Fluctuations in the Bardeen-Cooper-Schrieffer Hamiltonian induced by finite particle number

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The fluctuations properties of the BCS Hamiltonian which are induced in finite systems are explored. It is shown that for very large particle numbers the static-path approximation is an excellent approximation, while for small particle numbers, the random-phase-approximation corrections should be taken into account, especially for particle numbers small enough to cause the normal- to superconducting-phase transition. A correlated mean field containing quantal fluctuations is introduced and compared with the Hartree-Bogoliubov mean field.

I. INTRODUCTION

Phase transitions in many-body systems appear in the thermodynamic limit of infinite particle number, or equivalently for infinite volume. For finite systems, no singularity occurs in the partition function or in the thermodynamic response of the system.

An interesting question about the singular behavior of many-body systems is to what extent effects due to a finite number of particles still display a thermodynamic response which is reminiscent of a phase transition. On general grounds, one expects that, for large particle numbers, the singularities of the free energy will be smoothed. For small particle numbers, one expects that the fluctuations induced by the correction to the standard Hartree [or Hartree+random-phase-approximation (RPA) corrections] approximation, will be so strong as virtually to wipe out any signature of the phase transition of the large-N limit. We wish to study this question in interacting fermionic systems.

In previous works (Ref. 1), the Lipkin model (Ref. 2) and pairing Hamiltonian in a single energy shell were studied in the case of relatively small particle numbers. A comparison between the Hartree mean field and exact calculations showed no remnant of the second-order phase transition.

In the limit of large particle numbers, that is, in the limit of infinite degeneracy, the models of Ref. 1 do display second-order phase transitions since their static action, in the functional-integral representation for the partition function, is proportional to N; that is, these models admit a $1/N$ expansion around the mean field (Ref. 3).

Small-amplitude quantal corrections (that is, imaginary-time-dependent Gaussian fluctuations), if well behaved, do not appreciably contribute for large systems since their relative weight to the static action goes to 0 in the large-N limit as $1/N$. The remaining large-amplitude quantal fluctuations, which are associated with the tunneling between the stable Hartree phases (Ref. 1), cancel the singularity caused by small quantal fluctuations which diverge (much in the same way of the standard Gaussian model) for some energy below the barrier height. In other words, large quantal fluctuations associated with the imaginary-time axis are strong enough to destroy the phase transition caused by the Gaussian fluctuations in the imaginary-time order parameter. Since we know that the specific heat of the pairing Hamiltonian shows only the discontinuity associated with the static gap, we are led to the conclusion (although we have no rigorous proof) that this might be a general feature of quantal fluctuations for $1/N$ theories. That is that quantal fluctuations (which are one dimensional and with nearest-neighbor coupling given by the time derivative) always cancel singular behavior caused by tunneling between the potential barrier in the mean-field thermodynamic response. Of course, quantal fluctuations have no effect on the phase transition in the static order parameter.

The inclusion of the fluctuations in Ref. 1 was also carried out within the framework of the RPA-SPA (static-path approximation), where static fluctuations, at any order, and Gaussian quantal fluctuations were included. The effect of these fluctuations, for the particle numbers considered, was, as expected, to cancel the signature of a phase transition on the thermal response for those models.

In the past, static fluctuations have also been studied in Ref. 4 in the BCS Hamiltonian for finite particles in the framework of the SPA. However, no quantal fluctuations around the static approximation of the BCS Hamiltonian were considered. The goal of this paper is to include the quantal fluctuations within the framework of the RPA-SPA.

II. THE RPA-SPA FORMULATION

Let us consider the BCS Hamiltonian

$$\hat{H}=\hat{H}_0-G\sum_{k,l>0}a_k^\dagger a_{\bar{k}}^\dagger a_{\bar{l}}a_l \ , \tag{2.1}$$

where the labels $k,l,\bar{k},\bar{l}$ refer to single-electron states and to their time reversal. The single-particle Hamiltonian is defined as

