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Finite temperature effects and phase transitions in the pairing force problem: Variational approach

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Finite temperature effects in the pairing force problem are studied within the formalism of a variational approach. The formalism, which is free of the number fluctuations which are present in the standard Bardeen-Cooper-Schrieffer approach, allows for the description of thermally-induced phase transitions. An application of the method is discussed for the case of a two-level model.

I. INTRODUCTION

The study of temperature effects in finite nuclei has been the subject of recent publications.[1-9] The problem has been motivated both by experimental and theoretical evidence[1,2,6,8] concerning, particularly, the treatment of pairing correlations in nuclei at finite temperatures. In this paper we focus our attention on the treatment of the pairing Hamiltonian within a variational approach[12-14] at finite temperatures.

The temperature dependent treatment of pairing correlations[1,2,6,8] within the framework of the Bardeen-Cooper-Schrieffer (BCS) approximation, or within the equivalent Hartree-Fock-Bogoliubov method,[1,2] shows that the pairing gap Δ collapses at a certain value of the temperature, thus inducing a phase transition from the superfluid phase to the normal one.[6,8] This phase transition has been interpreted as the signature of a configuration blocking[8] which clearly affects the single-particle levels in the neighborhood of the Fermi level. Within the BCS approximation, the critical temperature, T_c, which produces the above-mentioned phase transition, has the value[8] $T_c \simeq \Delta(T=0)/2$, a value which is very similar to that associated with the pairing collapse in infinite systems.[15]

Considering the approximations posed by the BCS method, it would be interesting to know whether this phase transition occurs in a more accurate description of the pairing force. With this motivation in mind we perform the theoretical analysis which is presented here.

The variational approach to the pairing force problem was reported long ago for a two-level model,[12,13] and the method proved to be able to identify a domain, as a function of the pairing coupling constant G, where the BCS result strongly differs from the exact solution. This failure of the BCS method is particularly evident for small values of G far from the critical value G_c where the pairing gap Δ vanishes.[12,13] Moreover, the so-called F approach[12,13] may be successfully applied whenever the BCS approximation or its number conserving extensions does not work because of the weakness of the interaction.[13] Although the F approach has a natural boundary of validity,[12,13] the method seems to be a suitable one in order to investigate temperature-dependent effects without the limitations posed by the BCS approach.

In this paper, we extend the F approach for the finite temperature case. The formalism is presented in Sec. II, both for the $T=0$ case and for the finite T case, respectively. The theoretical details are discussed for a two-level model, and the results of the calculations are presented in Sec. III. Some conclusions are drawn in Sec. IV.

II. FORMALISM

In this section we shall briefly discuss the main features of the F method for the case of the pairing Hamiltonian at temperature $T=0$ (subsection A) and at finite T (subsection B).

A. The F method at $T=0$

This approximation has been presented in detail in Refs. 12 and 13. The starting point is the definition of a unitary transformation $\exp(iF)$ under which the approximate ground state $|\tilde{\phi}_0\rangle$ is written as

$$|\tilde{\phi}_0\rangle = \exp(iF)\,|\phi_0\rangle \;, \tag{1}$$

$|\phi_0\rangle$ being the unperturbed ground state. The operator F is determined by the variational condition

$$\delta\langle\tilde{\phi}_0\,|\,H\,|\,\tilde{\phi}_0\rangle = 0 \;, \tag{2}$$

assuming a given order in the series expansion of the operator $\exp(iF)$ in powers of F. The variation leads to a set of linear equations for the matrix elements of F. Once the structure of F is fixed, the eigenvalues of the Hamiltonian H are represented, at the same order in the series expansion in powers of F, by the diagonal matrix elements of the transformed Hamiltonian H' (Refs. 12 and 13):

$$H' = \exp(-iF)H\exp(iF) \;. \tag{3}$$

For the pairing-force Hamiltonian, we have

$$H = \sum_j \epsilon_j N_j - \frac{G}{4} \sum_{\substack{jm \\ j'm'}} a^\dagger_{jm} a^\dagger_{\overline{jm}} a_{\overline{j'm'}} a_{j'm'} \;, \tag{4}$$

where

$$N_j = \sum_m a^\dagger_{jm} a_{jm} \ , \tag{5}$$

and where $a^\dagger_{jm}$ (a_{jm}) are the creation (annihilation) operators of fermions in the shell model orbits (j,m), and where $a^\dagger_{\overline{jm}}$ ($a_{\overline{jm}}$) are the corresponding time reversed operators. In Eq. (4), G is the pairing coupling constant and ϵ_j are the single-particle energies.

