# Variational treatment of retarded phonon-induced electron pairing

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To treat the phonon-induced electron pairing in a way which allows for vortex corrections and retardation effects, we develop a method using a canonical transformation involving a variational function. This method is expected to be useful for developing a unified theory for phonon-induced electron pairing ranging between adiabatic and nonadiabatic behavior, or, respectively, between Copper-pair condensation in momentum space and bipolaron condensation in real space. To demonstrate the power of our variational treatment we determine for a model pairing potential, involving a temperature-dependent energy cutoff c(T) as a variational parameter, the thermodynamical properties of the conventional intermediate- and strong-coupling superconductors. Thus, we obtain results which compare well with those obtained by solving the Eliashberg equations.

### I. INTRODUCTION

The standard microscopic theory for superconductivity has been developed by Bardeen Cooper, and Schrieffer (BCS).<sup>1</sup> This theory was then generalized by Migdal and Eliashberg (ME).<sup>2,3</sup> Retardation and many-body effects of the electron-phonon interaction were included to some extent. In these theories only those electrons near the Fermi surface form strongly overlapping Cooper pairs. The coherence length  $\xi_0$  was such that  $\xi_0 k_F \sim 10^3 - 10^4$ , where  $k_F$  is the Fermi wave vector and  $k_F^{-1}$  the average distance between two electrons. Thus all thermodynamical and electrodynamical properties of the conventional superconductors were determined rather well.<sup>4,5</sup> This extraordinary success of the BCS and ME theories relies on the fact that  $\omega_{\rm ph}/E_F < 0.01$  and that then vertex renormalization of the electron-phonon coupling can be neglected ( $\omega_{ph}$  is a characteristic phonon energy). If, however, the electron-phonon coupling gets stronger, the adiabaticity of the coupling should break down due to the so-called local-lattice instability and then rather than Cooper pairs small polarons and bipolarons should form.<sup>6</sup> Theories for superconductivity involving small polarons and bipolarons have been developed in which all electrons in the Fermi sea pair with a short coherence length of the order of  $\xi_0 \sim 10k_F^{-1}$  (for smaller polarons) or smaller  $(\xi_0 \rightarrow 0 \text{ for small bipolarons})$ .<sup>7-12</sup> These small polaron and bipolaron theories do not yield the BCS theory in the weak-coupling and  $\omega_{\rm ph}/E_F \ll 1$  limit. Therefore it would be interesting to develop a unified theory yielding both BCS-type Cooper pair and bipolaron condensations. Note that after the discovery of high- $T_c$  oxides and other exotic high- $T_c$  materials such as doped fullerenes with very short coherence length  $\xi_0$ , some authors argued that superconductors with a size  $\xi_0$  for its pairs (to be of the order of  $10k_F^{-1}$  and comparable to the average interparticle spacing) exhibit behavior in between that of large overlapping Cooper pairs  $(\xi_0 k_F \gg 1)$  and that of Bose condensation of tightly bound bipolarons  $(\xi_0 k_F \sim 1)$ .<sup>13-15</sup> There are several papers dealing with the crossover

behavior between Cooper-pair and bipolaron condensation by using the negative-U Hubbard model or a twobody model attraction potential.<sup>13-15</sup> However, the important retardation of the electron-phonon coupling has been completely neglected.

Here we present a theory of superconductivity due to electron-phonon coupling which includes retardation effects and is expected to yield in the weak-coupling and  $\omega_{\rm ph}/E_F \ll 1$  limit Cooper-pair condensation and to yield for strong coupling also bipolaron condensation. Furthermore, this theory is expected to work also in the crossover regime. Using a canonical transformation together with a variational function, we determine the retarded phonon-induced attractive electron interaction. The variational function acts like a control parameter regulating adiabatic or nonadiabatic behavior. To demonstrate the usefulness of our approach, we use an approximation for the variational function such that we obtain an effective paring potential, similar to the one in BCS theory, describing an attractive interaction between electrons within an energy layer of width 2c(T) around the chemical constant  $\mu$ . Here c(T) is a temperaturedependent variational parameter to be determined such that the free energy becomes minimal. Thus, taking c(T)to be of the order of the Debye energy  $\omega_D$ , we calculate various quantities and compare with results obtained by using the Eliashberg theory. We show that for  $c \sim D$  one might get bipolaron condensation (D = bandwidth ofelectrons).

In Sec. II we outline our theory, in Sec. III we present results, and in Sec. IV we give our conclusions. Details of our analysis are given in the Appendix. We put  $\hbar = 1$ and  $k_B = 1$ .

#### **II. THEORY**

We start by using the Fröhlich Hamiltonian

$$H = \sum_{q,\gamma} \omega_{q,\gamma} b^{\dagger}_{q\gamma} b_{q\gamma} + \sum_{k,\sigma} (\epsilon_k - \mu) d^{\dagger}_{k\sigma} d_{k\sigma} + \frac{1}{\sqrt{N}} \sum_{q,\gamma} \sum_{k,\sigma} g_{q\gamma} (b^{\dagger}_{-q\gamma} + b_{q\gamma}) d^{\dagger}_{k+q\sigma} d_{k\sigma} .$$
(1)

The operator  $d_{k\sigma}^{\dagger}(d_{k\sigma})$  creates (annihilates) an electron with wave vector k and spin  $\sigma$ .  $\epsilon_k$  is the electron energy, and  $\mu$  is the chemical potential.  $b_{q\gamma}^{\dagger}(b_{q\gamma})$  creates (annihilates) a phonon of the  $\gamma$ th branch with frequency  $\omega_{q\gamma}$ .  $g_{q\gamma}$  is the electron-phonon coupling constant. In order to determine the thermodynamical properties of superconductors from a variational method, we derive the corresponding free energy F using Bogoliubov's thermodynamical variational principle:<sup>16</sup>

$$F(T) < F_0(T) = -\frac{1}{\beta} \ln \operatorname{Tr}[\exp(-\beta H_0)] + \operatorname{Tr}[\exp(-\beta H_0)(H - H_0)] + \mu N_e , \quad (2)$$

with  $\beta = 1/T$ ,  $N_e$  is the total number of electrons, and where  $F_0$  is an upper bound of the free energy F(T). Here  $H_0$  is a trial Hamiltonian approximating the original Hamiltonian H. We introduce a unitary operator  $\exp[-S(T)]$  and write

$$H_0 = \exp[-S(T)]H'_0 \exp[S(T)] .$$
 (3)