$$\hat{H}_0=\sum_i \varepsilon_i a_i^\dagger a_i \ . \tag{2.2}$$

In what follows we retain the symbols i,j for any single-particle state, while the symbols k,l will refer to a single-particle state in the interval $[\varepsilon_F-\omega_D,\varepsilon_F+\omega_D]$, where ω_D is the Debye cutoff frequency and ε_F is the Fermi energy. In terms of the pairing operators $\hat{P}_k^\dagger=a_k^\dagger a_{\bar{k}}^\dagger$ and $\hat{P}_k=a_{\bar{k}}a_k$, the interaction can be rewritten as

$$-G\sum_{k,l>0}\hat{P}_k^\dagger\hat{P}_l=-G\hat{P}^\dagger\hat{P}\ .$$

Define the quasispin operators as

$$\begin{aligned}J_x&=\tfrac{1}{2}(\hat{P}+\hat{P}^\dagger)=\sum_k J_x^{(k)}\ ,\\ J_y&=\frac{i}{2}(\hat{P}-\hat{P}^\dagger)=\sum_k J_y^{(k)}\ ,\\ J_z&=\tfrac{1}{2}(\hat{N}-1)=\sum_k J_z^{(k)}\ .\end{aligned}\tag{2.3}$$

From the above definition it follows that

$$\hat{P}^\dagger\hat{P}=J_x^2+J_y^2+J_z\ ,\tag{2.4}$$

which is the form most suited for a functional integral. The grand-canonical partition function is given by

$$Z(\beta,\alpha)=\left[\frac{\epsilon}{\pi G}\right]^M\int\prod_{n=1}^{M}(d\phi_{xn}d\phi_{yn})\times\exp-\frac{\epsilon}{G}\sum_{n=1}^{M}(\phi_{xn}^2+\phi_{yn}^2)\times\mathrm{Tr}\mathcal{T}\exp\left(-\epsilon\sum_{n=1}^{M}\mathcal{H}_n\right)\ .\tag{2.5}$$

In the above, $\mathcal{T}$ is the imaginary-time ordering operator, M is the number of time slices, and $\epsilon=\beta/M$; the limit as M goes to ∞ is understood in the above. The Hamiltonian in (2.5) is given by

$$\mathcal{H}_n=\mathcal{H}_0-GJ_z-2G(J_x\phi_{xn}+J_y\phi_{yn})-\mu\hat{N}\ ,\tag{2.6}$$

where μ is the chemical potential. Equation (2.5) is exact. To define the approximations used in this work, let us use the Fourier transform of the fields ϕ_{xn} and ϕ_{yn} defined as (Ref. 1)

$$\begin{aligned}\phi_{xn}&=\bar{\eta}_x+\sum_{p\,(\neq 0)}\eta_{xp}e^{-i\omega pt_n}\ ,\\ \phi_{yn}&=\bar{\eta}_y+\sum_{p\,(\neq 0)}\eta_{yp}e^{-i\omega pt_n}\ ,\end{aligned}\tag{2.7}$$

where $\omega=2\pi/\beta$, and consider the eigenvalue problem

$$[\partial_t+\overline{\mathcal{H}}+\delta\mathcal{H}(t)]\xi_{\mu p}(t)=\mathcal{E}_{\mu p}\xi_{\mu p}(t)\ .\tag{2.8}$$

The label μ and p refer to the quasispin and the time, respectively. The static Hamiltonian in (2.8) is given by

$$\overline{\mathcal{H}}=\hat{H}_0-GJ_z-2G(\bar{\eta}_xJ_x+\bar{\eta}_yJ_y)-\mu\hat{N}\tag{2.9}$$

and the perturbation is

$$\delta\mathcal{H}(t)=-2G\sum_{p\,(\neq 0)}(\eta_{xp}J_x+\eta_{yp}J_y)e^{i\omega pt}\ .\tag{2.10}$$

I shall first derive the SPA expression for the partition function by neglecting $\delta\mathcal{H}(t)$ and then the RPA-SPA expression by performing second-order perturbation theory on the thermodynamic potential inside the functional integral. Because of the very special form of the Hamiltonian (2.1), the static-path approximation to the partition function will be of the $1/N$ type, that is, the thermodynamic potential in the SPA will be proportional to the particle number; in the RPA-SPA, the quantal corrections, instead, will not be proportional to the particle number (they tend to a constant as $N\to\infty$) and thus in the thermodynamic limit they will not contribute.

