Pairing effects at finite temperature: Fermionic and bosonic contributions to the specific heat of a nucleus

F. Alasia, O. Civitarese, and M. Reboiro
Department of Physics, University of La Plata, 1900 La Plata, Argentina
(Received 30 June 1986)

The behavior of the specific heat, for a system with a finite number of nucleons interacting through a pairing force, is studied. The formalism is based on the finite temperature Bardeen-Cooper-Schrieffer plus random phase approximation treatment of the interaction. The fermionic and bosonic excitations are described, as a function of the temperature, both in the superfluid and normal phases.

I. INTRODUCTION

The study of nuclear properties at nonzero temperatures has been the subject of recent publications.[1-4] The interest in the problem has been motivated in part by the available experimental information about compound nucleus reactions at high energy.[5] From the theoretical side different approaches have been reported in connection with temperature dependent mean field[2,6] and collective[7,8] descriptions in schematic[1] and realistic models.[9-11]

The microscopic description of pairing effects in finite systems has the obvious advantage of a unified picture where fermionic and bosonic degrees of freedom result from the treatment of the same interaction within the Bardeen-Cooper-Schrieffer (BCS) and random phase approximation (RPA) methods, respectively.

The meaning of these effective degrees of freedom, namely, the quasiparticle (fermionic) and correlated RPA (bosonic) excitations, can be understood in terms of the contributions arising from the two-body interaction, which in the present case will be represented by a separable pairing force. The structure of these degrees of freedom, and their evolution at finite temperature, have been discussed in detail in a series of papers[2] which deal with a functional integral representation of the nuclear many-body grand partition function. From the results of these references[2] and from previously reported treatments of pairing effects at finite temperatures,[1,9,10] we shall assume that at relatively low temperatures the most important change with respect to the zero temperature case is given by the collapse of the pairing gap. The consequences of this collapse upon the quasiparticle spectrum are noticeable, and it could be possible to establish some analogies between this effect and the well-known phase transitions in extended systems.[12-14] Therefore, we have to treat the fermionic and bosonic sectors of the pairing Hamiltonian in two temperature domains, namely, at low temperature, before the collapse of the pairing gap, where the fermionic degrees of freedom are described by the BCS approximation, and the bosonic ones, pairing phonons, are described by the quasiparticle RPA; and at high temperatures, where the fermions obey the Fermi-Dirac statistics and the pairing phonons, of the addition and removal type, obey the Planck statistics. In the first case both the quasiparticle and phonon energies are temperature dependent, while in the second case, only the phonon energies are temperature dependent. This is a very important feature which, as we are going to show, influences the low and high temperature behavior of the specific heat. A similar description was advanced years ago by Matsubara,[15] and in his work the pairing Hamiltonian is treated perturbatively, also with the inclusion of a coupling term between fermions and bosons. In our case, since we have adopted the BCS plus RPA treatment, we have neglected this coupling, which is, for finite nucleon numbers, smaller than the independent quasiparticle and phonon terms.

The paper is organized in the following way: in Sec. II we present the theoretical elements of our description; the results are shown in Sec. III; and finally some conclusions are drawn in Sec. IV. For the sake of convenience the details of the formalism are presented in the Appendix.

II. FORMALISM

To start with, let us write the monopole pairing Hamiltonian

$$H=\sum_{jm} e_j a_{jm}^{\dagger} a_{jm} - G \sum_{\substack{j,m>0\\ k,l>0}} a_{jm}^{\dagger} a_{\overline{jm}}^{\dagger} a_{\overline{kl}} a_{kl} \ , \tag{1}$$

where e_j are the single particle energies; $a_{jm}^{\dagger}$ (a_{jm}) are the creation (annihilation) operators for fermions in the single particle orbits denoted by the index j; G is the strength of the monopole pairing force; and the states denoted by $\overline{jm}$ are time reversed single particle states. The Hamiltonian (1) can be written in the quasiparticle basis by following the standard BCS approach at finite temperature,[1,9] and the result is (the details are given in the Appendix)

