Recently, Xu et al. [5] using the BCS theory of superconductivity derived the Ginzburg–Landau free energy density from the BCS free-energy density for temperatures at T_c and near T_c, and found relations between the microscopic and phenomenological coefficients. However, the coefficients of the expansion are found to depend only on $N(0)$, the density of states at Fermi level and T_c, not on the material parameters like ω_D and T_c, since they have taken the limit $\omega_D/T_c \to \infty$ in their calculations.

In this paper, we will show new solutions for ΔF, the free-energy difference, the temperature dependence of the order parameter, the critical fields, the entropy and the specific heat jump, taking into account the finite value of ω_D/T_c at $T = T_c$ and near T_c, and to make the formulation complete, we consider both the s and d pairing symmetries.

In Section 2, starting from the BCS gap equation we will give the complete expression for the temperature dependence of the order parameter, then the complete expansion for the free-energy density will be obtained in Section 3. Our improvement on the previous results will naturally lead to the modification of the coefficients of the well-known Ginzburg–Landau equation. In Section 4, we will consider the thermodynamic properties of an s-wave superconductor with finite ω_D/T_c, we will see that for large ω_D/T_c, all the BCS results are reproduced. Analytical expressions for the thermodynamic properties of a d-wave superconductor are also given. Discussions and conclusions are given in Section 5.

2. Order parameter equation

Within the BCS scheme, one obtains the BCS gap equation as

$$\Delta_{\vec{k}} = \sum_{\vec{k}'} V_{\vec{k}\vec{k}'} \frac{\Delta_{\vec{k}'}}{2E_{\vec{k}'}} \tanh(E_{\vec{k}'}/2T), \tag{1}$$

where

$$E_{\vec{k}} = \sqrt{\varepsilon_{\vec{k}}^2 + \Delta_{\vec{k}}^2} \tag{2}$$

and

$$\Delta_{\vec{k}} = \Delta(T)\, g(\phi). \tag{3}$$

Here ϕ is the polar angle specifying the direction of electron of momentum $\vec{k}$ in the plane and for $g(\phi)$ we adopt the model $g(\phi) = 1$ (s-pairing) or $\cos 2\phi$ (d-pairing). The BCS scattering matrix element $V_{\vec{k}\vec{k}'}$ due to phonon mediated interaction is assumed to have the usual separable form

$$V_{\vec{k}\vec{k}'} = V g(\phi) g(\phi'), \tag{4}$$

only if both $\varepsilon_{\vec{k}}$ and $\varepsilon_{\vec{k}'}$ are smaller than the Debye energy ω_D, so the attractive constant V is finite in a certain strip of width $2\omega_D$ in the vicinity of the Fermi level.

Assuming a constant density of states at the Fermi level $N(0)$, we apply standard transformation to Eq. (1) and arrive at the following gap equation

$$\frac{1}{N(0)V} = \int_0^{2\pi} \frac{d\phi}{2\pi} g^2(\phi) \int_{-\omega_D}^{\omega_D} \frac{d\varepsilon_k}{2E_k} \tanh(E_k/2T). \tag{5}$$

By differentiating Eq. (5) with respect to T, we obtain

$$\frac{\mathrm{d}\Delta^2(T)}{\mathrm{d}T} = \frac{\dfrac{1}{T^2}\displaystyle\int_0^{2\pi}\frac{\mathrm{d}\phi}{2\pi}g^2(\phi)\int_0^{\omega_D}\mathrm{d}\varepsilon\,\mathrm{sech}^2(E/2T)}{\displaystyle\int_0^{2\pi}\frac{\mathrm{d}\phi}{2\pi}g^4(\phi)\int_0^{\omega_D}\mathrm{d}\varepsilon\left[\frac{\mathrm{sech}^2(E/2T)}{2TE^2} - \frac{\tanh(E/2T)}{E^3}\right]}. \tag{6}$$

If the notation $\langle g^n(\phi)\rangle = \int_0^{2\pi}(\mathrm{d}\phi/2\pi)g^n(\phi)$ is introduced, then at $T = T_c$ Eq. (6) can be written as

$$\frac{\mathrm{d}\Delta^2(T)}{\mathrm{d}T}\Big|_{T=T_c} = \frac{\langle g^2(\phi)\rangle 8T_c\tanh^2 y_c}{\langle g^4(\phi)\rangle\left[\dfrac{\tanh y_c}{y_c^2} - \dfrac{1}{y_c} - I_3\right]}, \qquad \text{where } y_c = \omega_D/2T_c \tag{7}$$

and

$$I_3 = \frac{16}{\pi^3}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^3}\tan^{-1}\left(\frac{y_c}{\left(n+\dfrac{1}{2}\right)\pi}\right). \tag{8}$$