Neglecting the effect of the perturbation (2.10) in (2.8), one obtains the SPA expression for the partition function, i.e.,

$$Z(\beta,\alpha)=\left[\frac{\beta G}{\pi}\right]\int d\bar{\eta}_x d\bar{\eta}_y e^{-\beta G(\bar{\eta}_x^2+\bar{\eta}_y^2)}\mathrm{Tr}\mathcal{T}e^{-\beta\overline{\mathcal{H}}}\ .\tag{2.11}$$

The Hamiltonian $\overline{\mathcal{H}}$ can readily be diagonalized by rotations in the quasispin space. Define for convenience $G_k=G$ and $G_j=0$ for $j\neq k$. The Hamiltonian $\overline{\mathcal{H}}$ can be rewritten as

$$\overline{\mathcal{H}}=\mathcal{A}^\dagger\left[\mathcal{E}_0-2\sum_j R_jJ_z\right]\mathcal{A}\ ,\tag{2.12}$$

where the quasienergies R_j are given by

$$R_j=\sqrt{q_j^2+G_j^2(\bar{\eta}_x^2+\bar{\eta}_y^2)}\tag{2.13}$$

with

$$q_j=G_j/2+\mu-\varepsilon_j\ .$$

$\mathcal{A}$ is the rotation operator in the quasispin space

$$\mathcal{A}=\exp\left[i\sum_j\theta J_z^{(j)}\right]\exp\left[i\sum_j\phi_jJ_y^{(j)}\right]\ .\tag{2.14}$$

The rotation angles are defined by the relations

$$\begin{aligned}G\bar{\eta}_x&=\Delta\cos\theta\ ,\\ G\bar{\eta}_y&=\Delta\sin\theta\ ,\\ q_j&=R_j\cos\phi_j\ ,\\ \Delta&=R_j\sin\phi_j\ ,\\ R_j&=\sqrt{q_j^2+\Delta^2}\ .\end{aligned}\tag{2.15}$$

The constant $\mathcal{E}_0$ is

$$\mathcal{E}_0=\sum_j(\varepsilon_j-\mu)\ .\tag{2.16}$$

The eigenvalues of $\mathcal{H}_0$ are therefore

$$\mathcal{E}[m_j]=\mathcal{E}_0-2\sum_j R_jm_j\ ,\tag{2.17}$$

where the m's are the eigenvalues of J_z and are denoted collectively by μ in Eq. (2.8). The SPA expression for the partition function now becomes

$$Z(\beta,\alpha)=\left[\frac{2\beta}{\pi G}\right]\int d\Delta\,\Delta\exp\left[-\frac{\beta}{G}\Delta^2-\beta\mathcal{E}_0+\beta\sum_j R_j+2\sum\ln[1+\exp(-\beta R_j)]\right] \tag{2.18}$$

(see also Ref. 4). In order to understand the physical meaning of the SPA expression (2.18), note first that the extrema of the integrand are obtained in correspondence of the familiar Hartree-Bogoliubov gap. In fact, the extrema of the argument of the exponential in (2.18) satisfy the condition

$$\frac{2\Delta}{G}=\sum_k\frac{\Delta}{R_k}\tanh\left[\frac{\beta R_k}{2}\right].$$

Moreover, deviations from self-consistent Δ are included in (2.18) each weighted according to their free energy. A limitation of (2.18) is that quantal RPA corrections are not included in (2.18). Such corrections are, however, included in the RPA-SPA, as the name suggests. The pairing coupling constant is $G=g\delta$, where δ is the single-particle level spacing at the Fermi surface. For δ small enough, the sums can be approximated by integrals and one the contribution from the interaction isolated from the free part. The final expression is

$$Z(\beta,\alpha)=Z_{\text{free}}\left[\frac{\beta}{\pi g\delta}\right]\int d\Delta\,\Delta\exp\left[\frac{\beta}{\delta}\mathcal{L}\right]. \tag{2.19}$$

