Thermal effects and the interplay between pairing and shape deformations

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The interplay between pairing and shape deformations at finite temperatures is studied with reference to an exactly soluble SU(2)×SU(2) model which is able to suitably mock up both superconductivity and the effects of long-range residual forces. Thermodynamic and ground state phase transitions are studied, both in the thermodynamic limit and in the case of a finite number of particles. Several independent quasiparticle approximations are analyzed with reference to the corresponding exact results.

I. INTRODUCTION

Thermal or statistical descriptions of nuclear systems have become quite frequent in the literature during the last decade, strongly motivated by the availability of experimental information concerning heavy-ion reactions (see, for example, Ref. 1). The sheer complexity of the problem has prompted the study of simple models (as, for instance, Refs. 2 and 3), and, from the theoretical point of view, much light has been shed on the intricacies of the nuclear many-body problem by studying the general properties and peculiarities of pseudospin Hamiltonians of the Lipkin type.[4,5]

In this sense, recourse to the formidable weaponry of atomic coherent states has provided a rather clear picture of several thermodynamic phase transitions that take place within the scope of these models.[4–11]

It is the aim of this paper to study, within the framework of an exactly soluble model, the interplay between thermal effects and two of the crucial ingredients of the nuclear many body problem, namely, superconductivity and deformation due to long-range residual forces. To this end, a suitable generalization of the thermal approach of Gilmore and Feng[7] is proposed, which allows one to apply their methodology to an SU(2)×SU(2) extension of the original Lipkin model.[4] The extended model[12] is able to mock up the interplay between pairing and shape deformations,[13–16] and allows thus for the introduction of thermal effects in a simple fashion. In this way, different independent quasiparticle approximations [thermal Bardeen-Cooper-Schrieffer (BCS), thermal Hartree-Fock-Bogoliubov] can be compared to exact results, at any temperature T, both in the thermodynamic limit and in the case of a finite number of particles.

The results obtained in this paper allow one to gain some insight into the machinery that underlies a significant amount of the work performed over the years in relation to the nuclear many-body problem, which, undoubtedly, revolves about the mean field approach. In other words, we deal here with a basic aspect of nuclear theory: that of describing the independent motion of an appropriately defined quasiparticle in *some* field (contributed to by other quasiparticles), and we study features of such an independent particle motion that arise as a consequence of temperature-related effects, showing that a special type of theoretical tool (atomic coherent states) can be advantageously employed.

The paper is organized as follows: the extended SU(2)×SU(2) model is described in Sec. II and exact free energies are discussed in Sec. III. The thermal BCS approximation is studied in Sec. IV, while both the thermal Hartree-Fock and the thermal Hartree-Fock-Bogoliubov approaches are dealt with in Sec. V. Some conclusions are drawn in Sec. VI.

II. DESCRIPTION OF THE MODEL

The model deals with N fermions distributed in two (2Ω)-fold degenerate single-particle (sp) levels, separated by the sp energy ϵ. Two quantum numbers characterize a given sp state. One of them adopts the values $\mu=-1$ (lower level) and $\mu=+1$ (upper level). The other, which may be called "p spin," singles out a state within the (2Ω)-fold degeneracy. Within this context one introduces Lipkin's quasispin operators[4]

$$\begin{aligned}
&\hat{J}_+=\hat{J}^\dagger_-=\sum_{p=1}^{2\Omega} C^\dagger_{p+}C_{p-}\ ,\\
&\hat{J}_z=\tfrac{1}{2}\sum_{p\mu}\mu C^\dagger_{p\mu}C_{p\mu}\ ,\\
&\hat{J}^2=\hat{J}_z^2+\tfrac{1}{2}(\hat{J}_+\hat{J}_-+\hat{J}_-\hat{J}_+)\ ,
\end{aligned}\tag{2.1}$$

and the corresponding SU(2) algebra. We shall denote with M the eigenvalues of $\hat{J}_z$ and with $J(J+1)$ the ones of $\hat{J}^2$. Further, we introduce some additional operators of the type (2.1), which, following Cambiaggio *et al.*,[12] we shall call quasispin pairing (qsp) operators. They are

$$\begin{aligned}
&\hat{Q}_+=\hat{Q}^\dagger_-=\sum_p C^\dagger_{p,+}C^\dagger_{p,-}\ ,\\
&\hat{Q}_0=\tfrac{1}{2}\sum_{p,\mu}C^\dagger_{p\mu}C_{p\mu}-\Omega=\tfrac{1}{2}\hat{N}-\Omega\ ,\\
&\hat{Q}^2=\hat{Q}_0^2+\tfrac{1}{2}(\hat{Q}_+\hat{Q}_-+\hat{Q}_-\hat{Q}_+)\ ,
\end{aligned}\tag{2.2}$$

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 the $\hat{J}$ operators [SU(2)×SU(2)]. Obviously, $\hat{Q}_+$ creates (and $\hat{Q}_-$ destroys) two particles which yield zero contribution to the M value, and which could then be said to "couple" to $M=0$ and $J=0$. Thus, the $\hat{Q}$ operators behave (formally) in the same way as the pairing ones of the theory of nuclear superconductivity.[2,3] We shall denote by Q_0 the eigenvalues of $\hat{Q}_0$ and by $Q(Q+1)$ the ones of $\hat{Q}^2$.

We are thus led to consider an extended [SU(2)×SU(2)] "Lipkin-like" Hilbert space of dimension

$$D=\begin{bmatrix} 4\Omega \\ N \end{bmatrix} , \tag{2.3}$$

as one deals with N undistinguishable particles that have to be "distributed" among 4Ω sp states. These states can be characterized by the eigenvalues J,Q,Q_0,M, although there exists yet a further symmetry to be accounted for, as every $\hat{Q}$ or $\hat{J}$ operator commutes with any of the $(2\Omega)!$ permutation operators that exchange two given p spins.[8]

This additional symmetry gives rise to a certain multiplicity $Y(J,Q)$ for a given $|J,Q,M,Q_0\rangle$ state. In order to label the members of that irreducible representation of the permutation group (for 2Ω objects) to which $|J,Q,M,Q_0\rangle$ belongs, one additional quantum number is needed. However, given the structure of the Hamiltonians to be studied in this work, no physical quantity will actually depend upon this extra-quantum number.

