HARTREE-FOCK THEORY IN EXACTLY SOLUBLE MODELS WITH A FINITE NUMBER OF PARTICLES

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ABSTRACT

A review is made of different exactly soluble models of a finite number of fermions, in order to study the properties of the Hartree-Fock approach, relating them to those of the exact Schrödinger solution. Particular attention is paid to the description of phase transitions.

RESUMEN

Para estudiar las propiedades de la aproximación Hartree-Fock se hace una revisión de los diferentes modelos con soluciones exactas de un número finito de fermiones relacionándolas a aquellas de la solución exacta de Schrödinger. Se pone atención especial a la descripción de las transiciones de fase.

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I. INTRODUCTION

Exactly soluble models have proved to be extremely useful in theoretical studies concerning the validity and/or usefulness of diverse theoretical approaches developed in order to investigate the manifold aspects of the quantum many-body problem.

Of these models, the most widely known is perhaps the so-called Lipkin Model[1], which is strongly appealing because of its elegance and simplicity, being based on SU2 algebra. In the present work, which is devoted to the Hartree-Fock (HF) approximation, we shall concern ourselves with the peculiarities of this basic theoretical approach both in the case of the Lipkin Model, and in that of some generalizations of it, guided by the fact that we have available the exact Schrodinger solution. Thus, we will be in a position to assert whether special features predicted within the HF context have their counterpart in the exact wavefunction.

The basic ingredient of the models to be described lies in the so-called quasi-spin algebra, which we discuss below.

II. QUASI-SPIN OPERATORS

The models that will occupy our attention deal with N particles, distributed in two (2Ω)-fold degenerate single-particle (s.p.) levels which are separated by the s.p. energy ε. We characterize the 2Ω lower states by $|p,\mu = -1\rangle$ and the 2Ω upper ones by $|p,\mu = 1\rangle$ (for $p = 1,2, \ldots 2\Omega$). Thus, each s.p. state is completely characterized by the two quantum numbers p and μ.

Lipkin et al.[1] introduced the operators

$$\hat{J}_+ = \hat{J}_-^\dagger = \sum_p c^\dagger_{p,+} \times c_{p,-} \ ,$$

$$\hat{J}_Z = \frac{1}{2} \sum_{p,\mu} \mu \, c^\dagger_{p,\mu} \, c_{p,\mu} \ , \tag{1}$$

where $c_{p,\mu}$ is the destruction operator for the single fermion state p,μ, while $c^\dagger_{p,\mu}$ creates a particle in that state. The operators (1) satisfy

commutation relations identical to those for angular momentum operators, thus the name quasi-spin (q.s.). We have then to deal with an SU2 algebra and there exists a Casimir operator

$$\hat{J}^2 = \hat{J}_Z^2 + \frac{1}{2}(\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+) , \tag{2}$$

which commutes with the three operators $\hat{J}_+$, $\hat{J}_-$ and $\hat{J}_Z$. Some of the 2^N many body states of our system can then be classified as eigenstates of $\hat{J}^2$ and $\hat{J}_Z$ labelled by quantum-numbers J, M such that

$$\begin{aligned} \hat{J}^2 \mid J,M\rangle &= J(J+1) \mid J,M\rangle , \\ \hat{J}_Z \mid J,M\rangle &= M \mid J,M\rangle . \end{aligned} \tag{3}$$

Lipkin's hamiltonian reads[1]

$$\begin{aligned} \hat{H}_L &= \frac{\varepsilon}{2} \sum_{\mu} \mu \, c^{\dagger}_{p,\mu} c_{p,\mu} + \frac{K}{2} \sum_{p_1,p_2} \sum_{\mu} c^{\dagger}_{p_1,\mu} c^{\dagger}_{p_2,\mu} c_{p_2,-\mu} c_{p_1,-\mu} \\ &= \varepsilon \hat{J}_z + \frac{K}{2} \sum_{\mu} \sum_{p_1} c^{\dagger}_{p_1,\mu} \left(\sum_{p_2} c_{p_2,\mu} c_{p_2,-\mu} \right) c_{p_1,-\mu} \\ &= \varepsilon \hat{J}_z + \frac{K}{2} (\hat{J}_+^2 + \hat{J}_-^2) . \end{aligned} \tag{4}$$

When the interaction, that does not affect the p-quantum number and is accordingly referred to as a monopole one, is switched off, the system will be found in its unperturbed ground state (u.g.s.)

$$\mid \text{u.g.s.} \rangle \equiv \mid J = \frac{N}{2} , \quad M = -\frac{N}{2} \rangle , \tag{5}$$

as it is easily seen from the definition (1), i.e., the lowest possible value of J_Z is obtained when all particles accomodate themselves in the lower level, and, acoordingly, the maximum possible value for J is the modulus of M_{MIN}.