The second derivative of $\Delta^2(T)$ in Eq. (5) with respect to T at T_c is then given by

$$\frac{\mathrm{d}^2\Delta^2(T)}{\mathrm{d}T^2}\Big|_{T=T_c} = \frac{8\langle g^2(\phi)\rangle\tanh y_c}{\langle g^4(\phi)\rangle\left[\dfrac{\tanh y_c}{y_c^2} - \dfrac{1}{y_c} - I_3\right]}(\alpha+\beta), \tag{9}$$

where

$$\alpha = 1 - \frac{2y_c}{\sinh 2y_c} - \frac{2\left[\dfrac{\tanh^2 y_c}{y_c} + I_3\right]}{\left[\dfrac{\tanh y_c}{y_c^2} - \dfrac{1}{y_c} - I_3\right]}, \tag{10}$$

$$\beta = \frac{\langle g^2(\phi)\rangle\langle g^6(\phi)\rangle}{\langle g^4(\phi)\rangle^2}\,\frac{\tanh y_c\left[\dfrac{\tanh^2 y_c}{y_c^3} - \dfrac{1}{y_c} - I_5\right]}{\left[\dfrac{\tanh y_c}{y_c^2} - \dfrac{1}{y_c} - I_3\right]^2} \tag{11}$$

and

$$I_5 = \frac{192}{\pi^5}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^5}\tan^{-1}\left(\frac{y_c}{\left(n+\dfrac{1}{2}\right)\pi}\right). \tag{12}$$

The Taylor's expansion of $\Delta^2(T)$ about T_c yields the following equation

$$\Delta^2(T) = (T-T_c)\frac{\mathrm{d}\Delta^2(T)}{\mathrm{d}T}\Big|_{T=T_c} + \frac{1}{2}(T-T_c)^2\frac{\mathrm{d}^2\Delta^2(T)}{\mathrm{d}T^2}\Big|_{T=T_c} + \dots \tag{13}$$

By substituting Eqs. (7) and (9) into Eq. (13), the temperature dependence of the order parameter near T_c is found to be

$$\Delta^2(T) = \frac{8T_c^2\langle g^2(\phi)\rangle \tanh y_c}{\langle g^4(\phi)\rangle\left[I_3 + \dfrac{1}{y_c} - \dfrac{\tanh y_c}{y_c^2}\right]}\left(1 - \frac{T}{T_c}\right)\left\{1 - \frac{1}{2}\left(1 - \frac{T}{T_c}\right)(\alpha + \beta)\right\}. \tag{14}$$

Up to this point we can see that the BCS approximation $y_c = \omega_D/2T_c \to \infty$ and $\langle g^n(\phi)\rangle = 1$ for any n, give the result for the $\Delta^2_{BCS}(T)$ of an s-wave superconductor as

$$\Delta^2_{BCS}(T) = \frac{8(\pi T_c)^2}{7\zeta(3)}\left(\frac{1 - T}{T_c}\right)\left\{1 - \frac{1}{2}\left(3 - \frac{93\zeta(5)}{[7\zeta(3)]^2}\right)\left(1 - \frac{T}{T_c}\right)\right\}, \tag{15}$$

where $\zeta(n)$ is the Rieman zeta function. The last term on the right hand side of Eq. (15) is a correction to BCS's approximation. Recently, Xu et al. [5] calculated the temperature dependence of the order parameter near T_c, their result is different from ours, our exact results show that their result is in error.

We now calculate the ratio $\Delta^2(T)/\Delta^2_{BCS}(T)$ as a function of ω_D/T_c for different T/T_c values.