It is shown in the Appendix that the above referred to multiplicity is given by

$$Y(J,Q)=\frac{(2\Omega+2)!(2\Omega)!(2J+1)(2\Omega+1)}{(\Omega+J+Q+2)!(\Omega+J-Q+1)!(\Omega-J+Q+1)!(\Omega-J-Q)!} , \tag{2.4}$$

where the possible values of J and Q are constrained by the relationships

$$\begin{aligned} &0\le J\le \Omega-|Q_0| , \\ &|Q_0|\le Q\le \Omega , \\ &|Q_0|\le J+Q\le \Omega . \end{aligned} \tag{2.5}$$

In studying ground states,[12] only the $J+Q=\Omega$ "band" needs to be considered. However, as soon as the temperature ceases to be zero, a host of states belonging to other bands will become "accessible"[17] as one endeavors to construct the corresponding statistical ensemble.

A useful concept is that of quasispin seniority, defined as[12]

$$v=2\Omega-2Q , \tag{2.6}$$

which indicates the *maximum* possible number of "unpaired" particles compatible with a given value of Q.

Two different Hamiltonians will be considered in this work. The first is a pure qsp Hamiltonian

$$\hat{H}=\epsilon\hat{J}_z-\frac{G}{2}\hat{Q}_+\hat{Q}_- ,\quad G>0 , \tag{2.7}$$

which mocks up the effects of a typical pairing force.[12]

The other one is of the form

$$\hat{H}=\epsilon\hat{J}_z-\frac{G}{2}\hat{Q}_+\hat{Q}_-+\frac{V}{2}(\hat{J}_+^2+\hat{J}_-^2) , \tag{2.8}$$

i.e., a monopole force[4] is added to (2.7), so as to mock up now the interplay between pairing and shape deformations.[13–16]

III. FREE ENERGIES

As the Hamiltonians (2.7) and (2.8) commute both with $\hat{J}^2$ and with $\hat{Q}^2$, the exact free energy at a given temperature T can be easily computed by recourse to

$$\begin{aligned} F&=-kT\ln \mathrm{Tr}(e^{-\beta\hat{H}}) \\ &=-kT\ln \sum_{J,Q} Y(J,Q)\mathrm{Tr}'e^{-\beta\hat{H}} , \end{aligned} \tag{3.1}$$

where k is Boltzmann's constant, $\beta=1/kT$, and Tr′ is the trace over that subspace characterized by J and Q. For the Hamiltonian (2.7) this reads

$$\mathrm{Tr}'e^{-\beta\hat{H}}=\sum_{M=-J}^{J}\exp\left[-\beta\left\{\epsilon M-\frac{G}{2}[Q(Q+1)-Q_0(Q_0-1)]\right\}\right] . \tag{3.2}$$

It will be useful later on to consider the thermodynamic limit of (3.1), that is, the situation in which $(2\Omega)\to\infty$ with N proportional to Ω. For this limit to exist, the coupling constants must satisfy the (scaling) condition

$$\begin{aligned} G&=\frac{g}{2\Omega},\quad g \text{ finite} , \\ V&=\frac{v}{2\Omega},\quad v \text{ finite} . \end{aligned} \tag{3.3}$$

Thermodynamic limits within the context of the Lipkin model[4] have been carefully studied by Gilmore and Feng.[7] We shall here endeavor to investigate the "BCS-like" aspects of them.

Let us introduce the quantities

$$\begin{aligned} q&=\frac{Q}{2\Omega} , \\ r&=\frac{J}{2\Omega} , \end{aligned} \tag{3.4}$$

which are to be regarded as continuous in the thermodynamic limit, and subject to the restrictions [cf. Eq. (2.5)]

$$\begin{aligned} &0<r<\tfrac{1}{2}-q_0 ,\\ &q_0<q<\tfrac{1}{2} ,\\ &q_0<r+q<\tfrac{1}{2} , \end{aligned} \tag{3.5}$$

with $q_0=\lim_{2\Omega\to\infty}|Q_0|/2\Omega$. Introducing, additionally, the quantities

$$\begin{aligned} &\phi_1(q,r)=(\tfrac{1}{2}+q+r) ,\\ &\phi_2(q,r)=(\tfrac{1}{2}-q-r) ,\\ &\phi_3(q,r)=(\tfrac{1}{2}+q-r) ,\\ &\phi_4(q,r)=(\tfrac{1}{2}-q+r) , \end{aligned} \tag{3.6}$$

and using Stirling's approximation, we immediately find the "entropy per particle" to be [cf. Eq. (3.14)]

$$s(r,q)=\lim_{2\Omega\to\infty}\frac{\ln Y(J,Q)}{2\Omega}=\sum_{i=1}^{4}\phi_i(r,q)\ln\phi_i(r,q) . \tag{3.7}$$