The action $\mathcal{L}$ in (2.19) is approximately size independent and is given by

$$\mathcal{L}=-\Delta^2-\omega_D^2+2\int_0^{\omega_D}R(\varepsilon)d\varepsilon +4\int_0^{\omega_D}d\varepsilon[\ln(1+e^{-\beta R(\varepsilon)})-\ln(1+e^{-\beta\varepsilon})] \tag{2.20}$$

with

$$R(\varepsilon)\sqrt{(g\delta/2-\varepsilon)^2+\Delta^2}\,. \tag{2.21}$$

Quantal corrections can be included by expanding the thermodynamic potential inside the functional integral up to second order in the perturbation in (2.8). The perturbation expansion is carried out in the basis defined by the time-dependent eigenstates of

$$[\partial_t+\overline{\mathcal{H}}]\xi_{\mu m}(t)=\mathcal{E}_{\mu m}\xi_{\mu m}(t)\,, \tag{2.22}$$

which, as before, are labeled by the eigenvalues of the rotated spin and by a time label associated with the time variable in (2.21),

$$\mathcal{E}_{\mu p}=\mathcal{E}_{\mu 0}+i\omega p\,,$$

with eigenstates

$$\xi_{\mu p}(t)=\xi_{\mu 0}e^{i\omega pt}\,,$$

where $\mathcal{E}_{\mu 0}$ and $\xi_{\mu 0}$ are the eigenvalues and eigenvectors of (2.9). The first-order correction to the quasienergies R_k is zero since the time average of the perturbation (2.10) is zero. The second-order correction gives

$$\delta\mathcal{E}_{\mu 0}=\sum_{(\nu n)\,[\neq(\mu 0)]}\frac{(\mu 0|\delta\mathcal{H}|\nu n)(\nu n|\delta\mathcal{H}|\mu 0)}{\mathcal{E}_{\mu 0}-\mathcal{E}_{\nu n}}\,. \tag{2.23}$$

Since the Hamiltonian (2.12) and the perturbation (2.10) are sums of independent Hamiltonians, each j term, in (2.17) is modified and, after some algebra, one finds that the corrections to R_k are of the type R_kD_k, where

$$D_k=\sum_{p\,(>0)}\left[(\cos^2\phi_k|F_{xp}|^2+|F_{yp}|^2)\frac{4R_k}{4R_k^2+\omega^2p^2}+\left[\frac{2\cos\phi_k}{R_k}\right](F_{xp}F_{y-p}-F_{x-p}F_{yp})\times\frac{\omega p}{4R_k^2+\omega^2p^2}\right]. \tag{2.24}$$

The variables F_{xp} and F_{ym} have the following expression:

$$F_{xp}=\eta_{xp}\cos\theta+\eta_{yp}\sin\theta\,,$$

$$F_{yp}=-\eta_{xp}\sin\theta+\eta_{yp}\cos\theta\,.$$

Finally, making use of the expansion

$$\text{Tr}\mathcal{T}\exp\left[-\epsilon\sum_{n=1}^{M}\mathcal{H}_n\right]=\prod_k\sum_{N=0}^{2}\binom{2}{N}e^{\beta R_k(N-1)(1+D_k)} =e^{\beta R_k+2\ln[1+e(-\beta R_k)]}\times e^{\beta R_kD_k-2F_k\beta R_kD_k}\,, \tag{2.25}$$

where the fermionic occupation numbers are given by

$$F_k=\frac{1}{1+e^{-\beta R_k}}\,,$$

one has, after performing the Gaussian integral over the variables η_{xp} and η_{yp},

$$Z(\beta,\alpha)=Z_{\text{free}}\left[\frac{\beta}{\pi g\delta}\right]\int d\Delta\,\Delta\exp\left[\frac{\beta}{\delta}\mathcal{L}\right]\mathcal{C}\,. \tag{2.26}$$

The quantal correction factor in (2.26) is given by

$$\mathcal{C}=\prod_{m\,(>0)}\left[\left[1-\sum_k A_{km}\right]\left[1-\sum_k B_{km}\right]+\left[\sum_k C_{km}\right]^2\right], \tag{2.27}$$

where the various factors are

$$A_{km}=\frac{2q_k^2G}{R_k}\frac{\tanh(\beta R_k/2)}{4R_k^2+\omega^2m^2}\,,$$
$$B_{km}=2R_kG\frac{\tanh(\beta R_k/2)}{4R_k^2+\omega^2m^2}\,, \tag{2.28}$$
$$C_{km}=\frac{2Gq_k}{R_k}\frac{\omega m\tanh(\beta R_k/2)}{4R_k^2+\omega^2m^2}\,.$$