We will use S(T) to introduce a variational function. Then one can rewrite  $F_0(T)$  as

$$F_{0}(T) = -\ln \operatorname{Tr} \{ \exp[S(T)] \exp(-\beta H_{0}) \exp[-S(T)] \} + \operatorname{Tr} \{ \exp[S(T)] \exp(-\beta H_{0}) \exp[-S(T)] \exp[S(T)] (H - H_{0}) \exp[-S(T)] \} + \mu N_{e}$$

$$= -\frac{1}{\beta} \ln \operatorname{Tr} [\exp(-\beta H_{0}')] + \operatorname{Tr} [\exp(-\beta H_{0}') (H' - H_{0}')] + \mu N_{e} , \qquad (4)$$

where

$$H' = \exp[S(T)]H \exp[-S(T)] .$$
<sup>(5)</sup>

The unitary transformation in Eq. (5) is performed by using

$$S(T) = \frac{1}{\sqrt{N}} \sum_{q,\gamma} \sum_{k,\sigma} \frac{g_{q\gamma}}{\omega_{q\gamma}} (b^{\dagger}_{-q\gamma} - b_{q\gamma}) \delta(k+q,k) d^{\dagger}_{k+q\sigma} d_{k\sigma} .$$
(6)

Here we introduce the variational function  $\delta(k', k)$ , which is a function of the energies of the incoming and outgoing electrons in the electron-phonon scattering process. Note that Eq. (6) corresponds to the usual unitary transformation yielding the effective attractive electronelectron interaction. This is a generalization of an incomplete Lang-Firsov transformation and accounts for finite phonon frequency effects or retardation effects. Depending on the choice for the variational function, we can describe the antiadiabatic limit  $(\omega \rightarrow \infty) \ \delta \rightarrow 1$  and the adiabatic limit  $(\omega \rightarrow 0) \delta \rightarrow 0$ . The variational function measures the polaron effect, i.e., the amount of lattice deformation caused by the electron. The effective electron-electron attraction results from the response of the lattice to the motion of the electrons, i.e, the nonadiabatic part of the electron-phonon interaction ( $\delta \neq 0$ ). Note that  $F_0(T)$  involves the Fröhlich Hamiltonian and not the reduced BCS Hamiltonian.<sup>1</sup>

The thermodynamical variational principle means that the variational function introduced by the unitary operator  $\exp[-S(T)]$  should be adjusted so that  $F_0(T)$  reaches a stable minimum. Note that the variational function is only used for  $H_0$ , while all parameters in H remain fixed. Using now the transformation S(T), we get

$$H' = H^0 + H^1 + [S, H^0] + [S, H^1] + \frac{1}{2}[[H^0, S], S] + O(g_{av}^3).$$

Here we have used  $H = H^0 + H^1$ , where  $H^1$  describes the interaction. The first-order terms in the transformed Hamiltonian H' are

$$H^{1} + [S, H^{0}] = \frac{1}{\sqrt{N}} \sum_{q\gamma} \sum_{k,\sigma} g_{q\gamma} (b^{\dagger}_{-q\gamma} + b_{q\gamma}) d^{\dagger}_{k+q\sigma} d_{k\sigma} - \frac{1}{\sqrt{N}} \sum_{q\gamma} \sum_{k,\sigma} g_{q\gamma} \delta(k+q,k) (b^{\dagger}_{-q\gamma} + b_{q\gamma}) d^{\dagger}_{k+q\sigma} d_{k\sigma} + \frac{1}{\sqrt{N}} \sum_{q\gamma} \sum_{k,\sigma} \frac{g_{q\gamma}}{\omega_{q\gamma}} (\epsilon_{k} - \epsilon_{k+q}) \delta(k+q,k) (b^{\dagger}_{-q\gamma} - b_{q\gamma}) d^{\dagger}_{k+q\sigma} d_{k\sigma} .$$

$$(7)$$

The variational function  $\delta$  can now be chosen such that the first two terms in Eq. (7) cancel for the states k and k+q within a range c(T) around the Fermi energy. For these states close to  $E_F$  giving low-energy excitations, the response of the lattice is strong and described in the antiadiabatic regime. On the other hand, for large excitation energies the behavior is rather adiabatic, because the response to the lattice is too slow to follow them. Correspondingly, we take

$$\delta(k',k) = \begin{cases} 1 & \text{if } |\epsilon_k - \mu| \le c(T), |\epsilon_{k'} - \mu| \le c(T) ,\\ 0 & \text{otherwise} . \end{cases}$$
(8)

The variational parameter c(T) is a temperaturedependent energy cutoff and should be of the order of the phonon energy. The third term on the right-hand side of Eq. (7) includes a factor  $(\epsilon_k - \epsilon_{k+q})$ , and so it is approximately zero when both  $\epsilon_k$  and  $\epsilon_{k+q}$  are within a layer of width 2c(T) near the Fermi surface. Then  $\{H^1+[S,H^0]\}$  can be neglected. The second-order terms in the equation for H' are given in the Appendix. Note that the residual term in Eq. (7) resulting from states away from  $E_F$  in the adiabatic regime  $[\delta(k+q,k)=0]$ contains the possibility of change-density waves corresponding to  $\langle c_{k+q\sigma}^{\dagger}c_{k\sigma}\rangle \neq 0$ . We will not consider such states here. Now, keeping only terms which renormalize the kinetic energy and the Cooper pairing contribution, we get  $H' \approx H'_0$ , with

$$H_{0}^{\prime} = \sum_{q,\gamma} \omega_{q\gamma} b_{q\gamma}^{\dagger} b_{q\gamma} + \sum_{k,\sigma} (\epsilon_{k} - \mu) \rho_{k} d_{k\sigma}^{\dagger} d_{k\sigma}$$
$$- \sum_{k} V_{k',k} (d_{k\uparrow}^{\dagger} d_{-k\downarrow}^{\dagger} d_{k'\uparrow} d_{k'\downarrow}^{\dagger} + \text{H.c.}) . \qquad (9)$$

Here  $\rho_k$  is the energy-dependent renormalization factor resulting from the polaron effect and is given by

$$\rho_{k} = 1 - \frac{1}{N} \sum_{q,\gamma} \frac{g_{q\gamma}^{2}}{\omega_{q\gamma}} [2n(\omega_{q\gamma}) + 1] \delta^{2}(k+q,k) , \quad (10)$$

with  $n(\omega)=1/[\exp(\beta\omega)-1]$ , and the interaction potential is given by

$$V_{k'k_{j}} = \frac{1}{N} \sum_{q} \frac{2g_{q}^{2}}{\omega_{q}} \delta(k',k)$$

Note that  $H'_0$  is different from the reduced BCS Hamiltonian<sup>1</sup> due to the renormalization factor  $\rho_k$ . Furthermore, both the kinetic energy and interaction  $V_{k',k}$  are affected by the variational function  $\delta(k',k)$ , e.g., by the cutoff c(T).  $V_{k',k}$  is illustrated in Fig. 1. While it has the same form as in BCS theory, the cutoff c(T) may differ. Using the mean-field approach, Eq. (9) can be rewritten as usual:



FIG. 1. Effective potential  $V(\epsilon_k, \epsilon_k)$  for phonon-induced attraction of two electrons with energies  $\epsilon'_k$  and  $\epsilon_k$  and opposite spin. c(T) and  $\mu$  denote the variational cutoff parameter and chemical energy, respectively.

with

$$\Delta_k = \sum_{i'} V_{k',k} \langle d_{k'\uparrow} d_{-k'\downarrow} \rangle \; .$$

Now, with these results and neglecting all terms of higher order than  $g_{g\gamma}^2$ , one gets

$$F_{0}(T) = E_{0} - \frac{2}{\beta} \sum_{k} \ln[1 + \exp(-\beta \sqrt{E_{k}^{2} + \Delta_{k}^{2}})]$$
$$- \sum_{k} \sqrt{E_{k}^{2} + \Delta_{k}^{2}}$$
$$+ \frac{1}{2} \sum_{k} \frac{\Delta_{k}^{2}}{\sqrt{E_{k}^{2} + \Delta_{k}^{2}}} \tanh\left[\frac{\beta}{2}\sqrt{E_{k}^{2} + \Delta_{k}^{2}}\right]$$
$$- \lambda' N(0)c^{2}N, \qquad (11)$$

where N is the total number of cells,  $E_0$  is a constant, and  $E_k = (\epsilon_k - \mu)\rho_k$ . The gap equation is given by

$$\Delta_{k} = \frac{1}{2N} \sum_{k'} V_{k',k} \frac{\Delta_{k'}}{\sqrt{E_{k'}^{2} + \Delta_{k'}^{2}}} \tanh\left[\frac{\beta}{2}\sqrt{E_{k'}^{2} + \Delta_{k'}^{2}}\right] .$$
(12)

Note the nonperturbative properties of the superconductivity theory (e.g., the exponential dependence of the gap function on the coupling is hidden in this equation). Using for simplicity and also for comparison with other results an Einstein model for the phonons  $(g_{q\gamma}=g_0, \omega_{q\gamma}=\omega_0), \rho_k$  becomes

$$\rho k = \begin{cases} 1 - \lambda' [2n(\omega_0) + 1] c(T) / \omega_0 & \text{if } |\epsilon_k - \mu| \le c(T) , \\ 1 & \text{otherwise} , \end{cases}$$

(13)

where  $\lambda' = 2g_0^2 N(0)/\omega_0$  and N(0) is the bare electron density of states at the Fermi surface. Then  $V_{k',k}$  is given by

$$V_{k',k} = \frac{2g_0^2}{\omega_0} \delta(k',k) .$$
 (14)

The effect of a direct Coulomb repulsion<sup>17</sup> can be included by rewriting Eq. (14) as

$$V_{k',k} = \frac{2g_0^2}{\omega_0} \delta(k'k) - U , \qquad (15)$$

where U involves a cutoff D different from c(T). D is of the order of the Fermi energy. With this form for  $V_{k',k}$ , the gap function becomes

$$\Delta_{k} = \begin{cases} \Delta_{0} , & |\boldsymbol{\epsilon}_{k} - \boldsymbol{\mu}| \leq c(T) , \\ -\Delta_{1} , & c(T) < |\boldsymbol{\epsilon}_{k} - \boldsymbol{\mu}| \leq D . \end{cases}$$
(16)

Substituting Eq. (15) into Eq. (12) and Eqs. (A9)-(A13), we get

$$\frac{1}{\lambda' - \mu^*} = \int_0^{c(T)} d\epsilon \frac{1}{\sqrt{\epsilon^2 \rho^2 + \Delta_0^2}} \tanh\left[\frac{\beta}{2}\sqrt{\epsilon^2 \rho^2 + \Delta_0^2}\right],$$
(17)

$$\mu^* = \frac{\mu_0}{1 + \mu_0 \ln[D/c(T)]} , \qquad (18)$$

where  $\mu_0 = UN(0)$ . With this, we have now completed the determination of  $F_0(T)$  [Eq. (11)]. Note that to obtain a stable minimum of the free energy  $F_0$  we have to adjust the variational parameter c(T) at each T.

From  $F_0(T)$  we determine all thermodynamical quantities. The results of such a determination are the following. First, for T=0 we find in the *normal state*  $(\Delta_0=0)$ , for the cutoff parameter,

$$c_n(0) = 2\omega_0/3 \tag{19}$$

and, for the free-energy,

$$F_0(0)_n = -4N(0)\lambda'\omega_0^2/27 . \qquad (20)$$

These results indicate that even for the normal state (n) the cutoff is a finite quantity and leads to a renormalized density of states,

$$N(0) \rightarrow N(0) / \rho_n . \tag{21}$$

For the superconducting state  $(\Delta_0 \neq 0)$ , we have [see (A19) and (A21)]

$$\Delta_0(0) = c_s(0)\rho_s(0) / \sinh\left[\frac{\rho_s(0)}{\lambda' - \mu^*}\right], \qquad (22)$$

$$\rho_{s}(0) = 1 - \lambda' \frac{c_{s}(0)}{\omega_{0}} , \qquad (23)$$

and the equation determining the cutoff  $c_s(T)$  [see (A22)]:

$$2(1-\lambda') - \left[2-3\lambda'\frac{c_s(0)}{\omega_0}\right] \operatorname{coth} \left[\frac{\rho_s(0)}{\lambda'-\mu^*}\right] - \frac{\lambda'\Delta_0^2(0)}{\omega_0 c_s(0)\rho_s(0)(\lambda'-\mu^*)} + \left[\frac{\Delta_0(0)\mu^*}{c_s(0)(\lambda'-\mu^*)}\right]^2 = 0.$$
(24)

When  $\rho_s(0)/(\lambda'-\mu^*) \gg 1$ , Eq. (22) reduces to (in BCS weak-coupling theory)

$$\Delta_0(0) = 2c_s(0)\rho_s(0)\exp\left[\frac{\rho_s(0)}{\lambda'-\mu^*}\right] . \qquad (25)$$

Second, for  $T \rightarrow T_c$ ,  $\Delta(T) \rightarrow 0$ , and then  $T_c$  is determined by [see (A23) and (A24)]

$$\frac{1}{\lambda' - \mu^*} = \int_0^{c(T_c)} d\epsilon \frac{1}{\rho(T_c)\epsilon} \tanh\left[\frac{\rho(T_c)\epsilon}{2T_c}\right], \quad (26)$$

$$\rho(T_c) = 1 - \lambda' [2n(\omega_0) + 1] \frac{c(T_c)}{\omega_0} .$$
(27)

When  $c(T_c)\rho(T_c)/T_c \gg 1$ , the integral in Eq. (26) can be done analytically and we get a similar result as in the BCS weak-coupling theory:

$$T_c = 1.134c(T_c)\rho(T_c)\exp\left[\frac{\rho(T_c)}{\lambda' - \mu^*}\right].$$
 (28)

