

The MCHF function can be expanded into functions of the basis representation

$$\psi = \sum_{n=0}^N \{ \cos \phi d_{-J; n-J}^J(-\beta) + \sin \phi d_{2-J; n-J}^J(-\beta) \} |n, c\rangle, \quad (16)$$

The results are given in Table 1. A comparison shows that the energy difference between the MCHF and the exact solution is by one order of magnitude smaller than the difference between the HF and the exact total energy.

4. Conclusion

The Lipkin^{2,3} model has been extended in order to provide a non-trivial HF solution for any value of the coupling parameter. The exact, the MCHF, and HF solutions have been calculated. The MCHF always

lies between the HF solution and the exact solution. The difference with the exact energy is normally by one order of magnitude smaller for the MCHF case than for the HF case. This encourages applications of the MCHF theory to real nuclei.

We would like to thank Prof. S. A. MOSZKOWSKI for stimulating discussion. One of us (A. F.) is indebted to the "Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina", to the "Deutscher Akademischer Austauschdienst", and to the Universidad de La Plata, Argentina for their support. Last but not least he wants to thank Dr. H. E. BOSCH for his hospitality during his stay at the "Laboratorio de Radiaciones, IIAE, Buenos Aires", where part of this work was done. One of us (A. P.) is indebted to the Deutsches Bundesforschungs-Ministerium for economic support. Thanks are also due to the staff of the Computer Center of "Yacimientos Petrolíferos Fiscales" for making computing time available to them and to Mr. J. CANTARD for numerous courtesies.

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