First we take $g(\phi) = 1$ for an s-wave superconductor, then Eqs. (14) and (15) yield the following result

$$\frac{\Delta_s^2(T)}{\Delta^2_{BCS}(T)} = \frac{7\zeta(3)\tanh y_c\left\{1 - \dfrac{1}{2}\left(1 - \dfrac{T}{T_c}\right)(\alpha + \beta_s)\right\}}{\pi^2\left[I_3 + \dfrac{1}{y_c} - \dfrac{\tanh y_c}{y_c^2}\right]\left\{1 - \dfrac{3}{2}\left(1 - \dfrac{31\zeta(5)}{(7\zeta(3))^2}\right)\left(1 - \dfrac{T}{T_c}\right)\right\}}, \tag{16}$$

where β_s, as defined in Eq. (11), becomes

$$\beta_s = \frac{\tanh y_c\left[\dfrac{\tanh^2 y_c}{y_c^3} - \dfrac{1}{y_c} - I_5\right]}{\left[\dfrac{\tanh y_c}{y_c^2} - \dfrac{1}{y_c} - I_3\right]^2}. \tag{17}$$

We can easily see that at $T = T_c$ and as $\omega_D/T_c \to \infty$, the ratio $\Delta_s^2(T)/\Delta^2_{BCS}(T)$ reduces to 1, as it should.

Next, we take $g(\phi) = \cos 2\phi$ for the d-wave superconductor, for this case $\langle g^2(\phi)\rangle = 1/2$, $\langle g^4(\phi)\rangle = 3/8$, $\langle g^6(\phi)\rangle = 5/16$, Eqs. (14) and (15) give the result

$$\frac{\Delta_d^2(T)}{\Delta^2_{BCS}(T)} = \frac{28\zeta(3)\tanh y_c\left\{1 - \dfrac{1}{2}\left(1 - \dfrac{T}{T_c}\right)(\alpha + \beta_d)\right\}}{3\pi^2\left[I_3 + \dfrac{1}{y_c} - \dfrac{\tanh y_c}{y_c^2}\right]\left\{1 - \dfrac{3}{2}\left(1 - \dfrac{31\zeta(5)}{(7\zeta(3))^2}\right)\left(1 - \dfrac{T}{T_c}\right)\right\}}, \tag{18}$$

again from Eq. (11), one finds $\beta_d = (10/9)\beta_s$. In the limits $T = T_c$ and weak coupling ω_d/T_c approaches ∞, one has to $\Delta_d^2(T)/\Delta^2_{BCS}(T) \to 4/3$.

These ratios, $\Delta_s^2(T)/\Delta^2_{BCS}(T)$ and $\Delta_d^2(T)/\Delta^2_{BCS}(T)$, written in terms of observable quantities such as the cutoff and the transition temperature for different $T = T_c$ values are shown in Fig. 1. The two sets of curves

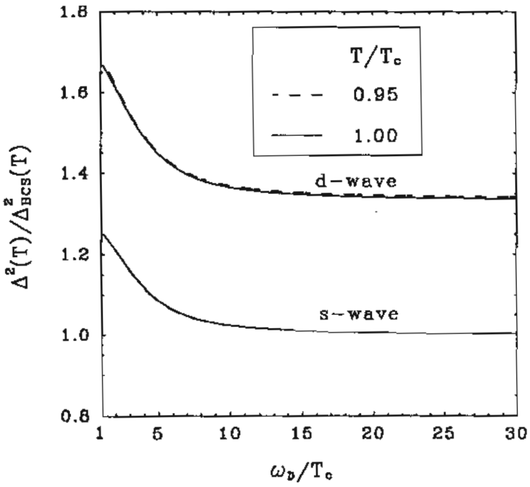

Fig. 1. Shows the variation of the dimensionless ratio $\Delta^2(T)/\Delta^2_{BCS}$ as a function of ω_D/T_c. Two different types of pairing, s and d, and two reduced temperatures T/T_c, are plotted.

behave quantitatively in the same way and almost insensitive to temperature variations. We note that $\Delta_d(T) > \Delta_s(T)$ for all parameter spaces.

3. Free energy difference

Thermodynamic properties depend on the free energy difference $\Delta F = F_S - F_N$ between the superconducting and normal states. The subscript S (N) refers to the superconducting (normal) state. The integral form of the ΔF can be written as

$$\Delta F = \int_0^{\Delta(T)} \mathrm{d}\Delta'(T)|\Delta'(T)|^2 \frac{\mathrm{d}(1/V)}{\mathrm{d}\Delta'(T)}. \tag{19}$$

Since, near T_c, the order parameter $\Delta(T)$ is very small, this allows Eq. (5) to be expressed as a series in powers of $(\Delta^2(T)/\varepsilon^2 + \omega_n^2)$, where $\omega_n = (n + 1/2)\pi T$ is the usual Matsubara frequency, n is an integer, and we find that Eq. (5) is converted into the following form:

$$\frac{1}{V} = 4T \sum_{n,m=0}^{\infty} \langle g^{2m+2}(\phi)\rangle(-1)^m \Delta^{2m}(T) \int_0^{\omega_D} \frac{N(0)\mathrm{d}\varepsilon}{\left(\varepsilon^2 + \omega_n^2\right)^{m+1}}. \tag{20}$$