It is obvious from (4) and (2) that

$$[\hat{H}_L , \hat{J}^2] = 0 , \tag{6}$$

which means that J is a good quantum number and that the exact solution is obtained by diagonalizing $\hat{H}_L$ within a given J-multiplet. Since the maximum value of J is $\frac{N}{2}$, the size of the matrix to be diagonalized is at most $(N+1)\times(N+1)$, a simple task if N is not too large. We see then that, with Lipkin's hamiltonian, only a few of the 2^N many-body states referred to above become relevant, and one is often interested just in the N+1 states pertaining to the J-multiplet that contains the u.g.s.

There are some additional operators of the type (1) that will be of interest too as the q.s. pairing (q.s.p.) operators introduced by Cambiaggio an Plastino[2]:

$$\hat{Q}_+ = \hat{Q}_-^\dagger = \sum_p c^\dagger_{p,+} \; c^\dagger_{p,-} \;,$$

$$\hat{Q}_o = \frac{1}{2} \sum_{p,\mu} c^\dagger_{p,\mu} \; c_{p,\mu} - \Omega = \frac{1}{2}\hat{N} - \Omega \;, \tag{7}$$

$$\hat{Q}^2 = \hat{Q}_o^2 + \frac{1}{2}(\hat{Q}_+ \hat{Q}_- + \hat{Q}_- \hat{Q}_+) \;,$$

where $\hat{N}$ is the number operator. It can be easily shown that the $\hat{Q}_i$ obey angular-momentum commutation rules. Moreover, any $\hat{Q}$-operator commutes with all $\hat{J}$-operators (SU2 × SU2). Obviously, $\hat{Q}_+$ creates (and $\hat{Q}_-$ destroys) two particles which yield zero contribution to the $\hat{J}_z$-value, and which could then be said to "couple" to M = 0. Thus, the $\hat{Q}$-operators behave in the same way as the pairing ones of the theory of nuclear superconductivity[3].

We see that a complete orthonormal basis exists characterized by the eigenvalues of the operators $\hat{J}^2$, $\hat{Q}^2$, $\hat{J}_Z$ and $\hat{Q}_o$, i.e., $|J,Q,M,Q_o\rangle$. The minimum possible value of Q_o is attained when N, the number of particles, is zero and then $Q_o = -\Omega$. The maximum Q_o obtains when $N = 4\Omega$, and then $Q_o = \Omega$. In the Lipkin Model one always has $N = 2\Omega$ and $Q_o = 0$.

Let us now consider the general multiplet $|Q,Q_o\rangle$. The eigenvalues of $\hat{Q}_o$ will depend only on the particle-number, which for given Q varies, according to (7) between

$$N_{MIN}\,(Q_o = -Q) = 2\Omega - 2Q \tag{8}$$

and

$$N_{MAX}\ (Q_o = Q) \;=\; 2\Omega + 2Q\,. \tag{9}$$

We can define a "seniority" quantum number v, which can be referred to as a q.s. seniority, as

$$v \;=\; N_{MIN}\ (Q_o = -Q)\,, \tag{10}$$

which indicates the number of particles not "paired" to M = 0, since

$$\hat{Q}_-\ |\,Q, -Q\,\rangle \equiv 0\,, \tag{11}$$

and so, v is the number of "unpaired" particles in a Q_- multiplet. From (8)

$$Q \;=\; \frac{1}{2}\,(2\Omega - v)\,. \tag{12}$$

Now, if for a given pair J, Q we have v unpaired particles, the minimum possible value for $\hat{J}_Z$ in this (J,Q)-multiplet is equal to -v/2. Consequently, the q.s. seniority fixes also the value of J:

$$J \;=\; v/2\,, \tag{13}$$

$$J + Q \;=\; \Omega\,. \tag{14}$$

So that the states pertaining to the above mentioned SU2 × SU2 multiplets are characterized by just three quantum numbers: v, Q_o and M.

In the case of the Lipkin Model (N = 2Ω), the u.g.s. has J = Ω, M = -Ω and Q = Q_o = 0. In the u.g.s. multiplet, only M varies, from -Ω to +Ω. For this multiplet v equals 2Ω. The remaining multiplets in the Lipkin Model can easily be characterized with the help of the q.s. seniority concept, since for them v decreases from its maximum value down to zero in steps of two.