Third, for the general case  $0 < T < T_c$ , we have, for the normal state  $[\Delta_0(T)=0]$  [see (A26) and (A27)],

$$F_{0}(T)_{n} = N(0)(1-\lambda')c_{n}^{2}(T) - N(0)c_{n}^{2}(T)\rho_{n}(T)$$

$$-4TN(0)\int_{c_{n}(T)}^{D}d\epsilon \ln\left[1+\exp\left[-\frac{\epsilon}{T}\right]\right]$$

$$-4TN(0)\int_{0}^{c_{n}(T)}d\epsilon \ln\left[1+\exp\left[-\frac{\rho_{n}(T)\epsilon}{T}\right]\right],$$
(29)

$$\rho_n(T) = 1 - \lambda' [2n(\omega_0) + 1] \frac{c_n(T)}{\omega_0} .$$
(30)

For the superconducting state, we find [see Eqs. (A28), (A29), and (A30)]

$$\frac{1}{\lambda'-\mu^{tar}} = \int_0^{c_s(T)} d\epsilon \frac{1}{\sqrt{\epsilon^2 \rho_s^2(T) + \Delta_0^2(T)}} \tanh\left[\frac{\beta}{2}\sqrt{\epsilon^2 \rho_s^2(T) + \Delta_0^2 T}\right],\tag{31}$$

$$F_{0}(T)s_{s} = N(0)(1-\lambda')c_{s}^{2}(T) - N(0)c_{s}(T)\sqrt{c_{s}^{2}(T)\rho_{s}^{2}(T) + \Delta_{0}^{2}(T)} - N(0)N(0)\frac{\Delta_{0}^{2}(T)}{\rho_{s}(T)}\ln\frac{c_{s}(T)\rho_{s}(T) + \sqrt{c_{s}^{2}(T)\rho_{s}^{2}(T) + \Delta_{0}^{2}(T)}}{\Delta_{0}(T)} + N(0)\frac{\Delta_{0}^{2}(T)}{\lambda' - \mu^{*}} - 4TN(0)\int_{c_{s}(T)}^{D}d\epsilon \ln\left[1 + \exp\left[-\frac{\epsilon}{T}\right]\right] - 4TN(0)\int_{0}^{c_{s}(T)}d\epsilon \ln\left[1 + \exp\left[-\frac{\sqrt{\rho_{s}^{2}(T)\epsilon^{2} + \Delta_{0}^{2}(T)}}{T}\right]\right],$$
(32)

$$\rho_{s}(T) = 1 - \lambda' [2n(\omega_{0}) + 1] \frac{c_{s}(T)}{\omega_{0}} .$$
(33)

Note again that the variational parameters  $c_n(T)$  and  $C_s(T)$  must be determined by minimizing  $F_0(T)_n$  and  $F_0(T)_s$ , respectively.

These results are now used for numerical calculations of the gap function, the critical magnetic field, and the specific heat.

## **III. RESULTS**

To check the validity of our approach, we compare for conventional intermediate- and strong-coupling superconductors our results obtained by using the formulas given in Sec. II with those obtained by solving the Eliashberg equations. Since we choose  $D/\omega_0 \gg 1$ , we refer to the adiabatic limit. The numerical results shown in Table I were calculated by using  $\lambda'$  and the corresponding  $\mu^*$  as input parameters. Note that these are not variational parameters and are chosen such that the observed  $T_c$  is obtained in deriving  $H'_0$ . (For the ratio  $D/\omega_0$  we take 100 in all calculations.) The ratio  $T_c/\omega_0$  [as well as  $2\Delta_0(0)/T_c$ ] is a measure of the coupling strength. The BCS weak-coupling limit corresponds to  $T_c/\omega_0 \rightarrow 0$ . Note that the critical field  $H_c$  is related to the condensation energy  $H_c^2(T)/8\pi = F_0(T)_n - F_0(T)_s$ . (The BCS value of this ratio is 0.168.) The normalized jump in the specific heat at  $T_c$  is given by

$$\Delta C(T_c)/C_n(T_c) = [C_s(T_c) - C_n(T_c)]/C_n(T_c)$$

where

$$C(T_c) = -\left[T\frac{\partial^2 F_0(T)}{\partial^2 T^2}\right]_{T=T_c}$$

(the BCS value is 1.426).  $\alpha$  denotes the isotope coefficient. Note that when  $\mu^*=0$ , we can see from Eqs. (25) and (26) that the only independent parameter is  $\lambda'$ and the phonon energy  $\omega_0$  can be used as an overall energy scale. So the dimensionless variational parameter  $c(T)/\omega_0$  and critical temperature  $T_c/\omega_0$  are functions of  $\lambda'$  only. Thus we get for the isotope coefficient  $\alpha = 0.5$ . When  $\mu^* > 0$ , our numerical results show that  $\alpha < 0.5$ . For comparison we show also the results obtained by Carbotte and co-workers and Wolf and Noer by solving the Eliashberg equations.<sup>5, 18-20</sup> Note that  $\omega_{ln}$  is given by

$$\ln\omega_{\ln}=2\int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega} \ln\omega$$

The values  $T_c / \omega_{\rm ln}$  correspond to our values  $T_c / \omega_0$ . While we get in general good agreement even for the strong-coupling superconductor Pb, there is a notable disagreement in the case of Hg with the strongest coupling. We expect this disagreement to result from (a) our use of an Einstein model for the phonons, which does not properly take into account lower-energy phonon modes and which are known to be important, 5, 18, 19 and (b) from our neglect of higher terms in the electron-phonon coupling in deriving  $H'_0$ .

In Fig. 2 we show results for the normalized gap function  $\Delta_0(T)/\Delta_0(0)$  as a function of the reduced temperature  $t = T/T_c$ . The deviation from the weak-coupling BCS results is obtained correctly. However, the devia-