We shall now employ the formidable weaponry of atomic-coherent states[6–11] in order to obtain some interesting results. Gilmore *et al.* have shown[6–8] that, for a wide variety of pseudospin operators $\hat{O}$ (that are functions of $\hat{J}_+$, $\hat{J}_-$, and $\hat{J}_z$), the following important inequality holds:

$$\frac{1}{(2J+1)}\mathrm{Tr}e^{-\beta\hat{O}}\geq\frac{1}{4\pi}\int\exp\{-\beta\langle J\Omega'|\hat{O}|J\Omega'\rangle\}d\Omega' , \tag{3.8}$$

with equality in the thermodynamic limit. In this relationship $|J\Omega'\rangle$ stands for an atomic-coherent state[6–11] and the trace is to be taken over a subspace of dimension $(2J+1)$. Within the present context, (3.8) translates into

$$\begin{aligned}\frac{1}{(2J+1)}\mathrm{Tr}'e^{-\beta\hat{H}}&=\frac{1}{(2J+1)}\sum_M e^{-\beta E(J,Q,M)}\\ &\geq\frac{1}{4\pi}\int\exp\{-\beta\langle JQ\Omega'|\hat{H}|JQ\Omega'\rangle\}d\Omega' ,\end{aligned} \tag{3.9}$$

where $E(J,Q,M)$ is the Mth eigenvalue of $\hat{H}$ within a given (J,Q) multiplet[12] and $|J,Q,\Omega'\rangle$ refers here to atomic-coherent states in the extended [SU(2)×SU(2)] Hilbert space. In the thermodynamic limit, we can replace sums over J,Q,M by integrals over r,q,Ω', and, by recourse to the saddle-point (or Laplace) method[6–8] we obtain

$$\phi(J,Q,\Omega')=\left\langle J,Q,\Omega'\left|\frac{\hat{H}}{2\Omega}\right|J,Q,\Omega'\right\rangle-kTs(r,q) , \tag{3.10a}$$

$$I_3=\frac{(2\Omega)^3}{4\pi}\int\int\int\exp\{-2\Omega\beta\phi(J,Q,\Omega')\}dr\,dq\,d\Omega' , \tag{3.10b}$$

$$\begin{aligned}f&=\lim_{2\Omega\to\infty}\frac{F}{2\Omega}=-kT\lim_{2\Omega\to\infty}(\ln I_3/2\Omega)\\ &=\min_{r,q,\Omega'}\{h(r,q,\Omega')-kTs(r,q)\}+O\left[\frac{\ln\Omega}{\Omega}\right] ,\end{aligned} \tag{3.10c}$$

where

$$h(r,q,\Omega')=\lim_{2\Omega\to\infty}\left\langle J,Q,\Omega'\left|\frac{\hat{H}}{2\Omega}\right|J,Q,\Omega'\right\rangle . \tag{3.11}$$

For the Hamiltonian (2.7) we easily find

$$\min_{\Omega'}h(r,q,\Omega')=-\epsilon r-\tfrac{1}{2}g(q^2-q_0^2) , \tag{3.12}$$

as[6–8]

$$\min_{\Omega'}\langle J,Q,\Omega'|\hat{H}|J,Q,\Omega'\rangle=\langle J,Q,-J|\hat{H}|J,Q,-J\rangle \tag{3.13}$$

so that we are finally led to

$$f=\min_{r,q}\{-\epsilon r-\tfrac{1}{2}g(q^2-q_0^2)-kTs(r,q)\} , \tag{3.14}$$

which, together with (3.10c) suggests that $s(r,q)$ plays the role of an entropy per particle, or "intensive" entropy.

IV. THE THERMAL BCS SOLUTION

A. Generalities

The finite-temperature BCS (FTBCS) equations have been derived by Goodman,[18] the main idea of the approach being that of suitably approximating $\hat{H}$ in the exponent of the density (or statistical) operator $\hat{\rho}$ (grand canonical ensemble). $\hat{H}$ is replaced there by an independent quasiparticle Hamiltonian.

The starting point is that of introducing quasiparticle operators $a^\dagger_{p\mu}$ (Ref. 12)

$$\begin{aligned}&a^\dagger_{p,\mu}=\cos\gamma C^\dagger_{p,\mu}-\mu\sin\gamma C_{p-\mu} ,\\ &a_{p,-\mu}=\cos\gamma C_{p,-\mu}+\mu\sin\gamma C^\dagger_{p,\mu} ,\end{aligned} \tag{4.1}$$

so as to be in a position to write an approximate density operator of the form

$$\hat{\rho}=K\exp\left\{-\beta\left[H_0+\sum_{p\mu}E_\mu a^\dagger_{p\mu}a_{p\mu}\right]\right\} , \tag{4.2}$$

where K is a normalization constant, H_0 the quasiparticle vacuum, and E_μ the quasiparticle energy (p independent within the present context). The single-quasiparticle density matrix and the corresponding pairing tensor become[18]

$$\begin{aligned}\langle a_{p\mu}^\dagger a_{q\tau}\rangle &= \mathrm{Tr}\left[\hat\rho a_{p\mu}^\dagger a_{q\tau}\right] = t_\mu \delta_{\mu\tau}\delta_{qp} ,\\ \langle a_{p\mu} a_{q\tau}\rangle &= \langle a_{p\mu}^\dagger a_{q\tau}^\dagger\rangle = 0 ,\end{aligned} \tag{4.3}$$

where t_μ is the occupation number

$$t_\mu = [1+\exp(\beta E_\mu)]^{-1} . \tag{4.4}$$

By inversion of (4.1) one obtains, with the aid of (4.3),

$$\langle C_{p\mu}^\dagger C_{q\tau}\rangle = \delta_{pq}\delta_{\mu\tau}[\cos^2\gamma t_\mu + \sin^2\gamma(1-t_{-\mu})] \tag{4.5}$$

and

$$\langle C_{p-}^\dagger C_{p+}^\dagger \rangle = \langle C_{p+} C_{p-}\rangle^* = \sin\gamma\cos\gamma(1-t_+ - t_-) . \tag{4.6}$$

For a system of independent quasiparticles the entropy attains the form

$$\begin{aligned} S &= -k\,\mathrm{Tr}\hat\rho\ln\hat\rho \\ &= -2\Omega k \sum_\mu [t_\mu \ln t_\mu + (1-t_\mu)\ln(1-t_\mu)] . \end{aligned} \tag{4.7}$$