This seniority classification of the different multiplets of the Lipkin Model constitutes one of the main advantages gained by the introduction of the operators $\hat{Q}$. Another is that, by allowing Q_o to vary, we can generalize the model to a variable number of particles.

Another interesting set of q.s. operators is the following[4]:

$$\hat{S}_+ = \hat{S}_-^\dagger = \sum_p c^\dagger_{p,+}\, c_{2\Omega-p+1,-}$$

$$\hat{S}_Z = \hat{J}_Z \,. \tag{15}$$

The $\hat{S}$-operators commute among themselves like angular momentum ones. If one wants to work simultaneously with these $\hat{S}$-operators and the above mentioned $\hat{J}$-ones, it is necessary to introduce

$$\hat{U} = \frac{1}{2} \sum_\mu \mu\, c^\dagger_{p,\mu}\, c_{2\Omega-p+1,\mu} \,, \tag{16}$$

in order to close the algebra. Besides, it is very useful to define

$$\begin{aligned}
\hat{V}_+ &= \hat{V}_-^\dagger = \frac{1}{2}(\hat{J}_+ + \hat{S}_+) \,, \\
\hat{W}_+ &= \hat{W}_-^\dagger = \frac{1}{2}(\hat{J}_+ - \hat{S}_+) \,, \\
\hat{V}_Z &= \frac{1}{2}(\hat{J}_Z + \hat{U}) \,, \\
\hat{W}_Z &= \frac{1}{2}(\hat{J}_Z - \hat{U}) \,,
\end{aligned} \tag{17}$$

obtaining two additional commuting q.s. sets, the $\hat{V}_-$ and the $\hat{W}_-$ operators (SU2 × SU2).

III. THE HARTREE-FOCK APPROXIMATION

In the case of the models discussed here, the HF approach is both elegant and transparent in its application.

The Lipkin Model is particularly relevant to the mixed-parity, HF treatment of nuclei by Bleuler et al.[5] One can consider the $\mu = \pm 1$ shells as representing subshells in the jj-coupling nuclear shell model having the same value of j and opposite parity. Whenever states have the same value of the quantum number p and opposite values of the shell quantum number, they must have opposite parity. The hamiltonian (4) conserves parity as the interaction always involves a simultaneous change in parity of two particles. The parity operator can be defined formally in terms of q.s. operators as a 180° rotation about the Z-axis

in q.s. space[6],

$$\hat{\Pi} = e^{i\Pi\hat{J}_Z} e^{i\phi} \quad , \tag{18}$$

where the choice of the phase factor $e^{i\phi}$ does not affect any physical result. Moreover, any hamiltonian built up with the operators $\hat{J}_+$, $\hat{J}_-$ and $\hat{J}_Z$ will commute with $\hat{J}^2$ and with the operators

$$\hat{n}_p = \sum_p c^{\dagger}_{p,\mu} c_{p,\mu} \quad , \tag{19}$$

defined for all values of p.

In searching for the HF solution one tries to retain in it as many symmetries as possible. For the hamiltonian (4) there exists a HF solution which conserves all symmetries, being an eigenstate of $\hat{J}^2$, of $\hat{\Pi}$ and of all $\hat{n}_p$. This is the u.g.s. (clearly a HF solution since the interaction term can produce only two-particle excitations on this state). Other solutions will violate some of these symmetries, and people have concentrated mostly on those which violate parity conservation. Such HF states are called "deformed" ones by Agassi, Lipkin and Meshkov[6]. The requirement that a trial function remains an eigenfunction of $\hat{n}_p$ restricts it to a very simple form. One needs only to consider s.p. states obtained by mixing a particular state having a given value of the quantum numbers p and μ with its partner in the other shell having the same p-value and opposite μ. A mixing of these two states corresponds simply to a rotation in q.s. space. The HF approach consists then in looking for the zero particle-zero hole (0p-0h) wave function in the rotated frame. The corresponding angle is that which will minimize the expectation value of a given hamiltonian, built up with the $\hat{J}$-operators, with respect to this wave function.