Equations (2.26)–(2.28) define the RPA-SPA approximation to the partition function. From (2.26), as anticipated, one can easily see that $\mathcal{C}$ is approximately δ independent since, for small level spacing, the sums over k in (2.27) can be replaced by integrals which are independent from the size of the system (i.e., from δ). That is,

$$\mathcal{C}=\prod_{m\,(>0)}\left[\left[1-\int_0^{\omega_D}d\varepsilon\,A(\varepsilon,m)\right]\left[1-\int_0^{\omega_D}d\varepsilon\,B(\varepsilon,m)\right]+\left[\int_0^{\omega_D}d\varepsilon\,C(\varepsilon,m)\right]^2\right], \quad (2.29)$$

$$A(\varepsilon,m)=\frac{2[q(\varepsilon)]^2g}{R(\varepsilon)}\frac{\tanh[\beta R(\varepsilon)/2]}{4[R(\varepsilon)]^2+\omega^2m^2},$$

$$B(\varepsilon,m)=2R(\varepsilon)g\frac{\tanh[\beta R(\varepsilon)/2]}{4[R(\varepsilon)]^2+\omega^2m^2}, \quad (2.30)$$

$$C(\varepsilon,m)=\frac{2gq(\varepsilon)}{R(\varepsilon)}\frac{wm\tanh[\beta R(\varepsilon)/2]}{4[R(\varepsilon)]^2+\omega^2m^2}.$$

III. A NUMERICAL EXAMPLE

Let us apply the formalism developed in the previous sections to superconducting small particles (Ref. 5), along the same lines of Ref. 4. The constants ω_D and g will be treated as parameters with typical values. We will consider the case $g=0.25$ and $\omega_D=100$ K (Ref. 6). The unperturbed electron levels hae been taken equidistant, as done in Ref. 4. The Fermi energy $\mu_{\rm free}$ in the free bulk case was taken to 10^4 K and therefore the level spacing δ is related to the particle number N by the relation $N\delta=2\mu_{\rm free}$. Thus, the chemical potential for the free electrons is $\mu_{\rm free}+\delta/2$; in the case where the pairing interaction is taken into account, the chemical potentials do not differ much from their free values—for $\delta=5$ K, $\mu_{\rm free}-\mu=0.6$ K, and for smaller values of δ, this difference approaches the value -0.05 K in both the SPA and in the RPA-SPA. The difference in the chemical potentials between the SPA and the RPA-SPA was found to be less than one part in 10^5 and therefore was neglected in the calculation.

As noted in Ref. 4, the mean-field gap and the critical temperature become lower as δ increases because of the finite-size effect. In Fig. 1, the behavior of the mean-field gap, that is, the maximum of the integrand of the SPA partition function (2.18), is shown as a function of the temperature for different δ. In Fig. 2, the RPA-SPA gap [that is, the maximum of the integrand in (2.26)] is displayed. From Fig. 1 we note that the gap and the critical temperature decrease as δ increases and that, already for $\delta=1$ K, the bulk behavior is reached. In the SPA, the gap disappears at about $\delta=13.3$ K. The inclusion of the quantal fluctuations in the RPA-SPA scheme modifies appreciably this behavior: the superconducting phase already disappears at about $\delta=7$ K reflecting the fact the quantal fluctuations become more important for small systems. Note also, from Fig. 2, that the critical temper-