For simplicity we restrict ourselves to the case of two levels, each of them with degeneracy $\Omega_i = 2j_i + 1$ ($i = 1,2$). The lower level ($i = 1$) is placed at the energy $\epsilon_1 = 0$ and the upper level has $\epsilon_2 = \epsilon$. We assume a system with N fermions. For this two-level system F has the structure[12,13]

$$F = fL_+S_- + f^*_- S_+L_- \ , \tag{6}$$

with

$$L_+ = \sum_{m>0} a^\dagger_{j_2 m} a^\dagger_{\overline{j_2 m}} = L^\dagger_-$$

and (7)

$$S_+ = \sum_{m>0} a^\dagger_{j_1 m} a^\dagger_{\overline{j_1 m}} = S^\dagger_- \ .$$

The operators L_+, L_-, S_+, and S_-, and the operators

$$L_Z = \tfrac{1}{2}(N_2 - \Omega_2) \ , \tag{8}$$

$$S_Z = \tfrac{1}{2}(N_1 - \Omega_1) \tag{9}$$

define two sets of quasispin operators. The L and S operators commute and within each set they follow the usual angular momentum commutation algebra.

The variation, up to second order in f, leads to the result[12,13]

$$f = \frac{-iG}{2}\left[\epsilon - \frac{1}{2}\left[N - 2 + \frac{\Omega_2 - \Omega_1}{2} G\right]\right] \ , \tag{10}$$

which has a pole at the value

$$\frac{\epsilon}{G} = \frac{1}{2}\left[N - 2 + \frac{\Omega_2 - \Omega_1}{2}\right] . \tag{11}$$

At $T = 0$, the energy, at the same order in powers of f, reads

$$E = -G\left[N - \frac{\Omega_1}{2}\right]\left\{1 + \frac{(G\Omega_2/4)}{\epsilon - \frac{G}{2}\left[N - 2 + \left[\frac{\Omega_2 - \Omega_1}{2}\right]\right]}\right\} . \tag{12}$$

This result is to be compared with the exact value and it has been shown in Refs. 12 and 13 that the agreement is quite reasonable provided that the ratio ϵ/G is far from the value given by Eq. (11). In the same region where both the approximate result, Eq. (12), and the exact one do not differ, the BCS result is rather poor. Therefore we can adopt Eq. (12) as a good representation of the exact solution and we can thus study the effects of the thermal degrees of freedom much more accurately than in the standard BCS approach.

B. The F method at $T \neq 0$

The inclusion of temperature dependent degrees of freedom in a finite fermionic system can be performed by using the standard techniques of quantum statistical mechanics,[16] namely, we define a density operator ρ in such a way that the expectation value,

$$f_j = \langle a^\dagger_{jm} a_{jm} \rangle = \mathrm{Tr}(\rho a^\dagger_{jm} a_{jm}) \ , \tag{13}$$

can be understood as the thermal occupancy of the single-particle orbit (j,m). In the grand canonical ensemble[16] we have

$$\rho = \frac{\exp[-\beta(H - \lambda N)]}{Z} \ , \tag{14}$$

and the partition function Z is therefore given by[16]

$$Z = \mathrm{Tr}\{\exp[-\beta(H - \lambda N)]\} \ , \tag{15}$$

where $\beta = 1/T$ is the inverse temperature, T being the temperature in units of energy.

In the present case, we can perform the series expansion of the transformed Hamiltonian H' [see Eq. (3)], and by replacing the ground state expectation values for the corresponding traces, we get for the different terms which appear in the second order variation (with $g = G/\epsilon$)

$$\langle H \rangle = \tfrac{1}{2}(N - \Omega_2) + \Omega_2 f_2 - \frac{G}{2}(\Omega_1 f_1^2 + \Omega_2 f_2^2) \ , \tag{16}$$

$$\langle [H,F] \rangle = \frac{G}{2}(f - f^*)\Omega_1\Omega_2[f_1^2(f_2 - \tfrac{1}{2}) - f_2^2(f_1 - \tfrac{1}{2})] \ , \tag{17}$$