According to the FTBCS methodology, one should now minimize the free energy with respect to both the angle γ and the occupation number t_μ,

$$F = \min_{t_\mu,\gamma} \langle \hat H - T\hat S\rangle , \tag{4.8}$$

where the so-called "entropy-operator"

$$\hat S = -k\ln\hat\rho \tag{4.9}$$

has been introduced. The minimization procedure is carried out subject to the "number-conserving" constraint

$$N = \langle \hat N\rangle = \mathrm{Tr}\left[\hat\rho \sum_{p\mu} C_{p\mu}^\dagger C_{p\mu}\right] . \tag{4.10}$$

The procedure just described is tantamount to that of directly minimizing the grand canonical potential $\hat H - T\hat S - \lambda\hat N$, with a Lagrange multiplier λ taking care of (4.10). By recourse to the finite-temperature version of Wick's theorem, and with the aid of (4.6), one finds

$$\langle \hat H\rangle = 2\Omega\left[\frac{\epsilon}{2}(t_+ - t_-) - \frac{G}{2}\{2\Omega\sin^2\gamma\cos^2\gamma(1-t_+-t_-)^2 + [t_+ - \sin^2\gamma(t_- + t_+ - 1)][t_- - \sin^2\gamma(t_- + t_+ - 1)]\}\right] , \tag{4.11}$$

$$\langle \hat N\rangle = 2\Omega[t_- + t_+ + 2\sin^2\gamma(1-t_+-t_-)] , \tag{4.12}$$

so that, after introduction of

$$d = \frac{N}{2\Omega} = 1 + \frac{2Q_0}{2\Omega} = 1 + 2q_0 \tag{4.13}$$

one solves for $\sin^2\gamma$ in terms of t_+ and t_- in (4.12)

$$\sin^2\gamma = \frac{d - t_+ - t_-}{2(1-t_+-t_-)} \tag{4.14}$$

and recasts $\langle \hat H\rangle$ as

$$\frac{\langle \hat H\rangle}{2\Omega} = \frac{\epsilon}{2}(t_+ - t_-) - \tfrac{1}{8}g(d - t_+ - t_-)(2 - d - t_+ - t_-) , \tag{4.15}$$

where, as usual,[19] we have neglected the "self-energy" contribution [the last term in the curly braces on the rhs of (4.11)] of the pairing force, as its contribution vanishes when $\Omega\to\infty$. A first point to be made here is that the rhs of (4.15) does not depend upon the degeneracy Ω. A second, and a very important point indeed, is that, by substituting into (4.15)

$$\begin{aligned} r &= \tfrac{1}{2}(t_- - t_+) ,\\ q &= \tfrac{1}{2}(1 - t_+ - t_-) , \end{aligned} \tag{4.16}$$

the present value of $\langle \hat H\rangle$ becomes identical to the one obtained in Sec. III [cf. Eq. (3.12)] by recourse to coherent-atomic states. Moreover, by substituting (4.16) into (4.7) we also reproduce the result (3.7), as the sum $t_+ + t_-$ can be confined, without loss of generality, to lie in the interval $0 < t_+ + t_- < 1$. As $t_- > t_+$ ($E_- < E_+$) and $\sin^2\gamma$ is a definite positive quantity, we arrive again, within the present approach, at the situation described by the set of restrictions (3.5). Consequently, we are led to conclude that the thermal BCS approach is exact in the thermodynamic limit within the present context. Further, by evaluating

$$\langle \hat N^2\rangle = N^2 + 2N - \frac{N^2}{2\Omega} - 2\Omega(t_+ + t_- - 2t_+t_-) \tag{4.17}$$

we find that also at finite temperatures we regain the $T=0$ result

$$\frac{\langle \hat N^2\rangle - \langle \hat N\rangle^2}{\langle \hat N\rangle^2} \alpha \frac{1}{N} . \tag{4.18}$$

B. The case $N = 2\Omega$

Thus far our results apply for any given number N of particles ($\le 4\Omega$). We shall restrict ourselves herefrom to the so-called[12] "Lipkin case" in which N equals 2Ω. In this situation we have, consequently, $Q_0 \equiv 0$ and $\sin^2\gamma = \frac{1}{2}$ [cf. Eq. (4.14)]. The free energy per particle acquires the shape

$$f = \frac{\epsilon}{2}(t_+ - t_-) - \tfrac{1}{8}g(1 - t_+ - t_-)^2 + kT\sum_\mu [t_\mu \ln t_\mu + (1-t_\mu)\ln(1-t_\mu)] , \tag{4.19}$$

an expression that must be minimized with respect to the t's, paying due respect to the restriction

$$0 < t_+ + t_- < 1 . \tag{4.20}$$

By taking the corresponding derivatives and equating to zero we are thus led to the gap equation

$$-w + 1 = \{1 + \exp[(\tfrac{1}{2}\epsilon + \tfrac{1}{4}gw)/kT]\}^{-1} + \{1 + \exp[(-\tfrac{1}{2}\epsilon + \tfrac{1}{4}gw)/kT]\}^{-1} , \tag{4.21}$$

or, equivalently,

$$w = 1 - t_+ - t_- , \tag{4.22}$$

and the occupation numbers t_μ adopt the appearance (remember that the "number of particles" is explicitly taken care of [cf. (4.13) and (4.14)])

$$t_\mu = \{1 + \exp[(\tfrac{1}{2}\mu\epsilon + \tfrac{1}{4}gw^{-1})/kT]\} , \tag{4.23}$$

so that the independent quasiparticle energy becomes

$$E_\mu = \tfrac{1}{2}\mu\epsilon + \tfrac{1}{4}gw . \tag{4.24}$$

It is worth noticing that w is linearly related both to q and to the gap Δ (Ref. 18)

$$\Delta = \frac{g}{2}\sin\gamma\cos\gamma(1 - t_+ - t_-) = \tfrac{1}{4}gw , \tag{4.25}$$

so that, if we denote by Δ_0 the zero temperature gap, we get

$$\Delta = w\Delta_0 . \tag{4.26}$$

Of course, one could have gotten the gap equation (4.25) by following the standard FTBCS treatment.[18] We chose here a "direct-minimization" procedure because it resembles somewhat more closely the "exact" one.