$$H=H_0+H_{11}+H_{20}+H_{22}+H_{40}+H_{31}+H_{\text{qp-qp}} \ . \tag{2}$$

The behavior of the finite temperature BCS solutions has been discussed in detail in Refs. 1 and 9, and the main difference between this approach and the zero temperature one is due to the thermal collapse of the pairing gap parameter Δ, which occurs at temperatures of the order of $T_c=0.5\Delta(T=0)$.[1,9] Therefore we have to consider two different phases, namely, the superfluid phase, for $T<T_c$, and the normal one, for $T>T_c$. The normal phase would correspond, for the single particle degrees of freedom, to an open shell system partially filled with fermions which obey the Fermi-Dirac statistics. The two quasiparticle excitations, treated in the finite temperature RPA (Refs. 3, 7, and 9) are the solutions of the Hamiltonian

$$H(\mathrm{RPA})=H(\mathrm{qp})+H_{22}+H_{40} \ , \tag{3}$$

which can be written as the harmonic one

$$H(\mathrm{RPA})=H_0(\mathrm{RPA})+\sum_n W_n\Gamma_n^\dagger\Gamma_n \ , \tag{4}$$

where

$$H_0(\mathrm{RPA})=H_0-\sum_{jn} Y_{jn}^2\Omega_j(1-2f_j)W_n \ , \tag{5}$$

and the phonon creation (annihilation) operators $\Gamma_n^\dagger$ (Γ_n) are given by

$$\Gamma_n^\dagger=\sum_j (X_{jn}P_j^\dagger-Y_{jn}P_j) \ ,$$
$$\Gamma_n=(\Gamma_n^\dagger)^\dagger \ . \tag{6}$$

The corresponding definitions are given in the Appendix.

The energies W_n are solutions of the determinant[9]

$$\left\| \begin{matrix} -1+G\sum_j 2\Omega_jK_j^2E_j(1-2f_j)/d_j & GW_n\sum_j\Omega_jK_j(1-2f_j)/d_j \\ GW_n\sum_j\Omega_jK_j(1-2f_j)/d_j & -1+G\sum_j 2\Omega_jE_j(1-2f_j)/d_j \end{matrix} \right\| =0 \ , \tag{7}$$

where $K_j=(U_j^2-V_j^2)$ and $d_j=4E_j^2-W_n^2$.

For values of $T>T_c$ we have to describe explicitly the addition and removal modes[16] of an open shell system, where the phonon energies are given by the solutions of the following equations:

$$\begin{aligned} &\sum_{j>F}\Omega_j(1-2n_j)/(2\epsilon_j-W_{a,n})-\sum_{k\leq F}\Omega_k(1-2n_k)/(2\epsilon_k+W_{a,n})=1/G \ , \\ &\sum_{j>F}\Omega_j(1-2n_j)/(2\epsilon_j+W_{r,n})-\sum_{k\leq F}\Omega_k(1-2n_k)/(2\epsilon_k-W_{r,n})=1/G \ , \end{aligned} \tag{8}$$

where $\epsilon_j=e_j-\lambda$ for $j>F$ and $\epsilon_k=\lambda-e_k$ for $k\leq F$. With the index F we have denoted the position of the Fermi level λ, and $W_{a,n}$ ($W_{r,n}$) are the energies of the addition (removal) excitations. The factors n_j are the fermionic occupation numbers,

$$n_j=[1+\exp(e_j-\lambda)/T]^{-1} \ ,$$

and the phonon addition (removal) creation operators are given by

$$\begin{aligned} \Gamma_{a,n}^\dagger&=\sum_{j>F}a_n(j)B_j^\dagger+\sum_{k\leq F}a_n(k)B_k \ , \\ \Gamma_{r,n}^\dagger&=\sum_{j>F}r_n(j)B_j+\sum_{k\leq F}r_n(k)B_k^\dagger \ , \end{aligned} \tag{9}$$

respectively. The operators $B_j^\dagger$ (B_j) create (annihilate) a pair of fermions. The amplitudes a_n and r_n are defined in the Appendix. For $T>T_c$, and in the basis of addition and removal modes, the RPA Hamiltonian can be written