$$\begin{aligned}\langle [[H,F],F] \rangle = {} & 2ff^*\Omega_1\Omega_2[f_1^2(f_2 - \tfrac{1}{2}) - f_2^2(f_1 - \tfrac{1}{2})] \\ & + Gff^*\,\Omega_1\Omega_2\left[(\Omega_1 + \Omega_2 - 4)f_1^2 f_2^2 + f_1 f_2^2(1 - \Omega_1) + f_1^2 f_2(1 - \Omega_2) + \frac{f_1 f_2}{2}(\Omega_1 f_1 + \Omega_2 f_2)\right. \\ & \left. + (f_1^2 - f_2^2)\frac{(\Omega_2 - \Omega_1)}{4} + (\Omega_1 - 2)f_1^3(\tfrac{1}{2} - f_2) + (\Omega_2 - 2)f_2^3(\tfrac{1}{2} - f_1)\right] \ ,\end{aligned} \tag{18}$$

where the quantities f_1 and f_2 are the single particle occupancies

$$f_1 = 1/[1+\exp(-\beta\lambda)]\ ,$$
$$f_2 = 1/\{1+\exp[\beta(\epsilon-\lambda)]\}\ . \tag{19}$$

The Lagrange multiplier λ is fixed by the number condition

$$N = \Omega_1 f_1 + \Omega_2 f_2\ , \tag{20}$$

which has the solution

$$\lambda = -\frac{1}{\beta}\ln[R+(R^2-r)^{1/2}]\ , \tag{21}$$

with

$$R = [\alpha\Omega_1+\Omega_2-N(\alpha+1)]/2\alpha N$$

and

$$r = (N-\Omega_1-\Omega_2)/\alpha N\ ,$$

where $\alpha = \exp(\beta\epsilon)$. The minimization of the energy, up to second order in f, yields

$$f = -iGB/(2B+GA)\ , \tag{22}$$

where

$$B = f_1^2(f_2-\tfrac{1}{2}) - f_2^2(f_1-\tfrac{1}{2})$$

and

$$\begin{aligned} A ={}& (\Omega_1+\Omega_2-4)f_1^2 f_2^2 + f_1 f_2^2(1-\Omega_1) \\ & + f_1^2 f_2(1-\Omega_2) + \frac{f_1 f_2}{2}(\Omega_1 f_1+\Omega_2 f_2) \\ & + (f_1^2-f_2^2)\left[\frac{\Omega_2-\Omega_1}{4}\right] + (\Omega_1-2)f_1^3(\tfrac{1}{2}-f_2) \\ & + (\Omega_2-2)f_2^3(\tfrac{1}{2}-f_1)\ . \end{aligned}$$

Finally, the energy for $T \neq 0$ reads

$$E(T\neq 0) = \frac{N-\Omega_2}{2} + \Omega_2 f_2 - \frac{G}{2}(\Omega_1 f_1^2 + \Omega_2 f_2^2) + \frac{\Omega_1\Omega_2 G^2 B^2}{2(2B+GA)}\ . \tag{23}$$

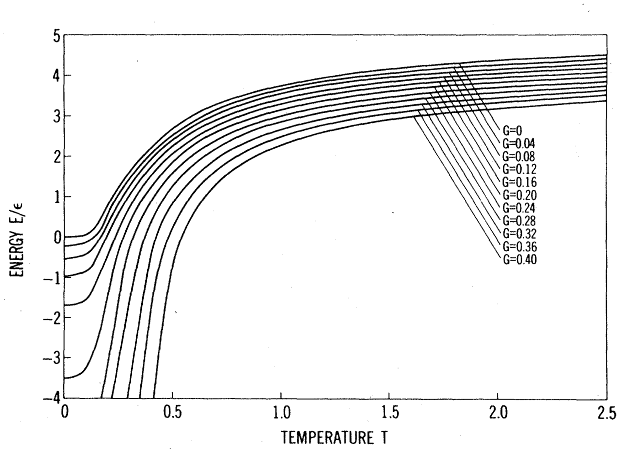

FIG. 1. Energy as a function of T for different values of the coupling constant G. The temperature T is given in units of ϵ and the curves correspond to the symmetric case.