It must be pointed out that $w = 0$ is always a solution to the gap equation, and that, moreover, the number-conserving restriction (4.10) is automatically satisfied whenever $t_+ + t_- = 1$, in which case the angle γ is left undetermined and the pairing force contribution vanishes ($\Delta = q = 0$, $v = N$). This is the only solution, at *all* temperatures, for

$$g < 4\epsilon , \tag{4.27}$$

and the corresponding t_μ become

$$t_- = 1 - t_+ = [1 + \exp(-\tfrac{1}{2}\epsilon/kT)]^{-1} , \tag{4.28}$$

i.e., the usual Fermi distribution, with the spectrum of the unperturbed Hamiltonian $\epsilon\hat{J}_z$. This solution could certainly be called a "strange" one, as the occupation probability $t_- \to 1$ and not to zero as $T \to 0$. The present, "thermal," method, yields thus the exact nonsuperconducting ground state at $T = 0$ (the one with $Q = 0$, $J = N/2$), as one of the solutions of the gap equation, something that does not happen in the case of the ordinary ($T = 0$) treatment.[12]

For $g > 4\epsilon$, the gap equation allows for other solutions, and they should be compared with the one previously discussed. The "ordinary" superconducting solution ($w = 1$, $v = 0$) is the "lowest-lying" (energy wise) at $T = 0$ (as expected). As T starts to rise, the gap (and w) decreases, eventually vanishing at some critical temperature $T = T_c$. For $T > T_c$, $w = 0$ becomes once more the only solution to the gap equation. By expansion of (4.21) around $w = 0$, one is led to the conclusion that T_c is that temperature for which

$$8kT_c\cosh^2(\epsilon/4kT_c) = g , \tag{4.29}$$

an expression that, for $\epsilon = 0$, reduces itself to the well-known result that applies for the so-called "degenerate model."[18] In studying the solutions to (4.29) two different situations arise, according to whether g is larger or smaller than $g_c = 4.4668\epsilon$:

(i) $g > g_c$. There are two solutions. However, as the smaller of these corresponds to the disappearance of a local maximum of the free energy (4.19), only one of them attains physical meaning.

(ii) $g < g_c$. There is no solution for T_c, meaning that the gap, as T increases, will "suddenly" vanish, as depicted in Fig. 1, where the gap is plotted as a function of T. The behavior of the mean energy per particle, $E(T) = \langle \hat{H}/2\Omega \rangle$, is illustrated, for different values of $N = 2\Omega$ and two values of g (smaller and greater than the critical one, respectively), in Fig. 2(a). ($g = 4.2$ and $g = 5.0$; ϵ is set equal to unity and kT is measured in units of ϵ.) The curve labeled FTBCS is that for the case $\Omega = \infty$. Two different types of "discontinuities" are seen to occur (i.e., first order and second order transitions). For $g = 4.2$ ($< g_c = 4.4668$), $E(T)$ exhibits a discontinuity at $T = T_c$, while, when the coupling constant reaches the value $g = 5$, the slope of E is the one that suffers a discontinuity. (The entropy S exhibits, in this respect, a similar behavior.) For $T > T_c$, all the state functions behave as those that correspond to the unperturbed Hamiltonian (i.e., the one with $g = 0$). All discontinuities are smoothed out when the number of particles is finite. As the number of particles increases, the corresponding results become closer and closer to those of the thermodynamic limit (see, for example, Fig. 3).

One should also notice [cf. Eq. (4.19)] that in the thermodynamic limit, the state of the system is univocally determined by t_+ and t_- (or, equivalently, by q and r), which in turn are functions of the temperature. As T grows from zero to infinity, the evolution of the system can then be followed in the "q-r" plane. At $T = 0$ the system "starts" either from $q = \frac{1}{2}, r = 0$ (superconducting state) or from $q = 0, v = \frac{1}{2}$ (unperturbed, or "normal,"

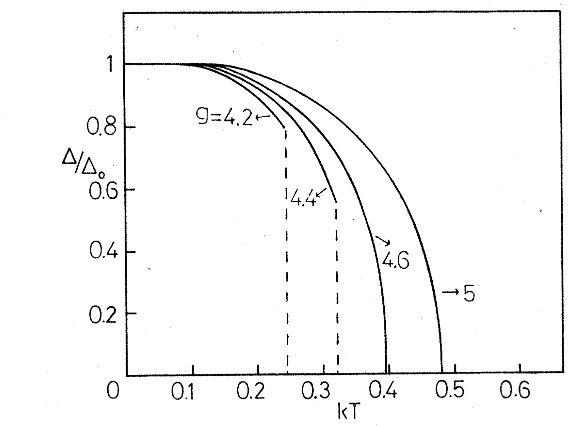

FIG. 1. Gap as a function of the temperature. Δ_0 is the gap at $T=0$. Both g and kT are expressed in units of ϵ.

state). At $T=\infty$ both q and r vanish, as the entropy is maximized by these zero values.