$$H(\mathrm{RPA})=H_0(\mathrm{RPA})+\sum_n W_{a,n}\Gamma_n^\dagger(a)\Gamma_n(a) + \sum_m W_{r,m}\Gamma_m^\dagger(r)\Gamma_m(r) \ , \tag{10}$$

where

$$H_0(\mathrm{RPA})=H_0(\mathrm{s.p.})-\sum_{m,j>F}\Omega_j(1-2n_j)W_{r,m}\,|r_m(j)|^2+\sum_{n,k\leq F}\Omega_k(1-2n_k)W_{a,n}\,|a_n(k)|^2 \tag{11}$$

is the RPA contribution to the ground state energy, which in the superfluid case corresponds to the quantity H_0(RPA) given by Eq. (5). Both in the normal and superfluid cases the terms H_0(s.p.) and H_0 are the contributions originating in the fermionic sector of the Hamiltonian.

With the above described formalism we can calculate the specific heat. We obtain the following results:

(a) Fermionic contributions to the specific heat at $T<T_c$:

$$\begin{aligned} C=&\sum_j 2\Omega_j(1-f_j)f_jE_j^2/T^2+(d\lambda/dT)\left[N+\sum_j\Omega_j\{(e_j-\lambda)[2(1-f_j)f_j/T+(1-2f_j)/E_j]-1\}\right] \\ &+\Delta(d\Delta/dT)\left[(2/G)-\sum_j\Omega_j[2(1-f_j)f_j/T+(1-2f_j)/E_j]\right] . \end{aligned} \tag{12}$$

(b) Fermionic contributions to the specific heat at $T>T_c$:

$$C=\left[\sum_j 2\Omega_j e_j^2 n_j(1-n_j)-\left[\sum_j 2\Omega_j n_j(1-n_j)e_j\right]^2\Big/\left[\sum_j 2\Omega_j n_j(1-n_j)\right]\right]\Big/T^2 . \tag{13}$$

(c) Bosonic contributions at $T<T_c$: in this case the phonons obey the statistical distribution given by the occupation numbers

$$n_{\text{phonons}}=[\exp(W_n/T)-1]^{-1} ,$$

and in consequence the mean value of the energy can be written as

$$E_{\text{phonons}}=H_0(\text{RPA})+\sum_n W_n n_{\text{phonons}} , \tag{14}$$

and the contribution to the specific heat is given by the value of the derivative

$$C=dE_{\text{phonons}}/dT .$$

(d) Bosonic contributions at $T>T_c$: again in this case the addition and removal phonons obey the Planck statistics, given by the occupation numbers n_{phonons}, where the energies W_n are the solutions of Eq. (8). In consequence we can calculate the contribution to the specific heat from the energy

$$E_{\text{phonons}}=H_0(\text{RPA})+\sum_r W_r n_{\text{phonons}}(W_r)+\sum_a W_a n_{\text{phonons}}(W_a) . \tag{15}$$

We have omitted the detailed formulae of the bosonic contributions because of their lengthy expressions in terms of the formal solutions of the RPA equations.

The other terms of the Hamiltonian, H_{31} and $H_{\text{qp-qp}}$, can be treated perturbatively. The first term, H_{31}, represents the coupling between quasiparticles (fermions) and phonons (bosons), while the second one, $H_{\text{qp-qp}}$, is a residual quasiparticle-quasiparticle interaction.[17]

Let us summarize the results of this section: starting from the Hamiltonian, Eq. (1), we have introduced fermionic and bosonic degrees of freedom by performing the temperature dependent BCS and RPA transformations; the fermionic and bosonic sectors of the transformed Hamiltonian contribute to the total excitation energy and with them we have evaluated the temperature dependence of the specific heat; both fermionic and bosonic contributions have been obtained for values of T above and below the critical value T_c.