Table The usua	I. Input (	data λ' an 1 is used.	$\mu^*$ used $\sigma$ refers to	for our calculation of the isotone of	ations and r defficient. T	esults. The resu	ults of Car	cbotte and ature. $\Delta$ t	l co-workers (R he gan function	efs. 5, 18, $c(T)$ the	and 19) we specific he	re obtained b	y solving the	e Eliashberg eq nagnetic field (	uations. 1. ).
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				zneng er	aı.	-					Caluo	N-OO DITE OI		-	
System	х	<b>*</b> п	$T_c/\omega_0$	$2\Delta(0)/T_c$	$\gamma T_c^2$ $H_c^2(0)$	$\left[ \frac{\Delta C}{C_n} \right]_{T=T_c}$	$h_c(0)$	α	System	<b>*</b> π	$T_c/\omega_{ m ln}$	$2\Delta(0)/T_c$	$\frac{\gamma T_c^2}{H_c^2(0)}$	$\left[\frac{\Delta C}{C_n}\right]_{T=T_c}$	<i>h</i> <sub>c</sub> (0)
-	BCS			3.528	0.168	1.426	0.576		BCS			3.528	0.168	1.426	0.576
7	0.389	0.123	0.0349	3.644	0.164	1.536	0.562	0.420	Ta	0.11	0.0349	3.673	0.162	1.63	0.550
ŝ	0.397	0.123	0.0384	3.667	0.163	1.558	0.558	0.425	Sn	0.11	0.0385	3.705	0.160	1.68	0.544
4	0.417	0.127	0.0459	3.719	0.161	1.613	0.551	0.429	П	0.135	0.0457	3.753	0.158	1.74	0.538
S	0.423	0.123	0.0505	3.758	0.159	1.657	0.546	0.438	In	0.125	0.0503	3.791	0.156	1.79	0.533
9	0.456	0.117	0.0701	3.952	0.153	1.912	0.525	0.456	V <sub>3</sub> Si	0.102	0.0698	3.933	0.150	1.99	0.515
٢	0.465	0.119	0.0742	3.996	0.152	1.984	0.519	0.457	<b>Nb</b>	0.11	0.0742	3.964	0.150	1.97	0.518
œ	0.505	0.117	0.0978	4.229	0.144	2.558	0.490	0.465	Nb <sub>0.75</sub> Zr <sub>0.25</sub>	0.10	0.0981	4.187	0.143	2.22	0.498
6	0.533	0.121	0.1136	4.528	0.139	3.087	0.467	0.466	Nb <sub>3</sub> Ge	0.122	0.1136	4.364	0.137	2.61	0.471
10	0.547	0.112	0.1278	4.789	0.134	3.847	0.436	0.473	Pb	0.131	0.1283	4.497	0.132	2.77	0.466
11	0.563	0.101	0.1460	5.203	0.128	5.541	0.379	0.479	Hg	0.11	0.1466	4.591	0.134	2.49	0.488

S



FIG. 2. Dependence of the normalized gap function  $\Delta_0(T)/\Delta_0(0)$  on the reduced temperature  $T/T_c$ . The dashed line is the result of BCS theory; the curves 3, 7, and 10 refer to the corresponding set of input data given in Table I and used for the numerical calculations.



FIG. 3. (a) Deviation function D(t) for the critical magnetic field as a function of  $T^2 = (T/T_c)^2$ . The dashed line is the result of BCS theory. The numbers refer to the set of input data given in Table I and used for the numerical calculations. (b) The results for the deviation function D(t) obtained by solving the Eliashberg equations for several intermediate- and strong-coupling superconductors. [see Carbotte and co-workers (Refs. 5, 18, and 19)].

tion in the strong-coupling case (curve 10) may be too large.  $^{21,22}$ 

In Figs. 3 and 4 the deviation function for the critical magnetic field,

$$D(T) = \frac{H_c(T)}{H_c(0)} - (1 - t^2) ,$$

is given. We show for comparison also the results by Carbotte and co-workers.<sup>5,18,19</sup> Again, good agreement is obtained, except for the case of Hg (curve 11). The reasons for this were discussed already.

Regarding the renormalized density of states in the normal state of the electron-phonon coupling system, we remark the following. As was pointed out in Sec. II, near the Fermi surface within a layer of width  $2c_n(T)$  the density of states is renormalized as  $N(0)/\rho_n(T)$  [and  $N(0)/\rho_n(T) \rangle N(0)$ ]. In Fig. 5 the important renormal-



FIG. 4. (a) Deviation function D(t) for the critical magnetic field as a function of  $t^2 = (T/T_c)^2$  for two sets of input data (see Table I). (b) The results of Carbotte's and co-workers for the deviation function D(t) obtained by solving the Eliashberg equations for NB (dashed line) and Nb<sub>0.75</sub>Zr<sub>0.25</sub> (solid line).

Renormalization Factor (1/9<sub>n</sub>





FIG. 5. Renormalization factor  $1/\rho_n(T)$  as a function of  $(T/T_c)^2$  or several sets of input data (see Table I).

ization factor  $1/\rho_n(T)$  is given as a function of  $(T/T_c)^2$ . Obviously, all curves are straight lines and can be put into the form

$$1/\rho_n(T) = 1/\rho_n(0) + A (T/T_c)^2, \qquad (34)$$

where A is a numerical factor. Note that this renormalization factor for the density of states at the Fermi surface corresponds to the Eliashberg<sup>5</sup> renormalization function

$$Z_n(\omega=0,T) = 1 + \lambda + \frac{\pi^2}{3} \lambda \left\langle \left[\frac{1}{\omega}\right]^2 \right\rangle T^2, \qquad (35)$$

with

$$\left\langle \left[ \frac{1}{\omega^2} \right] \right\rangle = 2 \int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega^3} .$$
 (36)

Obviously, the temperature dependence of the renormalization factor  $1/\rho_n$  and  $Z_n$  is the same. Note that the temperature dependence of  $\rho_n(T)$  comes mainly from the temperature dependence of the energy cutoff  $c_n(T)$ . This is a remarkable success of our approach. Contrary to  $c_n(T)$ , which is an increasing function of temperature  $T < T_c$ ,  $c_s(T)$  is always a decreasing function of T.

In Fig. 6 we present results for the variational cutoff



FIG. 6. Energy cutoff variational parameters  $c_n(T)$  and  $c_s(T)$  as functions of  $T/T_c$  for  $\lambda'=0.465$  and  $\mu^*=0.119$ .

parameters  $c_n(T)$  and  $c_s(T)$ , using  $\lambda'=0.465$  and  $\mu^*=0.119$ . The decrease of the cutoff  $c_s(T)$  with increasing temperature means that the phonon-induced attraction between electrons becomes less and less effective due to thermal fluctuations. Furthermore, since  $c_s(T) > c_n(T)$  for  $T < T_c$ , one gets

$$1/\rho_s(T) > 1/\rho_n(T)$$
 when  $T < T_c$ . (37)

This is different from Eliashberg theory,<sup>5,23</sup> where

$$Z_s(\omega = \Delta_0, T = 0) < Z_n(\omega = 0, T = 0)$$
 (38)

Here  $Z_s(\omega = \Delta_0, T = 0)$  is the renormalization factor at the gap edge in the superconducting state at T = 0. As was shown by Scalapino<sup>24</sup> in the case of a retarded strong-coupling, the correction of the condensation energy with respect to BCS weak coupling arises primarily from the difference between  $Z_n(\omega)$  and  $Z_s(\omega)$  and is approximately given by

$$N(0)\operatorname{Re}\int d\omega [Z_n(\omega) - Z_s(\omega)]\omega .$$
(39)

As discussed by Scalapino, the net effect of retardation is to lower the condensation energy below the BCS value since this correction should be negative. Using the approximation  $Z_n(\omega) \approx Z_n$  and  $Z_s(\omega) \approx Z_s$ , where  $Z_n$  and  $Z_s$  are constants, it follows that  $Z_s > Z_n$ , consistent with our result. So we conclude that our  $\rho_s < \rho_n$  is correct and accounts correctly for a retardation effect.