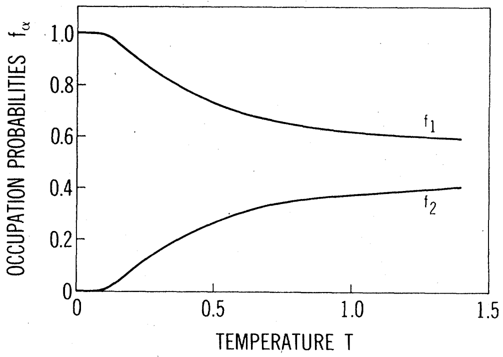

FIG. 2. Thermal occupancies f_j as a function of temperature T.

III. RESULTS AND DISCUSSION

In this section we shall show the results for the case of a symmetric two-level model where $\Omega_1 = \Omega_2 = N$. The thermal occupancies which fulfill the number condition are given by

$$f_1 = 1/[1+\exp(-\beta\epsilon/2)]\ ,$$
$$f_2 = 1/[1+\exp(\beta\epsilon/2)]\ , \tag{24}$$

where the value $\lambda = \epsilon/2$, which results from the solution of Eq. (21), has been used. The energy [Eq. (23)] can thus be calculated and the result is

$$E(T) = Nf_2 - \frac{GN}{2}(f_1^2+f_2^2) + \frac{G^2N^2B^2}{8(2B+GA)}\ , \tag{25}$$

where, for the symmetric case only, the coefficients A and B are given by

$$A = (N-2)(4f_1^2f_2^2 - 3f_1f_2 + \tfrac{1}{2}) \tag{26}$$

and

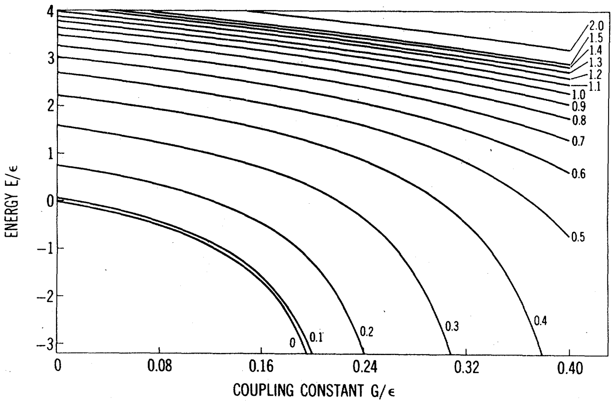

FIG. 3. Energy as a function of the coupling constant G for various T values and for $N = 10$.

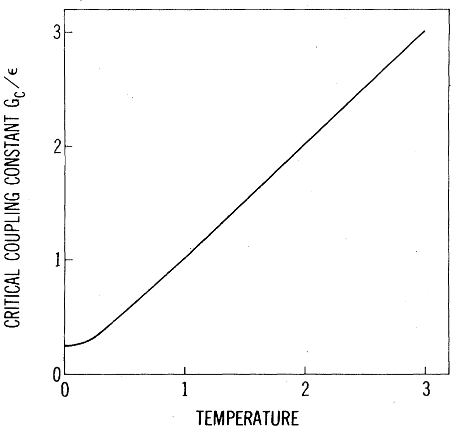

FIG. 4. Critical coupling constant G_c [see Eq. (28)] as a function of temperature for $N=10$.

$$B=(f_1-f_2)(f_1f_2-\tfrac{1}{2})\,, \tag{27}$$

respectively. The results of Eq. (25) are shown in Fig. 1 for various values of G. For $T=0$ the curves, as a function of G, show the behavior corresponding to Eq. (12); they decrease as G increases and they reach a saturation value for the temperature T which is of the order of the separation energy between both levels. Of course, this result is related to the temperature dependence of the occupation factors f_j, as is shown in Fig. 2.

The behavior of the energy, as a function of the coupling constant G, is shown in Fig. 3 for various values of the temperature T. As seen in this figure, the pole which at $T=0$ occurs for $G_c \simeq 0.2$ moves to higher values of G as T increases. It eventually disappears for $T>1$.

The temperature dependence of the critical G_c value, which at $T=0$ is given by the estimate Eq. (11), is shown in Fig. 4. The critical G_c value has an almost linear dependence upon T. In fact, the critical value of G_c corresponds to

$$G_c=\frac{(f_1-f_2)(f_1^2+f_2^2)}{(N-2)(4f_1^2f_2^2-3f_1f_2+\frac{1}{2})}\,. \tag{28}$$

This is the value at which the denominator in Eq. (25) vanishes. It is easy to see that it follows the limit

$$\lim_{T\to\infty} G_c=\infty\,. \tag{29}$$

The inclusion of thermal degrees of freedom washes out the pole which appears in the second-order expansion in terms of f increasing the domain of validity of this approximation.