III. RESULTS AND DISCUSSION

In this section we shall discuss the results of our calculations for the case of neutrons in the nucleus ^{115}Sn. We have considered the neutron closed shell $N=50$ as the inert core and the particles which are interacting through the pairing force are 15 neutrons in the shell $50\leq N\leq 82$. The single particle levels are taken from Ref. 18 and the pairing coupling constant G is fixed at the value $G=0.16$ MeV. We have obtained for the gap parameter at zero temperature the value $\Delta(T=0)=1.56$ MeV. The solutions of the finite temperature BCS equations are shown in Fig. 1, where the temperature dependent gap parameter is shown as a function of the nuclear temperature T. From the results shown in Fig. 1 we can extract the value $T_c=0.85$ MeV for the critical temperature. The contribution to the excitation energy due to quasiparticle excitations is shown in Fig. 2, together with the bosonic contributions. The dominant contribution to the total excitation energy corresponds to fermionic degrees of freedom, which for $T>T_c$ depends almost linearly on T. The phonon contribution to the total excitation energy is also a linear function of T for $T>T_c$. The behavior of the RPA solutions at both sides of the critical point $T=T_c$ is shown in Fig. 3. In this figure, the temperature dependence of the RPA energies is shown, and, as expected, the more pronounced change as a function of T is exhibited by the superfluid phase, which displays the collapse of the first RPA root, and for the low-energy excitations, a trend similar to that of the gap is observed. For $T>T_c$ the energy splitting of the roots between addition and removal phonons is observed, with the decrease of the excitation energies corresponding to removal phonons and the increase of the excitation energies to addition phonons. The fermionic and bosonic excitations included in this way are the building blocks for the estimate of the total specific heat of the system, which is shown in Fig. 4.

The temperature dependence of the total specific heat, as shown in Fig. 4, suggests a strong analogy with the results of the treatment of pairing correlations in extended systems, particularly with the results of the Landau[13] and Feyman[14] theories of Λ transitions.

In the present case, however, some differences appear as a consequence of the finite size of the single particle space and due to the presence of a finite number of particles. Although the transition between the superfluid $(T<T_c)$

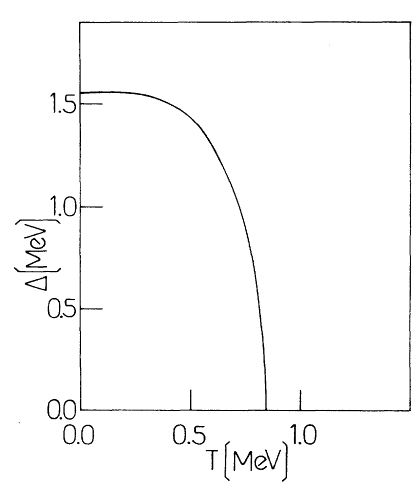

FIG. 1. Pairing gap Δ as a function of the temperature T.

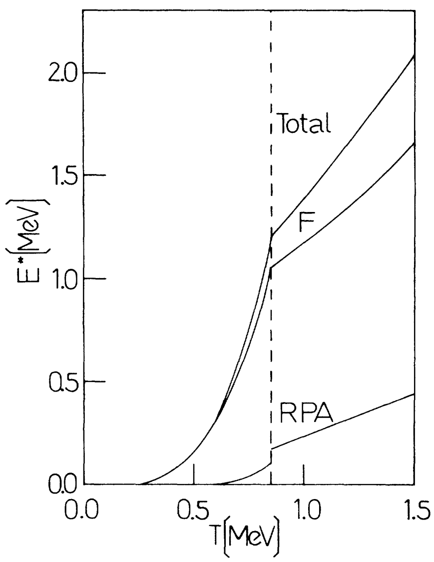

FIG. 2. Excitation energy E^* for the fermionic (F) and bosonic (RPA) degrees of freedom as a function of T. The total value is indicated (Total). The dashed line denotes the value of T_c.