As a further demonstration of the validity of our approach, we calculate the condensation energy at T=0 for the strong-coupling case Pb. This renormalized density of states at the Fermi surface,  $N^*(0)$ , which is equal to  $N(0)/\rho_n(0)$  in our theory, can be obtained from a specific-heat measurement  $\gamma = \frac{2}{3}\pi^2 k_B^2 N^*(0)$ .<sup>5,18</sup> One gets  $N^*(0)=1.35\times10^{34}$  erg/cm<sup>3</sup> and a condensation energy of  $2.68\times10^4$  erg/cm<sup>3</sup> using the experimental result  $T_c=7.2$  K. The experimental value obtained from critical-field measurements<sup>24</sup> is  $2.56\times10^4$  erg/cm<sup>3</sup>. The BCS result is  $\frac{1}{2}N^*(0)\Delta_0^2=3.10\times10^4$  erg/cm<sup>3</sup>, and the result obtained by solving the Eliashberg equations<sup>24</sup> is  $2.49\times10^4$  erg/cm<sup>3</sup>. Again, we find reasonable agreement between our result and the experimental one.

## **IV. CONCLUDING REMARKS**

We have proposed a simple approach based on a canonical transformation and variational principle to determine the properties of the conventional superconductors. The resultant pairing potential includes retardation effects and is similar to the BCS one, but involves a temperature-dependent cutoff. The temperaturedependent cutoff  $c_s(T)$  takes care of the fact that the phonon-induced attraction between electrons is not instantaneous, but retarded, and should be affected by the thermal fluctuations of the quasiparticles. This retardation effect causes the renormalization function to be different for the normal and superconducting states, which lowers the condensation energy. The generally good agreement between our numerical results and those by Carbotte and co-workers obtained by solving the Eliashberg equations is likely due to including such retardation effects. Our results show that the thermodynamical properties of the conventional superconductors are mainly determined by the ratio  $T_c/\omega_0$ . This conclusion agrees with that by Carbotte.<sup>5</sup>

The physical meaning of the coupling constant  $\lambda'$  in our work is different from  $\lambda$  in the Eliashberg theory. Our  $\lambda'$  has to be considered as a bare coupling constant. It is determined by  $(T_c/\omega_0)$ . Comparing our formula for the gap function  $\Delta_0(0)$  with that of the BCS theory  $(\Delta_0(0) \sim 1/\sinh[-(\lambda-\mu^*)^{-1}])$ , we find the relationship

$$\lambda \approx \lambda' / \rho_s(0) = \lambda' / [1 - \lambda' c_s(0) / \omega_0]$$
.

As an example, for  $\lambda'=0.465$  (to mimic Nb), we get  $\lambda \approx 0.71 [c_s(0)=0.739]$  and for  $\lambda'=0.547$  (to mimic Pb) we get  $\lambda \approx 1.06 [c_s(0)=0.887]$ .

In this work we have presented numerical results for the adiabatic case,  $\omega_{\rm ph}/E_F \ll 1$ . Note that in the Migdal-Eliashberg theory it is very difficult to take into account the vertex renormalization of the electronphonon coupling, which is necessary if  $\omega_{\rm ph}/E_F$  is not small.<sup>25</sup> However, our treatment, canonical transformation, can be extended to the nonadiabatic case where  $\omega_{\rm ph}/E_F$  is not small and where bipolaronic formation is expected. It is well known that when  $\omega_0/t \gg 1$ , the socalled antiadiabatic limit, the electron-phonon interaction becomes instantaneous and H can be transformed to the negative-U Hubbard model.<sup>26</sup> (t is the nearestneighbor electron hopping integral.) This can be seen by putting the variational function  $\delta(k',k) = 1$ , for all  $\epsilon'_k, \epsilon_k$ , which implies the energy cutoff c = D (D = bandwidth). Thus, using again a single Einstein phonon, one has

$$H' = \exp(S)H \exp(-S) ,$$
  
$$S = \sum_{i,\sigma} \frac{g_0}{\omega_0} (b_i^{\dagger} - b_i) d_{i\sigma}^{\dagger} d_{i\sigma} .$$

Here S becomes the usual canonical transformation in the antiadiabatic limit for the (Holstein) model Hamiltonian<sup>6</sup>

$$H = \sum_{i} \omega_0 b_i^{\dagger} b_i - \sum_{\langle ij \rangle, \sigma} t d_{i\sigma}^{\dagger} d_{j\sigma} + \sum_{i, \sigma} g_0 (b_i^{\dagger} + b_i) d_{i\sigma}^{\dagger} d_{i\sigma} .$$

Here  $g_0$  is the coupling constant. If then  $U = -2g_0^2/\omega_0$ 

and the electron-electron interaction is strong enough, bipolarons form and they can condense into the superfluid state at a lower temperature.<sup>8,12</sup> Thus we obtain within our approach also the Bose condensation of bipolarons. Note, of course, that the above transformation yields a different  $H'_0$  for the bipolaron case.<sup>8,12</sup>

Since, as shown, our canonical transformation includes both limits  $\omega/\epsilon_F >> 1$  and  $\omega/\epsilon_F << 1$ , one should expect our approach to be applicable also for the intermediate case  $\omega \sim \epsilon_F$ . It would be interesting to determine  $H'_0$  also for this crossover region.

We have neglected all higher-order terms in the coupling constant in performing the unitary transformation. If  $T_c/\omega_0$  is large, the higher-order terms may play a role and should be include.d Also, it would be interesting to use different forms for the variational function  $\delta(k',k)$ . Our choice for  $\delta(k',k)$  was only for simplicity and for a comparison with previous results. Keeping a k',k dependence of  $\delta(k',k)$ , one could give different phonons a varying weight, and by varying  $\delta(k',k)$  between 0 and 1, one may account for the amount of lattice deformation which follows the electrons.