We define thus a "self-consistent" representation "a", in which the basis and the s.p. states are connected by the unitary transformation

$$\begin{pmatrix} a_{p,-} \\ a_{p,+} \end{pmatrix} = \begin{pmatrix} \cos\frac{\beta}{2} & -i\sin\frac{\beta}{2} \\ -i\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} \begin{pmatrix} c_{p,-} \\ c_{p,+} \end{pmatrix} . \tag{20}$$

The inverse transformation reads

$$\begin{pmatrix} c_{p,-} \\ c_{p,+} \end{pmatrix} = \begin{pmatrix} \cos\frac{\beta}{2} & i\sin\frac{\beta}{2} \\ i\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} \begin{pmatrix} a_{p,-} \\ a_{p,+} \end{pmatrix} , \tag{21}$$

and allows us to relate the $\hat{J}$-operators in the old basis to those in the new one:

$$\begin{aligned} \hat{J}_x(c) &= \frac{1}{2}\left[\hat{J}_+(c) + \hat{J}_-(c)\right] = \hat{J}_x(a) , \\ \hat{J}_y(c) &= \frac{i}{2}\left[\hat{J}_-(c) - \hat{J}_+(c)\right] = \cos\beta\ \hat{J}_y(a) - \sin\beta\ \hat{J}_z(a) , \\ \hat{J}_z(c) &= \cos\beta\ \hat{J}_z(a) + \sin\beta\ \hat{J}_y(a) . \end{aligned} \tag{22}$$

In q.s. space this corresponds to

$$\begin{aligned} |\, c \,\rangle &= R(-\beta)\,|\, a \,\rangle , \\ |\, a \,\rangle &= R(\beta)\,|\, c \,\rangle , \end{aligned} \tag{23}$$

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

Since the HF state will be the Op-Oh state in the "a"-representation, it wil have the form[7]

$$\begin{aligned} |0,a\rangle \equiv |\, J,-J,a \,\rangle &= R(\beta)\,|\, 0,c \,\rangle \\ &= \sum_M |M,c\rangle\langle M,c\,|\,R(\beta)\,|\,0,c\,\rangle = \sum_{M=-J}^{J} d^J_{M,-J}(\beta)\,|\, M,c \,\rangle , \end{aligned} \tag{24}$$

where $|M,c\rangle = |J,M,c\rangle$. The functions d are defined by Edmonds[8], although the phase convention (21) requires the replacement of his $\sin\frac{\beta}{2}$ by $i\sin\frac{\beta}{2}$[7]. The absolute squares of the amplitudes in (24) represent a binomial distribution, as found by Agassi et al.[6].

We see that the dynamics of the problem will determine β, but for any hamiltonian that we may construct with the q.s. operators $\hat{J}$, the

structure of the HF state will be that given by (24).

Notice, that the rotation (21) preserves the form of the operators $\hat{Q}$ defined in Eq. (7).

Finally, if one builds up a hamiltonian with the $\hat{V}$- and $\hat{W}$-operators of (17), it is not sufficient to perform a rotation which mixes the $|\, p,\mu\,\rangle$ state with the $|\, p,-\mu\,\rangle$ one, as (21) does. Looking at the definition of the $\hat{S}$-operators, Eq. (15), it is clear that one must also mix the s.p. orbital $|\, p,\mu\rangle$ with $|2\Omega-p+1,-\mu\,\rangle$. This is conveniently done in two steps, i.e., one performs the two successive rotations

$$\begin{pmatrix} c_{2\Omega-p+1,-} \\ c_{p,+} \end{pmatrix} = \begin{pmatrix} \cos\frac{\beta}{2} & -i\sin\frac{\beta}{2} \\ -i\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} \begin{pmatrix} a_{2\Omega-p+1,-} \\ a_{p,+} \end{pmatrix} \tag{25}$$

and

$$\begin{pmatrix} a_{p,-} \\ a_{p,+} \end{pmatrix} = \begin{pmatrix} \cos\frac{\alpha}{2} & -i\sin\frac{\alpha}{2} \\ -i\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{pmatrix} \begin{pmatrix} b_{p,-} \\ b_{p,+} \end{pmatrix} . \tag{26}$$

As a result of (25) and (26) both the V-q.s. and W-one rotate around the x-axis, the former in an angle $(\alpha+\beta)$, the latter acording to $(\alpha-\beta)$.

IV. SPIN-FLIP MODEL

In order to obtain the exact solution corresponding to the hamiltonian (4), it is necessary to diagonalize it. A simpler hamiltonian, a special case of the Lipkin Model, has been studied by Plastino and Moszkowski[9], for which both the exact many-body problem and the HF one can be solved analytically. We shall consider it as our first application. The hamiltonian reads[9]

$$\hat{H}_{PM} = \varepsilon \hat{J}_Z - K\left[\frac{1}{2}\left(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+\right) - \text{"forward scattering" terms}\right]. \tag{27}$$