The most significant result of the present work is shown in Fig. 5, where the specific heat

$$C=\frac{dE}{dT} \tag{30}$$

is shown as a function of T and for various values of G. The peak value at $T\simeq 0.2$ for $G=0$ increases with G and there is practically no change in its position.

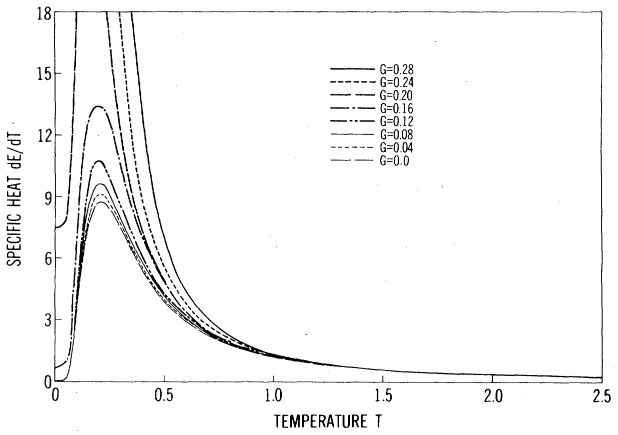

FIG. 5. Specific heat [see Eq. (30)], as a function of temperature T for different values of the coupling constant G and for $N=10$.

This tendency in the behavior of the specific heat could be related to the fact that, as is shown in Fig. 2, for this small value of T, in units of ϵ, there is a significant change of the occupation numbers f_j with respect to the $T=0$ situation with $f_1=1$ and $f_2=0$. The same behavior has been reported in the case of the BCS treatment of the pairing force.[6] We can conclude that it reflects the nature of the temperature-dependent phase transition rather than a pathology of the approximation adopted in order to describe pairing correlations, either the BCS approach or the present F method.

IV. CONCLUSIONS

In this work we studied the finite temperature version of a variational approach[12–14] to the pairing force problem. The inclusion of thermal degrees of freedom within this formalism shows the appearance of a phase transition which in the standard BCS approach has been interpreted[1,2,6,8] as the thermal collapse of the pairing gap. The present approach, which at $T=0$ gives better results than the standard BCS method, seems to be a suitable one for the study of pairing correlations at finite temperature. Concerning the poles which appear for certain values of the pairing coupling constant, in the $T=0$ limit of the variational approach, it is shown that they disappear in the finite temperature case. Within this treatment, the behavior of the specific heat shows the signature of a temperature-dependent phase transitions.

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[1] A. L. Goodman, Nucl. Phys. **A353**, 30 (1981).
[2] A. L. Goodman, Nucl. Phys. **A352**, 45 (1981).
[3] A. L. Goodman, Nucl. Phys. **A369**, 365 (1981).
[4] A. L. Goodman, Nucl. Phys. **A370**, 90 (1981).
[5] A. L. Goodman, Nucl. Phys. **A402**, 189 (1983).
[6] A. L. Goodman, Phys. Rev. C **29**, 1887 (1984).
[7] A. L. Goodman, Nucl. Phys. **A406**, 94 (1983).
[8] O. Civitarese, G. G. Dussel, and R. P. J. Perazzo, Nucl. Phys. **A404**, 15 (1983).
[9] O. Civitarese, R. A. Broglia, and C. H. Dasso, Ann. Phys. (N.Y.) **156**, 142 (1984).
[10] J. Rekstad *et al.*, Phys. Lett. **117B**, 384 (1982).
[11] J. O. Newton *et al.*, Phys. Rev. Lett. **46**, 1383 (1981).
[12] A. Mann, H. Nissimov, and I. Unna, Phys. Rev. **186**, 1104 (1969).
[13] M. Bishari, I. Unna, and A. Mann, Phys. Rev. C **3**, 1715 (1971).
[14] G. Bozzolo, J. Núñez, and A. Plastino, Phys. Rev. C **26**, 2692 (1982).
[15] A. A. Abrokosov, C. P. Gorkov, and I. E. Dzyaloshinski, in *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, 1963), p. 996.
[16] D. J. Thouless, in *The Quantum Mechanics of Many Body Systems* (Academic, New York, 1972).