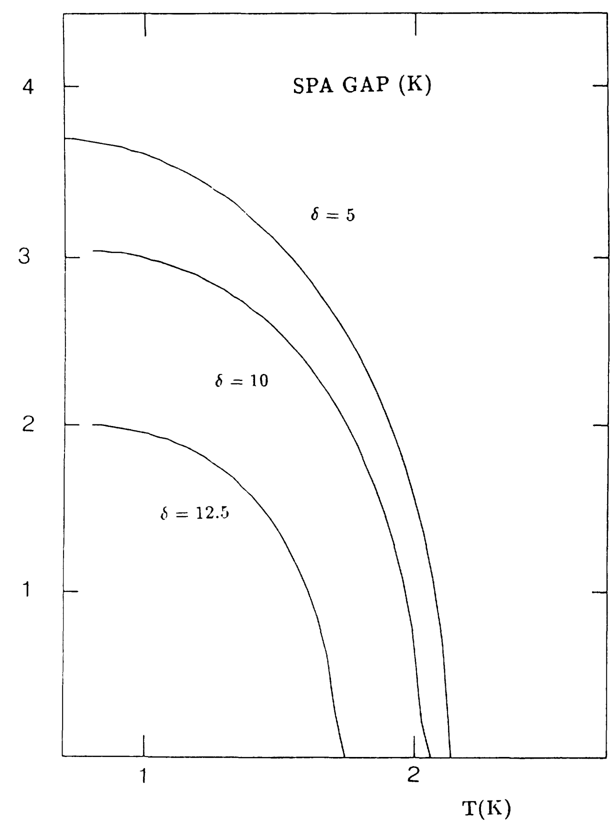

FIG. 1. Gap in K as a function of the temperature for several δ in the SPA.

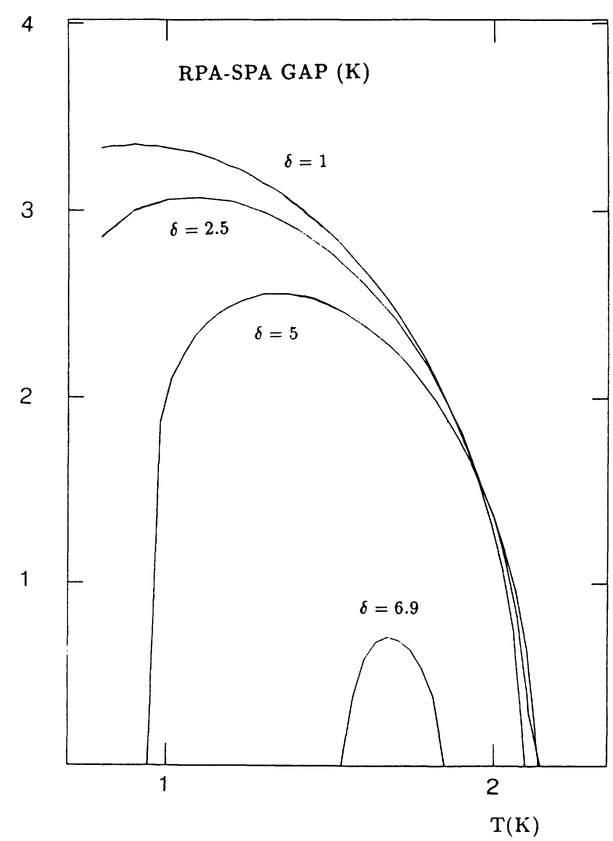

FIG. 2. Gap in K as a function of the temperature for several δ in the RPA-SPA.

ature in the RPA-SPA is roughly constant in the δ region where the superconducting phase exists and that the disappearance of the phase transition is due to the decreasing gap. In other words, quantal fluctuations, induced by finite particle number, affect the gap rather than the critical temperature itself. It should, however, be pointed out that these effects disappear for large systems.

The fact that the maximum of the integrand in the RPA-SPA expression (2.26) is reached for a value of Δ different from the Hartree value can be understood with the following argument. In the RPA-SPA, the effective action to be maximized as a function of Δ is

$$\mathcal{S}_{\rm eff}=\frac{\beta}{\delta}\mathcal{L}+\ln\mathcal{C} \ ,$$

while $\mathcal{L}$ is not very sensitive to the structure of the unperturbed single-particle levels, $\mathcal{C}$ is; depending on the structure of single-particle spectrum, $\mathcal{C}$ can be a strongly picked function of Δ for $\Delta=0$ or have a more complex behavior. In the case of large single-particle level spacing, the static action does not dominate and the maximum of the effective action is reached for $\Delta=0$, that is, this "correlated" mean field is totally dominated by the RPA corrections about the normal phase. For smaller level spacing, the static action tends to dominate and the correlated mean field does not differ from the standard Hartree-Bogoliubov mean field since, as pointed out above, the RPA corrections are roughly independent from the particle number.