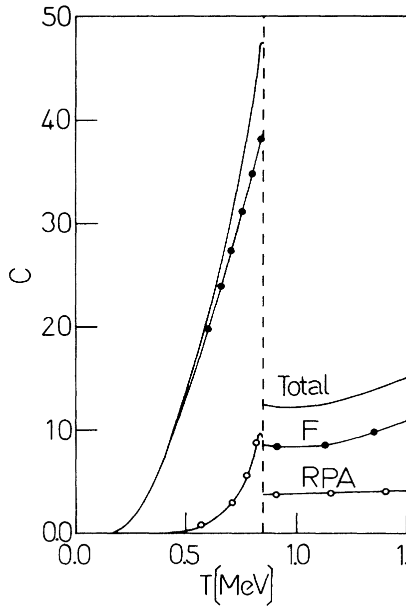

FIG. 4. Specific heat C as a function of the temperature T. The bosonic (RPA) and fermionic (F) contributions are denoted by open and filled circles, respectively, at both sides of the critical temperature T_c, which is denoted by the dashed line. The solid lines at each side of T_c correspond to the total value (Total) of C.

and the normal ($T > T_c$) phases is dominated by the collapse of the pairing gap, at the fermionic level, the bosonic contributions, especially due to the appearance of a vanishing collective energy at the critical temperature, are also important. In fact, the total specific heat receives an appreciable contribution from the bosons near the critical

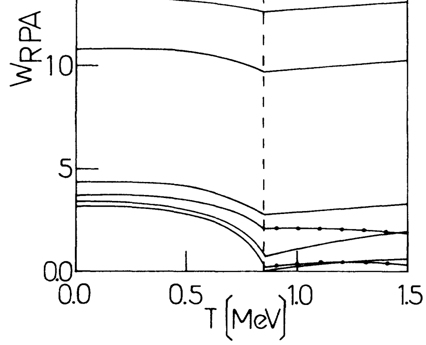

FIG. 3. Temperature dependent RPA solutions. The dashed line indicates the value of T_c, and in the normal phase ($T > T_c$) the solid lines correspond to addition modes and the dotted lines correspond to removal modes.

temperature. The value of the derivative of the specific heat is of the order of 40 MeV^{-1}, while for infinite systems, the same derivative is of the order of 60 MeV^{-1},[13] a value which is obtained when the corresponding formulae are written in comparable units, again a remarkable analogy to the above-mentioned theories of Λ transitions. This is a particularly interesting result because we are not dealing here with real bosons; instead, the bosonic degrees of freedom result from the linearization of two quasiparticle excitations within the RPA method. Finally, it should be noted that the specific heat displays a peak value as a function of T, a feature which has been associated with the fact that we are dealing with nucleons which are bound.[19]

IV. CONCLUSIONS

In order to summarize the results of the preceding section we can conclude as follows:

(1) The fermionic excitations display a transition from the superfluid to the normal phase which occurs at the critical temperature T_c. The signature of this phase transition is given by the increase of the specific heat near the critical temperature. The bosonic, temperature dependent spectrum shows the effect of the collapse of pairing correlations and also contributes to the specific heat near the critical temperature.

(2) At $T > T_c$ two quasiparticle excitations split up into addition and removal modes built on top of partially filled single particle states.

(3) The features of the fermionic and bosonic contributions to the specific heat near the critical point $T=T_c$ are similar to the same contributions in extended systems. We hope that these results can be of some use in connection with the problem of the temperature dependence of nuclear level densities,[10] particularly in view of the relationship between the specific heat and the level density parameter.

APPENDIX

A. Temperature dependent BCS equations

The finite temperature BCS treatment of the monopole pairing Hamiltonian gives the following results:[1,9]

$$\begin{aligned}
H_0 &= \sum_j (e_j-\lambda)2\Omega_j[U_j^2 f_j + V_j^2(1-f_j)] - \Delta^2/G , \\
H_{11} &= \sum_j [(e_j-\lambda)(U_j^2-V_j^2)+2U_jV_j]\hat{N}_j , \\
H_{20} &= \sum_j [(e_j-\lambda)2U_jV_j+(U_j^2-V_j^2)\Delta](\hat{P}_j^\dagger+\hat{P}_j) , \\
H_{22} &= \sum_{i,j} [-(G/2)(U_j^2U_i^2+V_j^2V_i^2)(\hat{P}_j^\dagger\hat{P}_i+\hat{P}_i^\dagger\hat{P}_j)] , \\
H_{40} &= \sum_{i,j} [(G/2)(U_j^2V_i^2+U_i^2V_j^2)(\hat{P}_i^\dagger\hat{P}_j^\dagger+\hat{P}_j\hat{P}_i)] , \\
H_{31} &= \sum_{i,j} [GU_iV_i(U_j^2-V_j^2)(\hat{N}_i\hat{P}_j+\hat{P}_j^\dagger\hat{N}_i)] , \\
H_{\text{qp-qp}} &= \sum_{i,j} (-GU_iU_jV_iV_j\hat{N}_i\hat{N}_j) ,
\end{aligned} \tag{A1}$$