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## APPENDIX: DETERMINATION OF THERMODYNAMICAL FUNCTIONS

Here we give mathematical details of the analysis performed in Sec. II. The upper bound of the free energy is

$$F_{0}(T) = -\frac{1}{\beta} \ln \operatorname{Tr}[\exp(-\beta H'_{0})] + \operatorname{Tr}[\exp(-\beta H'_{0})(H' - H'_{0})] + \mu N_{e} . \quad (A1)$$

Here  $H'_0$  is given by Eq. (9) and involves the variational cutoff parameter c(T). H' is the transformed Hamiltonian [Eq. (7)]. The second-order terms in H' can be collected as follows:

$$[S,H^{1}] + \frac{1}{2}[[H^{0},S],S] = \frac{1}{2N} \sum_{q,\gamma} \sum_{q',\gamma'} \sum_{b,f,k,k',\sigma} \frac{g_{q\gamma}g_{q'\gamma'}}{\omega_{q\gamma}\omega_{q'\gamma'}} (b^{\dagger}_{-q\gamma} - b_{q\gamma})(b^{\dagger}_{-q'\gamma'} - b_{q'\gamma'})(\epsilon_{k+q} - \epsilon_{k}) \\ \times \delta(k+q,k)\delta(k'+q',k')[d^{\dagger}_{k+q\sigma}d_{k'\sigma}\delta_{k'+q',k} - d^{\dagger}_{k'+q'\sigma}d_{k\sigma}\delta_{k+q,k'}] \\ + \frac{1}{2N} \sum_{q,\gamma} \sum_{q',\gamma'} \sum_{b,f,k,k',\sigma} \frac{g_{q\gamma}g_{q'\gamma'}}{\omega_{q\gamma}} (b^{\dagger}_{-q\gamma} - b_{q\gamma})(b^{\dagger}_{-q'\gamma'} - b_{q'\gamma'}[2\delta(k+q,k) \\ -\delta(k+q,k)\delta(k'+q',k')]) \\ \times [d^{\dagger}_{k+q\sigma}d_{k'\sigma}\delta_{k'+q',k} - d^{\dagger}_{k'+q'\sigma}d_{k\sigma}\delta_{k+q,k'}] \\ - \frac{1}{2N} \sum_{q,\gamma} \sum_{k,\sigma} \sum_{bfk',\sigma'} [2\delta(k+q,k) - \delta(k+q,k)\delta(k'-q,k')]d^{\dagger}_{k+q\sigma}d_{k\sigma}d^{\dagger}_{k'-q\sigma'}d_{k'\sigma'}.$$
(A2)

Here  $\delta_{k'+q',k}$  is the Kronecker  $\delta$  symbol. Substituting  $H'_0$  and H' into Eq. (A1) and omitting all terms of higher order in  $g^2_{q\gamma}$ , we get, as an upper bound of the free energy;

$$F_{0}(T) = E_{0} - \frac{2}{\beta} \sum_{k} \ln[1 + \exp(-\beta\sqrt{E_{k}^{2} + \Delta_{k}^{2}})] - \sum_{k} \sqrt{E_{k}^{2} + \Delta_{k}^{2}}$$
$$+ \frac{1}{2} \sum_{k} \frac{\Delta_{k}^{2}}{\sqrt{E_{k}^{2} + \Delta_{k}^{2}}} \tanh\left[\frac{\beta}{2}\sqrt{E_{k}^{2} + \Delta_{k}^{2}}\right] - \lambda' N(0)c^{2}N , \qquad (A3)$$

where  $\beta = 1/T$ , N is the total number of cells,  $E_0$  is a constant, and

$$E_k = (\epsilon_k - \mu)\rho_k \quad . \tag{A4}$$

Here the renormalization factor  $\rho_k$  is given in Eq. (10). For the sake of simplicity, we assumed an Einstein model for the phonons:  $g_{q\gamma} = g_0$  and  $\omega_{q\gamma} = \omega_0$ . In deriving (A3) we have used

$$\frac{1}{N}\sum_{q,\gamma}\frac{g_0^2}{\omega_0^2}[2n(\omega_0)+1]\delta^2(k+q,k)(\epsilon_{k+q}-\mu)=0.$$
(A5)

This is true because  $(\epsilon_{k+q} - \mu)$  is an odd function.

The gap function  $\Delta_k$  is determined by minimizing  $F_0(T)$ . Thus

$$\Delta_{k} = \frac{1}{N} \sum_{k'} V(k',k) \langle d_{-k'\downarrow} d_{k'\uparrow} \rangle$$
  
=  $\frac{1}{2N} \sum_{k'} V(k',k) \frac{\Delta_{k'}}{\sqrt{E_{k'}^{2} + \Delta_{k'}^{2}}} \tanh\left[\frac{\beta}{2}\sqrt{E_{k'}^{2} + \Delta_{k'}^{2}}\right].$   
(A6)

Here V(k',k) is the effective electron-electron interaction,

$$V(k',k) = \frac{2g_0^2}{\omega_0} \delta(k',k) - U , \qquad (A7)$$

where U is a phenomenological parameter introduced in order to take into account the effect of the Coulomb repulsion.<sup>17</sup> As a consequence of the assumed form of the variational function  $\delta(k',k)$  [see Eq. (5)], the gap function has the form

$$\Delta_k = \begin{cases} \Delta_0 , & |\epsilon_k - \mu| \le c(T) , \\ -\Delta_1 , & c(T) < |\epsilon_k - \mu| \le D . \end{cases}$$
(A8)

Here D is the higher-energy cutoff (bandwidth), which is of the same order of magnitude as the Fermi energy. The parameter c(T) is obtained by minimizing  $F_0(T)$ . Then,

$$\Delta_{0} = (\lambda' - \mu_{0}) \int_{0}^{c(T)} d\epsilon \frac{\Delta_{0}}{\sqrt{\epsilon^{2} \rho^{2} + \Delta_{0}^{2}}}$$
  
 
$$\times \tanh\left[\frac{\beta}{2}\sqrt{\epsilon^{2} \rho^{2} + \Delta_{0}^{2}}\right]$$
  
 
$$-\mu_{0} \int_{c(T)}^{D} d\epsilon \frac{-\Delta_{1}}{\sqrt{\epsilon^{2} + \Delta_{1}^{2}}} \tanh\left[\frac{\beta}{2}\sqrt{\epsilon^{2} + \Delta_{1}^{2}}\right]$$
(A9)

$$\Delta_{1} = \mu_{0} \int_{0}^{c(T)} d\epsilon \frac{\Delta_{0}}{\sqrt{\epsilon^{2} \rho^{2} + \Delta_{0}^{2}}} \tanh\left[\frac{\beta}{2}\sqrt{\epsilon^{2} \rho^{2} + \Delta_{0}^{2}}\right] -\mu_{0} \int_{c(T)}^{D} d\epsilon \frac{-\Delta_{1}}{\sqrt{\epsilon^{2} \rho^{2} + \Delta_{1}^{2}}} \tanh\left[\frac{\beta}{2}\sqrt{\epsilon^{2} \rho^{2} + \Delta_{1}^{2}}\right],$$
(A10)

where  $\mu_0 = UN(0)$ . For  $c\beta \gg 1$ , one gets then the solutions

$$\frac{1}{\lambda' - \mu^*} = \int_0^c d\epsilon \frac{1}{\sqrt{\epsilon^2 \rho^2 + \Delta_0^2}} \tanh\left[\frac{\beta}{2}\sqrt{\epsilon^2 \rho^2 + \Delta_0^2}\right],$$
(A11)

$$\Delta_1 = \frac{\mu^*}{\lambda' - \mu^*} \Delta_0 , \qquad (A12)$$

and

$$\mu^* = \frac{\mu_0}{1 + \mu_0 \ln[D/c(T)]} .$$
 (A13)