In order to display the rather strong dependence of the correlated mean-field from the single-particle spectrum, it is interesting to consider the special case where all levels are degenerate and coupled by the pairing potential. It is easy to show that, at low temperatures, the correlated mean field is smaller than the Hartree-Bogoliubov mean field, but as the temperature is increased, the correlated mean field becomes larger and disappears at a critical temperature slightly higher than the one given by the uncorrelated mean field. The persistency of this effect for large particle numbers on model Hamiltonians which display second-order phase transitions is still under investigation.

As mentioned in the Introduction, quantal fluctuation becomes large at temperatures lower than the critical temperature and eventually the Gaussian quantal corrections to the static path become unstable and higher-order corrections must be taken into account. Physically this represents the onset of tunneling between the normal and the superconducting phases. Thus, the Gaussian quantal corrections included in the RPA-SPA scheme are expected to be stronger around the normal unstable phase. This is in agreement with the disappearance of the gap at low temperatures as shown in Fig. 2.

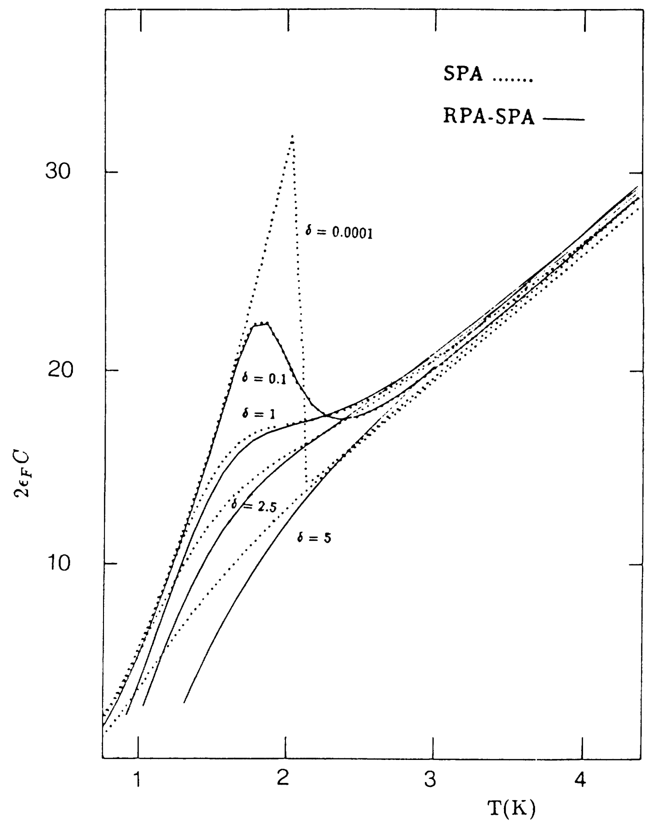

FIG. 3. Specific heat multiplied by $2\varepsilon_F$ in both the SPA and RPA-SPA for several δ values. For small δ the two approaches give the same results.

In Fig. 3 is shown the behavior of the specific heat (multiplied by $2\varepsilon_F$) as a function of the temperature for different δ. Note that fluctuations, both static and quantal, destroy the signature of the phase transition for $\delta<0.1$ K. For the specific heat, no appreciable contribution comes from the quantal fluctuations for the values of δ where the existence of the phase transition can be inferred. Note also that the effect of the quantal fluctuations is to decrease the specific heat, again this is a consequence of the single-particle spectrum which was taken in the calculation.

[1]G. Puddu, P. F. Bortignon, and R. A. Broglia, Ann. Phys. (N.Y.) **206**, 409 (1991).
[2]H. Lipkin, N. Meshkov, and A. Glick, Nucl. Phys. **62**, 188 (1965).
[3]J. W. Negele, Rev. Mod. Phys. **54**, 913 (1982).
[4]B. Muhlschleger, D. J. Scalapino, and R. Denton, Phys. Rev. B **6**, 1767 (1972).
[5]W. P. Halperin, Rev. Mod. Phys. **58**, 553 (1986), and references therein.
[6]A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).