V. PAIRING PLUS MONOPOLE FORCE

We shall now turn our attention to the Hamiltonian (2.8), with the hope of gaining some insight into the interplay among three competing effects: temperature, pairing (favors seniority zero), and monopole force (favors seniority $v=N$). Working out things as in Sec. IV (see also Refs. 7 and 8), one easily obtains

$$\min_{\Omega'} h(r,q,\Omega') = -\epsilon r - \tfrac{1}{2}g(q^2-q_0^2), \quad r<\frac{\epsilon}{2v}$$
$$= \left[-vr^2-\frac{\epsilon^2}{4v}\right] - \tfrac{1}{2}g(q^2-q_0^2), \quad r>\frac{\epsilon}{2v}\ . \tag{5.1}$$

In the thermodynamic limit the monopole interaction does not play any role for $v<\epsilon$. The question we want to answer now could be posed as follows: Can a thermal Hartree-Fock-Bogoliubov (FTHFB) treatment of the Hamiltonian (2.8) reproduce the exact results (5.1)?

By recourse to the Bloch-Messiah theorem,[20] the corresponding FTHFB transformation can be accomplished by first performing a HF transformation among "particle" operators ($C_\mu^\dagger$), followed by a BCS one in the corresponding "rotated" basis. The first step is, then,

$$C'^{\dagger}_{p+} = \cos\alpha C^{\dagger}_{p+} - i\sin\alpha C^{\dagger}_{p-}\ ,$$
$$C'^{\dagger}_{p-} = -i\sin\alpha C^{\dagger}_{p+} + \cos\alpha C^{\dagger}_{p-}\ . \tag{5.2}$$

The pairing term $-\frac{1}{2}G\hat{Q}_+\hat{Q}_-$ of the Hamiltonian is left invariant after application of (5.2), so that the "rotated" Hamiltonian reads now

$$\hat{H} = \epsilon(\hat{J}'_z\cos2\alpha + \hat{J}'_y\sin2\alpha) + V[\hat{J}'^2_x - (\hat{J}'_z\sin2\alpha - \hat{J}'_y\cos2\alpha)^2] - \frac{G}{2}\hat{Q}_+\hat{Q}_-\ , \tag{5.3}$$

where the primed operators are constructed with the $C'^{\dagger}_\mu$. Neglecting terms that vanish in the thermodynamic limit, and assuming for the sake of simplicity $N=2\Omega$, we are straightforwardly led to

$$\frac{1}{2\Omega}\langle \hat{H}\rangle = -\frac{\epsilon}{2}(t_- - t_+)\cos2\alpha - \tfrac{1}{4}v\sin^2 2\alpha(t_+ - t_-)^2 - \tfrac{1}{2}g\sin^2\gamma\cos^2\gamma(1-t_+-t_-)^2\ . \tag{5.4}$$

The recipe is then that of minimizing $\langle \hat{H} - T\hat{S}\rangle$, taking care of the number conserving restriction (see Sec. IV), with respect to t_+, t_-, γ, and α. The last variable is easily dealt with, the result being

$$\cos2\alpha = 1 \text{ for } t_- - t_+ < \epsilon/v\ ,$$
$$\cos2\alpha = \frac{\epsilon}{v(t_- - t_+)} = \frac{\epsilon}{2vr} \text{ for } t_- - t_+ > \frac{\epsilon}{v}\ , \tag{5.5}$$

where, once again, we are using the abbreviations

$$r=(t_- - t_+)/2\ ,$$
$$q=(1-t_+-t_-)/2\ , \tag{5.6}$$

so that one is immediately led to (5.1), and thus to the conclusion that the FTHFB approach is exact in the thermodynamic limit, a result that holds for a variety of pseudospin Hamiltonians (even if one adds a term of the form

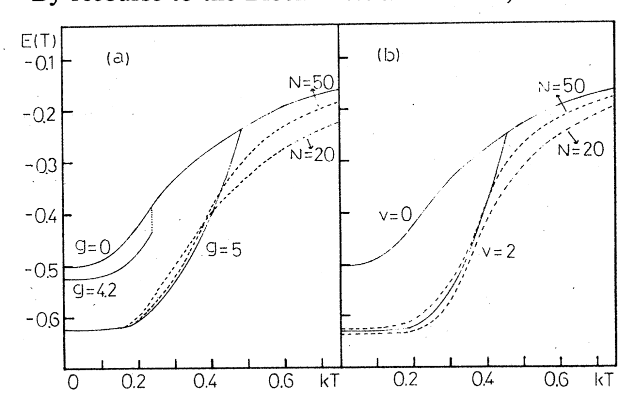

FIG. 2. Mean energy per particle $E(T)$ as a function of temperature for different pairing coupling constants (a) and different monopole strengths (b). N denotes the number of particles. Full lines correspond to the thermodynamic limit.

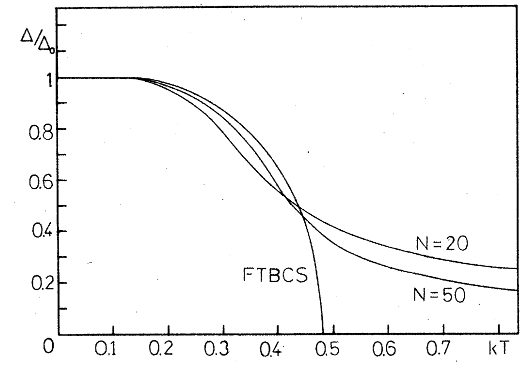

FIG. 3. The behavior of the relative gap as a function of temperature for the exact FTBCS treatment (thermodynamic limit) and for $N=50$ and 20. The pairing coupling constant is $g/\epsilon=5.0$.