At T = 0 one finds

$$\frac{1}{\lambda' - \mu^*} = \int_0^c d\epsilon \frac{1}{\sqrt{\epsilon^2 \rho^2 + \Delta_0^2}}$$
(A14)

and

$$F_{0}(0) = -\sum_{k} \sqrt{E_{k}^{2} + \Delta_{k}^{2}} + \frac{1}{2} \sum_{k} \frac{\Delta_{k}^{2}}{\sqrt{E_{k}^{2} + \Delta_{k}^{2}}} - \lambda' N(0) c^{2} N .$$
 (A15)

The remaining integrals can be easily performed. For the normal state  $(\Delta_0=0)$ , we have

$$F_0(0)_n = -N(0)\lambda' c_n^2(0) [1 - c_n(0)/\omega_0] .$$
 (A16)

Obviously, after minimizing  $F_0(0)$  with respect to  $c_n(0)$ , we get for the cutoff

$$c_n(0) = 2\omega_0/3 \tag{A17}$$

and

$$F_0(0) = -4N(0)\lambda'\omega_0^2/27 .$$
 (A18)

For the superconducting state  $(\Delta_0 \neq 0)$ , we have

$$\Delta_0(0) = c_s(0)\rho_s(0) / \sinh\left[\frac{\rho_s(0)}{\lambda' - \mu^*}\right]$$
(A19)

and

$$F_{0}(0) = N(0)(1-\lambda')c_{s}^{2}(0) - N(0)c_{s}^{2}(0)\rho_{s}(0) \operatorname{coth}\left[\frac{\rho_{s}(0)}{\lambda'-\mu^{*}}\right], \quad (A20)$$

with

$$\rho_s(0) = 1 - \lambda' \frac{c_s(0)}{\omega_0} .$$
(A21)

After differentiating  $F_0(0)_s$  with respect to  $c_s(0)$ , we get

$$2(1-\lambda') - \left[2-3\lambda'\frac{c_s(0)}{\omega_0}\right] \operatorname{coth} \left[\frac{\rho_s(0)}{\lambda'-\mu^*}\right],$$
$$-\frac{\lambda'\Delta_0^2(0)}{\omega_0 c_s(0)\rho_s(0)(\lambda'-\mu^*)} + \left[\frac{\Delta_0(0)\mu^*}{c_s(0)(\lambda'-\mu^*)}\right]^2 = 0$$
(A22)

for determining  $c_s(0)$ . For  $T \rightarrow T_c$ ,  $\Delta(T) \rightarrow 0$ , one finds

$$\frac{1}{\lambda'-\mu^*} = \int_0^{c(T_c)} d\epsilon \frac{1}{\rho(T_c)\epsilon} \tanh\left[\frac{\rho(T_c)\epsilon}{2T_c}\right], \quad (A23)$$

with

$$\rho_{(T_c)} = 1 - \lambda' [2n(\omega_0) + 1] \frac{c(T_c)}{\omega_c} . \qquad (A24)$$

This determines  $T_c$ . At  $T_c$  the free energy is given by

$$F_{0}(T_{c}) = N(0)(1-\lambda')c^{2}(T_{c}) - N(0)c^{2}(T_{c})\rho(T_{c}) - 4T_{c}N(0)\int_{c(T_{c})}^{D}d\epsilon \ln\left[1+\exp\left[-\frac{\epsilon}{T_{c}}\right]\right]$$

$$-4T_{c}N(0)\int_{0}^{c(T_{c})}d\epsilon \ln\left[1+\exp\left[-\frac{\rho(T_{c})\epsilon}{T_{c}}\right]\right].$$
(A25)

Again,  $c(T_c)$  is determined by minimizing  $F_0(T_c)$ .

For the general case of  $0 < T < T_c$ , we have, for the normal state,

$$F_{0}(T_{n}) = N(0)(1-\lambda')c_{n}^{2}(T) - N(0)c_{n}^{2}(T)\rho_{n}(T) - 4TN(0)\int_{c_{n}(T)}^{D} d\epsilon \ln\left[1 + \exp\left[-\frac{\epsilon}{T}\right]\right]$$

$$-4TN(0)\int_{0}^{c_{n}(T)} d\epsilon \ln\left[1 + \exp\left[-\frac{\rho_{n}(T)\epsilon}{T}\right]\right],$$
(A26)

with

$$\rho_n(T) = 1 - \lambda' [2n(\omega_0) + 1] \frac{c_n(T)}{\omega_0} .$$
(A27)

Furthermore, for the superconducting state, one gets

$$\frac{1}{\lambda'-\mu^*} = \int_0^{c_s(T)} d\epsilon \frac{1}{\sqrt{\epsilon^2 \rho_s^2(T) + \Delta_0^2(T)}} \tanh\left[\frac{\beta}{2}\sqrt{\epsilon^2 \rho_s^2(T) + \Delta_0^2(T)}\right]$$
(A28)

and

$$F_{0}(T)_{s} = N(0)(1-\lambda')c_{n}^{2}(T) - N(0)c_{s}(T)\sqrt{c_{s}^{2}(T)\rho_{s}^{2}(T) + \Delta_{0}^{2}(T)} - N(0)\frac{\Delta_{0}^{2}(T)}{\rho_{s}(T)}\ln\frac{c_{s}(T)\rho_{s}(T) + \sqrt{c_{s}^{2}(T)\rho_{s}^{2}(T) + \Delta_{0}^{2}(T)}}{\Delta_{0}(T)}$$

$$-4TN(0)\int_{0}^{c_{s}(T)}d\epsilon\ln\left[1 + \exp\left[-\frac{\sqrt{\rho_{s}^{2}(T)\epsilon^{2} + \Delta_{0}^{2}(T)}}{T}\right]\right]$$

$$+N(0)\frac{\Delta_{0}^{2}(T)}{\lambda' - \mu^{*}} - 4TN(0)\int_{c_{s}(T)}^{D}d\epsilon\ln\left[1 + \exp\left[-\frac{\epsilon}{T}\right]\right], \qquad (A29)$$

with

$$\rho_{s}(T) = 1 - \lambda' [2n(\omega_{0}) + 1] \frac{c_{s}(T)}{\omega_{0}} , \qquad (A30)$$

 $c_n(T)$  and  $c_s(T)$  can be determined by minimizing  $F_0(T)_n$  and  $F_0(T)_s$ , respectively, Unfortunately, these equations cannot be solved analytically.

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