It is easily seen that a "spin-flip" interaction, i.e., one

that only exchanges the p-quantum number (p-spin) of the interacting particles is given by (27), where one just substracts the diagonal elements from the combination $\frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+)$. The term to be substracted, let us denote it by $\hat{\Gamma}$, has the form

$$\hat{\Gamma} = \frac{1}{2}\hat{N}\quad\hat{\phi}\ , \tag{28}$$

where $\hat{\phi}$ is a two-body operator which commutes with both $\hat{J}^2$ and $\hat{J}_Z$. Now

$$|\hat{H}_{PM}, \hat{J}^2| = |\hat{H}_{PM}, \hat{J}_Z| = 0\ , \tag{29}$$

so that the exact ground-state solution will be that one, belonging to the multiplet $J = N/2$, whose $\hat{J}_Z$-value is such that the energy is a minimum. This value depends upon the strength of the interaction, as will be seen below.

The u.g.s. is $|J = \frac{N}{2}\ ,\ M = -\frac{N}{2}\rangle$. Within this J-multiplet th operator $\hat{\phi}$ always yields zero:

$$\hat{\phi}\ |\ J = \frac{N}{2}\ ,\ M\rangle \equiv 0\ , \tag{30}$$

so we shall forget it in what follows. Setting $\varepsilon = 1 (k = K/\varepsilon)$ we rewrite (27) as

$$\hat{H}_{PM} = \hat{J}_Z - k\left(\hat{J}^2 - \hat{J}_Z^2 - \frac{1}{2}\hat{N}\right)\ . \tag{31}$$

For $k = 0$ the ground state energy is $E_0 = -\frac{N}{2}$. If we switch on the interaction and let k grow, the u.g.s. will become unstable when the expression (31), for $M = -\frac{N}{2} + 1$, is smaller than $-\frac{N}{2}$. This happens for $k = 1/(N-1)$. At this value, the quantum number M of the interacting ground state jumps from $-N/2$ to $(-N/2 + 1)$. This latter value will again become unstable as k continues growing, and so on. One gets several "phase transitions" in M until the value zero for the eigenvalue of $\hat{J}_Z$ is attained. The "phase transition" between $M = -n$ and $M = (-n+1)$ occurs at

$$k = \frac{1}{2n - 1}\ . \tag{32}$$

In particular, for n=1 we get k=1 as the critical coupling constant for which the ground state of the interacting system reaches M=0, a critical value which is independent of N. The ground state energy for $k > 1$ is given by

$$E(M=0) = -kN^2/4. \tag{33}$$

In order to use the HF theory we perform the transformation (20) and, with the help of (22), obtain

$$\langle HF \mid \hat{H}_{PM} \mid HF \rangle \equiv \langle H \rangle = \frac{N}{2}\left[-\cos\beta - \frac{k}{2}(N-1)\sin^2\beta\right], \tag{34}$$

and

$$\frac{\partial\langle H\rangle}{\partial\beta} = \frac{N}{2}\left[\sin\beta - k(N-1)\sin\beta\cos\beta\right]. \tag{35}$$

The angle β which minimizes $\langle H \rangle$ may then adopt the values

$$\left.\begin{aligned} &\beta = 0 \quad \text{(trivial solution)}, \\ &\cos\beta = \frac{1}{k(n-1)} \quad \left(\text{for } k > \frac{1}{N-1}\right) \end{aligned}\right\}. \tag{36}$$

We see that the HF theory predicts a phase transition exactly at the point where the Schrödinger solution exhibits one. However, the remaining phase transitions [see Eq. (32)] are not seen within the HF framework. The HF energy is, for k larger than $(N-1)^{-1}$,

$$E_{HF} = \frac{N}{4}\left(-k(N-1) - \frac{1}{k(N-1)}\right), \tag{37}$$

which for $k \gg 1$ and N finite not necessarily too large

$$E_{HF} \approx -\frac{k}{4}N(N-1). \tag{38}$$

Comparing (37) or (38) with (33) one sees that $E_{HF}/E_{exact} \to 1$ as $N \to \infty$, i.e., the HF approximation is exact in the thermodynamical limit.

V. THE LIPKIN HAMILTONIAN AND HF THEORY

We return now to the hamiltonian (4) and treat it within the HF framework. Equation (22) yields[6]

$$\langle \text{HF} \mid \hat{H}_L \mid \text{HF} \rangle = -\varepsilon J \{\cos\beta + k(J-1/2)\,(1-\cos^2\beta)\} \,. \quad (39)$$

The HF solution is obtained by choosing β to minimize the expectation value (39). Setting $\varepsilon=1$ as before, we obtain two solutions:

a) for $k(N-1) \leq 1$

$$\beta = 0 \,, \quad E_{HF} = -\frac{N}{2} \,; \quad (40)$$

b) for $k(N-1) > 1$

$$\cos\beta = \frac{1}{k(N-1)} \,, \quad E_{HF} = \frac{N}{4}\left[-k(N-1) - \frac{1}{k(N-1)}\right]. \quad (41)$$

Comparing with (36) and (37) we see that the HF treatment of $\hat{H}_L$ predicts a phase transition at the same value of k than in the spin-flip case. Moreover, the analytical expression for the HF energy is identical in both cases.