where

$$\begin{aligned}
&\hat{N}_j = \sum_m \alpha_{jm}^\dagger\alpha_{jm} , \quad \hat{P}_j^\dagger = \sum_{m>0} \alpha_{jm}^\dagger\alpha_{j\bar{m}}^\dagger , \\
&\hat{P}_j = (\hat{P}_j^\dagger)^\dagger .
\end{aligned} \tag{A2}$$

The operators $\alpha_{jm}^\dagger$ (α_{jm}) are quasiparticle creation (annihilation) operators and the thermal averages f_j are defined by the expectation value

$$f_j = \langle \alpha_{jm}^\dagger \alpha_{jm} \rangle_T . \tag{A3}$$

The structure of the gap parameter Δ, the BCS occupation numbers U_j and V_j, and the quasiparticle energies E_j are determined by the variational treatment of the Hamiltonian

$$H(\text{qp}) = H_{11} + H_{20} = \sum_{jm} E_j \alpha_{jm}^\dagger \alpha_{jm} , \tag{A4}$$

with the condition $H_{20}=0$; their values are given by

$$\begin{aligned}
&E_j = [(e_j-\lambda)^2+\Delta^2]^{1/2} , \\
&U_j^2 = \tfrac{1}{2}[1+(e_j-\lambda)/E_j] , \\
&V_j^2 = 1-U_j^2 , \\
&\Delta = G\sum_j \Omega_j U_j V_j (1-2f_j) ,
\end{aligned} \tag{A5}$$

with $\Omega_j = j+\frac{1}{2}$, and

$$f_j = [1+\exp(E_j/T)]^{-1} , \tag{A6}$$

where the temperature T is given in units of energy.

The parameter λ is the Lagrange multiplier associated with the conservation of the average number of particles, which at finite T can be written as

$$N = \sum_j 2\Omega_j[U_j^2 f_j + (1-f_j)V_j^2] . \tag{A7}$$

B. Finite temperature RPA equations

The forward and backward going amplitudes of the correlated two quasiparticle excitations are defined by[9]

$$\begin{aligned}
X_{jn} &= \Lambda_n[a_n(U_j^2-V_j^2)-b_n]/(2E_j-W_n) , \\
Y_{jn} &= \Lambda_n[a_n(U_j^2-V_j^2)+b_n]/(2E_j+W_n) ,
\end{aligned} \tag{A8}$$

respectively. The normalization constant Λ_n is given by

$$\Lambda_n = \left[\sum_j \Omega_j(1-2f_j) \left\{ \frac{[a_n(U_j^2-V_j^2)-b_n]^2}{(2E_j-W_n)^2} - \frac{[a_n(U_j^2-V_j^2)+b_n]^2}{(2E_j+W_n)^2} \right\} \right]^{-1/2} , \tag{A9}$$

where

$$\begin{aligned}
a_n &= GW_n \sum_j \left[\frac{(U_j^2-V_j^2)\Omega_j(1-2f_j)}{4E_j^2-W_n^2} \right] , \\
b_n &= -1 + G\sum_j \left[\frac{(U_j^2-V_j^2)^2 2E_j\Omega_j(1-2f_j)}{4E_j^2-W_n^2} \right] .
\end{aligned} \tag{A10}$$