$-\frac{1}{2}g\hat{Q}_+\hat{Q}_-$). Taking now the derivatives of $\langle \hat{H} - T\hat{S} \rangle$ with respect to the t_μ and, afterwards, equating to zero, one finds the corresponding critical ("gaplike") equations

$$w = 1 - t_+ - t_- \,, \tag{5.7}$$

$$1 - w = (1 + e^{\epsilon'_+})^{-1} + (1 + e^{\epsilon'_-})^{-1} \,, \tag{5.8}$$

$$2r = (1 + e^{\epsilon'_-})^{-1} - (1 + e^{\epsilon'_+})^{-1} \,, \tag{5.9}$$

$$\epsilon'_\mu = \tfrac{1}{2}\mu\epsilon + \tfrac{1}{4}gw \text{ for } r < r_c = \epsilon/2v$$

$$= \mu v r + \tfrac{1}{4}gw \text{ for } r > r_c \,, \tag{5.10}$$

where the ϵ'_μ are, of course (independent) quasiparticle energies.

A. A pure monopole force

It may be of interest to consider first, in the present vein, the case $g = 0$. FTHFB reduces itself to a thermal HF approach and the Hamiltonian to the ordinary Lipkin one.[4] Equation (5.8) is trivially solved and $w = 0$ (zero gap). For $r < r_c$ (5.9) is also trivially solved, and one finds

$$r = \tfrac{1}{2}\tanh(\epsilon/4kT), \quad r < r_c \,, \tag{5.11}$$

which immediately leads to a critical temperature

$$kT_c = \left[\ln \left[\frac{v+\epsilon}{v-\epsilon} \right] \right]^{-1} \frac{\epsilon}{2} \,, \tag{5.12}$$

such that for $T > T_c$ the influence of the monopole interaction entirely vanishes. The system "evolves" as T increases in a form similar to that corresponding to the pairing Hamiltonian (2.7). This kind of behavior of the monopole interaction as the temperature grows has been extensively studied by Gilmore and Feng,[7] although from a different point of view, and is related to the crossover theorem[7] which relates ground state ($T = 0$) phase transitions, that arise as the *coupling constant* changes, with those that appear as T grows (for a fixed value of v). At $T = T_c$ a phase transition takes place, and a discontinuity in the *slope* of $E(T)$ (or of S) ensues, although no discontinuity whatsoever is to be detected, neither in $E(T)$ [see Fig. 2(b)] or in S. As expected, one finds, as in the preceding section, that the mean energies for N finite tend to the FTHF values as N grows. As here the gap obviously vanishes, the q,r plane trajectory of the system (cf. Sec. IV) runs always along the r axis, and the phase transition takes place when r "crosses" the critical value T_c.

B. The pairing versus monopole competition

Returning now to the full Hamiltonian, the set (5.8), (5.9) has to be simultaneously solved. The main result one obtains is that, for a nonzero gap, one has always $r < r_c$ (α equals zero), and, conversely for $r > r_c$ and $\alpha \neq 0$ the gap always vanishes. For T high enough, both α and γ become zero and things are arranged as if one were dealing only with the unperturbed Hamiltonian. The interplay between both interactions is illustrated in Fig. 4. At $T = 0$, the ground state will be the superconducting one ($q = \frac{1}{2}$, $r = 0$) for

$$g > g_c = 2 \left[v + \frac{\epsilon^2}{v} \right] \tag{5.13}$$

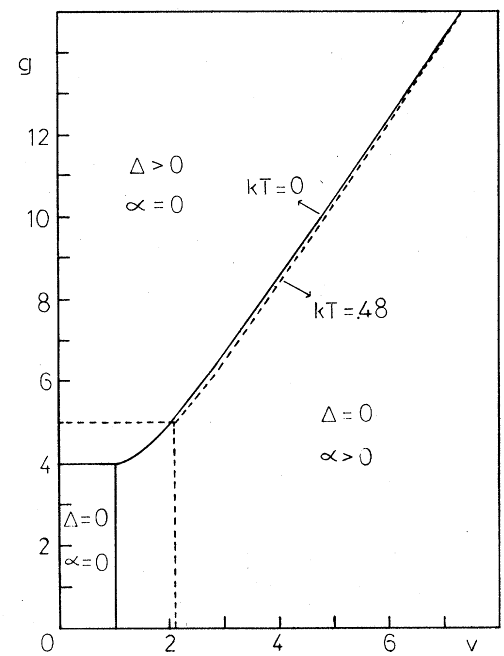

FIG. 4. Normal, superconducting, and "deformed" phases in the pairing coupling constant g vs monopole strength v plane. For more details see the text.

within the FTHFB framework (exact in the thermodynamic limit). For $g < g_c$, the ground state is "deformed" ($q = 0$, $r = \frac{1}{2}$, $\alpha \neq 0$). Finally, for $g < 4\epsilon$ and $v < \epsilon$, the system could be described as normal (nonsuper-

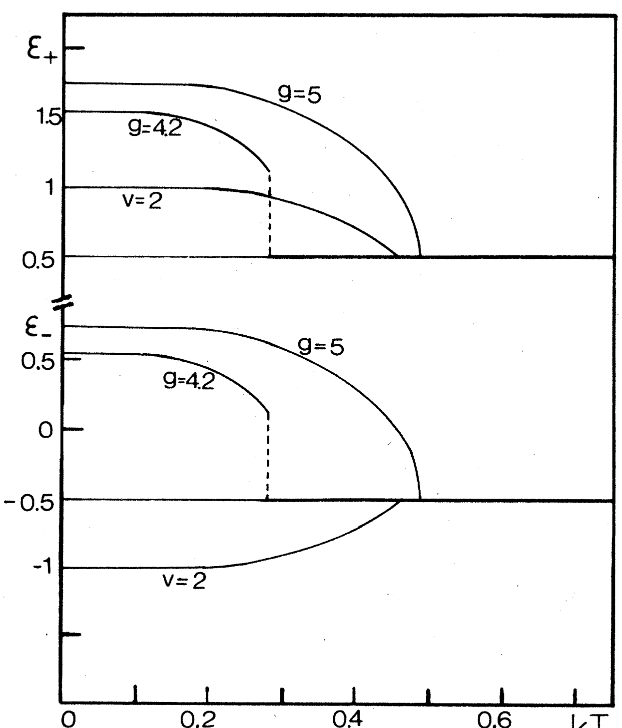

FIG. 5. Single-quasiparticle energies ($\epsilon_\mu - \lambda$) as a function of temperature for different coupling constants. λ is the chemical potential. When either g or v is finite, the other coupling constant is taken to be zero.

conducting) and "spherical."