However, the phase transitions that appear in both models are actually very different. In the Lipkin Model, when one studies the problem for a finite number of particles, one finds a critical coupling constant in the HF approach, but not in the exact solution. In the thermodynamical limit ($N \to \infty$), instead, the exact ground-state energy presents a second-order phase transition. In the spin-flip model one obtains a set of critical coupling constants in the exact solution, even for finite N. But they correspond to first-order phase transitions which are, indeed, level crossings. This means that when the coupling constant reaches a critical value, the energies of two different levels become equal so that before the phase transition the ground state is given by one of these levels and after it, by the other one. In the HF approach, only the first of these critical coupling constants is obtained.

The hamiltonian $\hat{H}_L$ has the drawback (from the HF viewpoint) of producing only two particle - two hole excitations. The u.g.s. therefore is already the HF state and only for not too small values of the inter-

action constant the unperturbed solution becomes unstable. It is desirable to have a model which yields for all values of the coupling constant a non-trivial HF solution in order to clarify this point. This will be considered in the next section. In the spin-flip model, although we do have a trivial HF solution, this coincides with the exact one, so that, when the u.g.s. becomes unstable this is because the exact eigenstate with $M=-N/2$, which represented the ground state before the phase transition, becomes now one of the excited states of the system.

VI. THE AFP MODEL

A model with the characteristics required at the end of the preceding section has been introduced by Abecasis, Faessler and Plastino[10]. The corresponding hamiltonian is

$$\begin{aligned}\hat{H}_{AFP} &= \frac{\varepsilon}{2}\sum_{p,\mu}\mu\, c^{\dagger}_{p,\mu}\, c_{p,\mu} + \frac{K}{2}\sum_{p,\mu,\nu}\nu\; c_{p,\nu}\sum_{q,\sigma,\tau}\sigma\, c^{\dagger}_{q,\sigma}\, c_{q,\tau} \\ &= \varepsilon\hat{J}_Z + \frac{K}{2}\{2\hat{J}^2 + 2\hat{J}_Z^2 + 2\hat{J}_Z(\hat{J}_+ - \hat{J}_-) + 2(-\hat{J}_+ + \hat{J}_-)\hat{J}_Z - \hat{J}_-^2 - \hat{J}_+^2\} \\ &= \varepsilon\hat{J}_Z + 2K\{\hat{J}_y^2 + \hat{J}_Z^2 + \hat{J}_x^2\}\,. \end{aligned} \tag{42}$$

In this case it is convenient to perform the HF transformation with a different phase than that of Eq. (20), namely,

$$\begin{pmatrix} a^{\dagger}_{p,-} \\ a^{\dagger}_{p,+} \end{pmatrix} = \begin{pmatrix} \cos\frac{\beta}{2} & \sin\frac{\beta}{2} \\ -\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} \begin{pmatrix} c^{\dagger}_{p,-} \\ c^{\dagger}_{p,+} \end{pmatrix}. \tag{43}$$

The s.p. transformation (43) corresponds in q.s.-space to the following rotation:

$$\begin{aligned} \hat{J}_x(c) &= \cos\beta\;\hat{J}_x(a) - \sin\beta\;\hat{J}_Z(a)\,, \\ \hat{J}_y(c) &= \hat{J}_y(a)\,, \\ \hat{J}_Z(c) &= \cos\beta\;\hat{J}_Z(a) + \sin\beta\;\hat{J}_x(a)\,. \end{aligned} \tag{44}$$

With Eqs. (43) and (44) we obtain (ε=1)

$$\langle HF \mid \hat{H}_{AFP} \mid HF \rangle = -J \cos\beta + k J \{2J \cos^2\beta + 1 + \sin^2\beta + 2\sin\beta\}, \tag{45}$$

where the angle β is found by solving the equation

$$2k\{(N-1)\cos\beta - \operatorname{cotg}\beta\} = 1 \quad . \tag{46}$$

The HF energies are quite close to the exact ones[10] and the overlap $\langle EXACT|HF \rangle$ is always greater than 95%[10].