For temperatures higher than T_c the amplitudes of the addition and removal pairing modes are given by

$$\begin{aligned}
a_n(j) &= \Lambda_n(a)/(2\epsilon_j - W_{a,n}) , \\
a_n(k) &= -\Lambda_n(a)/(2\epsilon_k + W_{a,n}) , \\
r_n(j) &= -\Lambda_n(r)/(2\epsilon_j + W_{r,n}) , \\
r_n(k) &= \Lambda_n(r)/(2\epsilon_k - W_{r,n}) ,
\end{aligned} \tag{A11}$$

with the normalization factors for addition and removal modes

$$\Lambda_n(a)=\left[\sum_{j>F}\Omega_j(1-2n_j)/(2\epsilon_j-W_{a,n})^2 + \sum_{k\leq F}\Omega_k(1-2n_k)/(2\epsilon_k+W_{a,n})^2\right]^{-1/2},$$

$$\Lambda_n(r)=\left[-\sum_{j>F}\Omega_j(1-2n_j)/(2\epsilon_j+W_{r,n})^2 - \sum_{k\leq F}\Omega_k(1-2n_k)/(2\epsilon_k-W_{r,n})^2\right]^{-1/2}, \quad \text{(A12)}$$

respectively. Equations (A11) and (A12) correspond to the finite temperature version of the formalism which has been presented in Ref. 16.

ACKNOWLEDGMENTS

This work was partially supported by CONICET (Argentina) and by the CICPBA (Argentina). M. Reboiro and O. Civitarese are fellows of the CONICET (Argentina); F. Alasia is fellow of the CICPBA (Argentina).

[1]A. L. Goodman, Nucl. Phys. **A352**, 30 (1981); **A352**, 45 (1981); Phys. Rev. C **29**, 1887 (1984).

[2]A. K. Kerman, S. Levit, and T. Troudet, Ann. Phys. (N.Y.) **148**, 436 (1983); A. K. Kerman and T. Troudet, *ibid.* **154**, 456 (1984), and references therein; T. Troudet, Nucl. Phys. **A441**, 676 (1985).

[3]D. Vautherin and N. Vinh Mau, Nucl. Phys. **A422**, 140 (1984); Phys. Lett. **120B**, 263 (1983).

[4]P. Bonche, S. Levit, and D. Vautherin, Nucl. Phys. **A436**, 265 (1985).

[5]J. Rekstad *et al.*, Phys. Lett. **117B**, 382 (1982); Phys. Scr. **T.5**, 45 (1983); Nucl. Phys. **A417**, 376 (1984).

[6]M. Brack and P. Quentin, Nucl. Phys. **A361**, 35 (1981).

[7]O. Civitarese, R. A. Broglia, and C. H. Dasso, Ann. Phys. (N.Y.) **156**, 142 (1984).

[8]W. Besold, P. G. Reinhart, and C. Toepffer, Nucl. Phys. **A431**, 1 (1984).

[9]O. Civitarese, G. G. Dussel, and R. P. J. Perazzo, Nucl. Phys. **A404**, 15 (1983).

[10]O. Civitarese and A. L. De Paoli, Nucl. Phys. **A440**, 480 (1985).

[11]G. Bozzolo and O. Civitarese, Phys. Rev. C **32**, 2111 (1985).

[12]P. G. De Gennes, *Superconductivity of Metals and Alloys* (Benjamin, New York, 1966), Chap. 4.

[13]L. D. Landau and E. Lifschitz, *Statistical Mechanics* (Pergamon, New York, 1959), Sec. 59.

[14]R. P. Feyman, *Statistical Mechanics* (Benjamin, Reading, Mass., 1972), p. 33, 343–350.

[15]T. Matsubara, Prog. Theor. Phys. **14**, 351 (1955).

[16]D. R. Bes and R. A. Broglia, Nucl. Phys. **80**, 289 (1968).

[17]We do not evaluate them in the present work and their effects will be discussed in a forthcoming paper in relation with the evaluation of single quasiparticle widths at finite temperature.

[18]R. A. Uher and R. A. Sorensen, Nucl. Phys. **86**, 1 (1966).

[19]O. Civitarese, G. G. Dussel, and A. Zuker, submitted to Phys. Rev. C.