For $T \neq 0$, the situation remains, *qualitatively,* the same. The "critical" values, however, change as T grows. Moreover, the ratio Δ/Δ_0 becomes smaller than unity in the superconducting region of Fig. 4, while $\frac{1}{2} > r > r_c$ in the deformed one. As the monopole interaction favors large values of J (Ref. 12) while the qsp one, on the other hand, tends to favor $J=0$ (Ref. 12), it is intuitively clear (just from the multiplet structure of our model) that there is a larger degree of "order" for a large J than for a small one. Consequently, for low temperatures, the monopole force is "downplayed" to a smaller extension than the qsp one by temperature effects. As a result, the separatrix between the "deformed" and the "superconducting" regions moves into the latter one as $T>0$.

Figure 5 displays the behavior of the independent quasiparticle energies for different situations. At $T=0$ they equal $\pm\frac{1}{2}v$ in the "deformed" case and $\pm\epsilon+\frac{1}{4}g$ in the superconducting one. As T grows, they tend to the unperturbed values $\pm\frac{1}{2}\epsilon$.

VI. CONCLUSIONS

The interplay between pairing and shape deformations, on one hand, and thermal effects, on the other, has been studied *within the framework of an exactly soluble model,* with the idea of gaining, *by comparison with the exact results,* some insight into the behavior of several independent quasiparticle approximations, mainly with respect to their ability to describe phase transitions. These phase transitions arise as a result of the competition between three different factors: a pairing-like force, a monopole interaction, and finite temperature effects, and a rich variety of situations thus ensues.

An important result is that all independent quasiparticle methods become exact in the thermodynamic limit. The intensive group quantum numbers q and r are thus identified with the occupation probabilities t_+ and t_-.

The thermal BCS approach is seen to yield the unperturbed ground state in a natural fashion, as a solution of the corresponding gap equation, a fact which suggests that the thermal approach may be useful even at $T=0$.

The interesting results of Refs. 1–4 can be straightforwardly generalized so as to encompass pairing-like effects. The theoretical approach used there is seen thus to be able to cope with a rich variety of ground state and thermodynamic phase transitions within a unified and simple context. As superconductivity is a crucial ingredient of the nuclear many body problem, we believe that the present effort is a useful complement to the work of Gilmore and Feng.[6–9]

APPENDIX: THE MULTIPLICITY FACTOR

In order to derive Eq. (4), we introduce first the operators:

$$\hat{n}_p = \sum_{\mu} C^{\dagger}_{p\mu} C_{p\mu} , \tag{A1}$$

which "count" the number of particles with a given p. Let P denote the number of particle "pairs" (i.e., eigenvalue of $\hat{n}_p$ equal to 2) and S the number of "hole pairs" (i.e., eigenvalue of $\hat{n}_p$ equal to 0). The value of Q will be determined by the configuration of the $P+S$ "paired" states while that of J by the remaining $2\Omega-P-S$, with eigenvalue of $\hat{n}_p$ equal to one.

If

$$J=\frac{2\Omega-P-S}{2}-K, \quad Q=\frac{P+S}{2}-L ,$$

the number of states, say M, with a given value of J,Q and $P+S$ is

$$\begin{aligned} M &= \begin{bmatrix} 2\Omega \\ P+S \end{bmatrix} \left[\begin{bmatrix} 2\Omega-P-S \\ K \end{bmatrix} - \begin{bmatrix} 2\Omega-P-S \\ K-1 \end{bmatrix} \right] \left[\begin{bmatrix} P+S \\ L \end{bmatrix} - \begin{bmatrix} P+S \\ L-1 \end{bmatrix} \right] \\ &= \frac{(2\Omega)!(2J+1)(2Q+1)}{\left[\frac{2\Omega-P-S}{2}-J\right]! \left[\frac{2\Omega-P-S}{2}+J+1\right]! \left[\frac{P+S}{2}-Q\right]! \left[\frac{P+S}{2}+Q+1\right]!} . \end{aligned} \tag{A2}$$

If there are N particles present, $0 \le N \le 4\Omega$, then $Q_0=\frac{1}{2}N-\Omega$, and, as a consequence,

$$|Q_0| \le Q \le \Omega . \tag{A3}$$

Moreover, as $|N-2\Omega| \le P+S \le 2\Omega$, J will satisfy

$$0 \le J \le \Omega - |\tfrac{1}{2}N-\Omega| = \Omega - |Q_0| . \tag{A4}$$

Clearly, $J+Q$ satisfies the relationship

$$0 \le J+Q \le \Omega . \tag{A5}$$

Now, for a given value of J and Q, $P+S$ will lie in the interval

$$2Q \le P+S \le 2\Omega-2J . \tag{A6}$$

Summing up expression (A2) with respect to $P+S$ over the interval (A6) one is led, finally, to Eq. (4). It is possible to verify that

$$\sum_{Q=Q_0}^{\Omega} \sum_{J=0}^{\Omega-Q} (2J+1) Y(J,Q) = \begin{bmatrix} 4\Omega \\ 2(Q_0+\Omega) \end{bmatrix} = \begin{bmatrix} 4\Omega \\ N \end{bmatrix} \tag{A7}$$

and

$$\sum_{Q=0}^{\Omega-J} Y(J,Q) = \begin{bmatrix} 2\Omega \\ \Omega-J \end{bmatrix}^2 - \begin{bmatrix} 2\Omega \\ \Omega-J-1 \end{bmatrix}^2 .$$

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