Possible phase transitions are not so clearly seen in this model as in the previous ones because neither the exact solution nor the HF are analytical. But plotting the ground-state energy versus the coupling constant it can be seen that there is a critical value for which the curvature of the function changes[11].

VII. Q.S. PAIRING PLUS MONOPOLE MODEL

We turn now our attention to the q.s. pairing plus monopole interaction studied in Ref. 2,

$$\hat{H} = \hat{J}_Z + \frac{k}{2}(\hat{J}_+^2 + \hat{J}_-^2) - \frac{g}{2}\hat{Q}_+ \hat{Q}_- \quad , \tag{47}$$

where we have set ε=1 and g is a positive coupling constant. As shown in Ref. 2, the last term in (47) has all the properties of the pairing interaction that plays a fundamental role in nuclear structure description[3].

In (47) we have two competing interactions, which act in different ways. On the one hand, the term $\hat{Q}_+ \hat{Q}_-$ favors states with J=0. As a matter of fact, for a hamiltonian of the form

$$\hat{H}_p = \hat{J}_Z - \frac{g}{2}\hat{Q}_+ \hat{Q}_- \quad , \tag{48}$$

the ground state will be $|J=0, \; M=0, \; Q=\Omega, \; Q_0=0\rangle$ for

$$g \geq \frac{4\Omega}{N}\left(2\Omega - \frac{N}{2} + 1\right)^{-1} \quad \text{(see Ref. 2)}.$$

The monopole force $\hat{J}_+^2 + \hat{J}_-^2$, instead, acts in such a way that the system tries to attain the maximum possible value of J. We are thus reminded of the competition between pairing and deformation in atomic nuclei[12].

The exact solution if found by diagonalizing $\hat{H}$ in the basis $|J, M, Q, Q_0 = 0\rangle$ and it should be remembered that the hamiltonian commutes both with $\hat{J}^2$ and $\hat{Q}^2$. It is found in Ref. 2 that if one varies g for a fixed value of k, the ground state of the system, which is always characterized by $J = \Omega$ for g sufficiently small, jumps abruptly to $J = 0$ at a given critical value of g. We have thus a phase transition from a "normal" to a "superconducting" phase. The system can be in its ground state only in one of these states ($J = \Omega$ or $J = 0$), according to the relative values of g and k (see Fig. 2 in Ref. 2).

In considering the present model from the point of view of the HF approach, a new feature makes its appearance: the abnormally occupied HF solution[13]. Within our context, this means that, after performing the transformation (20), the corresponding trial states are obtained by building up in the new basis "a" the Slater determinants $|J,M = -J,Q = \Omega - J,Q_0 = 0\rangle$. The novel feature referred to above consists in the fact that the J-value corresponding to the u.g.s. ($J=\Omega$) will not necessarily yield the lowest energy: other "abnormal" J-values may give lower energy.

Notice that the operators $\hat{Q}_+$ and $\hat{Q}_-$ are invariant under the transformation (21). After writing down $\hat{H}$ in terms of the operators "a" one obtains[2]

$$\langle HF|\hat{H}|HF\rangle = -J\cos\beta + \frac{k}{2}(1-2J)J\sin^2\beta - \frac{g}{2}(\Omega-J)(\Omega-J+1)\,, \tag{49}$$

which is to be minimized with respect to β. Two solutions exist:

a) for $k(2J-1) \leq 1$

$$\beta = 0, \quad E_{HF} = -J - \frac{g}{2}(\Omega-J)(\Omega-J+1)\,, \tag{50}$$

b) for larger values of the monopole coupling constant

$k(2J-1) > 1$ one gets

$$\cos\beta = \frac{1}{k(2j-1)} \equiv b^{-1} ,$$

$$E_{HF} = -\frac{J}{b}\frac{bJ}{2}\left(1-\frac{1}{b^2}\right) - \frac{g}{2}(\Omega - J)(\Omega - J + 1) \qquad (51)$$

The pairing force does not contribute to E_{HF} for $J = \Omega$. On the other hand, for $J = 0$, the monopole HF contribution is null.

The important point to be remarked here is that the transition between the "normal" and "superconducting" phases is fairly well predicted by the HF approach, i.e. the values of the corresponding "critical" coupling constants are similar both in the exact and in the HF treatment. On the other hand, the numerical value for the ground state energy may appreciably differ in both approaches[2].

VIII. SU2 × SU2 MODEL

An SU2 × SU2 model built up with the $\hat{V}$- and the $\hat{W}$-operators defined in section II, has been proposed by Cambiaggio and Plastino[4].

The hamiltonian reads

$$\hat{H}_s = \frac{\varepsilon}{2}\sum_{p,\mu}\mu\, c^{\dagger}_{p,\mu}\, c_{p,\mu} + \frac{k}{2}\left[\frac{1}{8}\sum_{p,q,\sigma,\tau}\sigma\,\tau\, c^{\dagger}_{p,\sigma}\, c^{\dagger}_{q,\tau}\,[c_{q,\tau}\, c_{p,\sigma} - c_{2\Omega-q+1,\tau} c_{2\Omega-p+1,\sigma}]\right.$$

$$\left. + \frac{1}{4}\sum_{p,q,\mu} c^{\dagger}_{p,\mu}\, c^{\dagger}_{q,-\mu}\,(c_{q,\mu}\, c_{p,-\mu} - c_{2\Omega-q+1,\mu}\, c_{2\Omega-p+1,-\mu})\right]$$

$$= \varepsilon\,\hat{J}_Z + \frac{K}{2}(2\hat{V}_Z\,\hat{W}_Z + \hat{W}_+\,\hat{V}_- + \hat{W}_-\,\hat{V}_+). \qquad (52)$$

Since $\hat{H}_s$ commutes both with $\hat{V}^2$ and $\hat{W}^2$, exact solutions are obtained by diagonalization within a given multiplet $|V, W, W_z, W_Z\rangle$. The u.g.s. is

$$|\text{u.g.s.}\rangle = |V = W = N/4,\ V_z = W_Z = -N/4\rangle . \qquad (53)$$

So, the exact ground state must be a linear combination of states pertaining to the multiplet V=W=N/4. Moreover, as $\hat{H}_s$ also commutes with $\hat{J}^2$, we can label the exact solutions with the q.s. J and write down the energy explicitly as

$$E_{J,N}\ (V=W=N/4) \ = \ - \ J \ + \ \frac{k}{2}\left[J(J+1) \ - \ 2W(W+1) \right] \ , \qquad (54)$$

with $J \leq N/2$ and $k = K/\varepsilon$ (we have taken $\varepsilon = 1$).

Studying the energy difference between two states of different J one finds a set of critical coupling constants $k_J = 1/J$. At $k = k_J$, the Lipkin q.s. of the ground state changes. So, the ground state of the system, which for k = 0 possesses the maximum possible J compatible with N, will run downward in J as k grows, passing through all possible values until it reaches J = 0 at k = 1.

In order to find the HF solutions for this model one performs the two successive transformations (25) and (26), and then determines α and β minimizing the expectation value of the hamiltonian with respect to the new (Op-Oh) state.

The HF solutions are two:

a) for $k\,\frac{N}{2} \leq 1$,

$$\alpha = \beta = 0 \ , \qquad E_{HF} = - \frac{N}{2}\left(1 - \frac{kN}{8} \right) ; \qquad (55)$$

b) for $k\,\frac{N}{2} \quad 1$,

$$\alpha = 0, \quad \beta = \arccos\left(\frac{2}{kN} \right) \ , \quad E_{HF} = - \frac{1}{2k} - \frac{kN^2}{16} \ . \qquad (56)$$

It has been shown that these HF solutions are obtained, even if one uses a more general trnsformation[14].

For small enough values of the interaction strength, the HF solution matches the exact one. Then, a phase transition is reached at a coupling constant which corresponds to the first critical value found in the exact solution. It is to be noted that the situation is similar to the one encountered in the spin-flip case of section IV. Both models present several first-order phase transitions which are actually level

crossings, as discussed in section V. In addition, HF theory "detects" only the first of these phase transitions.

IX. CONCLUSION

We have compared HF results to exact ones for different models whose main characteristic is that such exact solutions can be found without great trouble.

We have interested ourselves in answering the question: Can the HF approach reasonably predict qualitative features of many-body interacting systems, i.e., more specifically, phase transitions or level crossings?

The answer can be in the affirmative but not without reserves. It has been seen that in cases where several transitions existed, only one was predicted within the HF framework. The one transition "seen" by the selfconsistent approach is always the first one, i.e., that one occurring at the lowest possible critical constant.

Notice also that in all these models this first transition can always be associated with a radical departure from the properties associated with the u.g.s.

One may thus tentatively conclude that the HF theory is able to detect the passage from a "gas-like" state (as represented by the u.g.s.) to a "liquid-like" one. For larger values of the interaction strength, the one-body approach loses validity, as expected, and is no longer able to detect additional transitions.

Since HF theory is one of our main tools for trying to unravel the intricacies of the quantum many-body problem, probably more effort along the lines exposed in this review would be of some interest.

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