In order to obtain the free energy difference near T_c, one substitutes Eq. (20) into Eq. (19) and integrates to obtain

$$\Delta F(T,\omega_D) = 4T \sum_{n,m=0}^{\infty} (-1)^m \left(\frac{m}{m+1}\right)\langle g^{2m+2}(\phi)\rangle \frac{\Delta^{2m+2}(T)}{(2T_c)^{2m+1}} \int_0^{\omega_D/2T} \frac{\mathrm{d}xN(0)}{\left[x^2 + \left(\left(n+\frac{1}{2}\right)\pi\right)^2\right]^{m+1}}. \tag{21}$$

Retaining only the terms up to $\Delta^6(T)$, we have

$$\Delta F(T,\omega_D) = B_2(T_c,\omega_D)\Delta^4(T) + B_3(T_c,\omega_D)\Delta^6(T), \tag{22}$$

where

$$B_2(T_c,\omega_D) = \frac{N(0)\langle g^4(\phi)\rangle}{16T_c^2}\left[I_3 + \frac{1}{y_c} - \frac{\tanh y_c}{y_c^2}\right], \tag{23}$$

$$B_3(T_c,\omega_D) = \frac{N(0)\langle g^6(\phi)\rangle}{192T_c^4}\left[I_5 + \frac{1}{y_c} - \frac{\tanh^2 y_c}{y_c^3}\right]. \tag{24}$$

The utilization of Eq. (14) modifies ΔF to

$$\Delta F = -B_2(T_c,\omega_D)P^2\left(1-\frac{T}{T_c}\right)^2\left\{1+\left(1-\frac{T}{T_c}\right)\left(\frac{2Q}{P} - \frac{PB_3(T_c,\omega_D)}{B_2(T_c,\omega_D)}\right)\right.$$
$$\left. + \left(1-\frac{T}{T_c}\right)^2\left(\frac{Q^2}{P^2} - \frac{3QB_3(T_c,\omega_D)}{B_2(T_c,\omega_D)}\right)\right\}, \tag{25}$$

here

$$P = -T_c\frac{\mathrm{d}\Delta^2(T)}{\mathrm{d}T}\Big|_{T=T_c} \quad \text{and} \quad Q = \frac{T_c^2}{2}\frac{\mathrm{d}^2\Delta^2(T)}{\mathrm{d}T^2}\Big|_{T=T_c}.$$

The values of these derivatives have already been obtained [Eqs. (7) and (9)], hence P and Q are known.

4. Thermodynamic properties

Since the critical field can be obtained from the difference between the normal and superconducting state free energies, i.e. $(H_c^2(T)/8\pi) = -\Delta F$, where $H_c(T)$ is the thermodynamic critical field, then from Eq. (25), one has the critical field $H_c(T)$ near T_c as

$$\frac{H_c(T)}{1-T/T_c} = \frac{\langle g^2(\phi)\rangle\sqrt{32\pi N(0)}\,T_c\tanh y_c}{\sqrt{\langle g^4(\phi)\rangle\left[I_3 + \frac{1}{y_c} - \frac{\tanh y_c}{y_c^2}\right]}}\left\{1 - \frac{1}{2}\left(\alpha+\frac{\beta}{3}\right)\left(1-\frac{T}{T_c}\right) - \frac{\beta}{3}\left(\alpha + \frac{7}{6}\beta\right)\left(1-\frac{T}{T_c}\right)^2\right\}. \tag{26}$$

By taking the $\omega_D/T_c \to \infty$ limit and $\langle g^2(\phi)\rangle = 1 = \langle g^4(\phi)\rangle$ Eq. (26) gives the BCS critical field as

$$\frac{H_{c,BCS}(T)}{1-T/T_c} = \pi T_c\sqrt{\frac{32\pi N(0)}{7\zeta(3)}}\left\{1 - \frac{1}{2}\left(3 - \frac{31\zeta(5)}{(7\zeta(3))^2}\right)\left(1-\frac{T}{T_c}\right)\right.$$
$$\left. + \frac{31\zeta(5)}{(7\zeta(3))^2}\left(3 - \frac{31\zeta(5)}{14(\zeta(3))^2}\right)\left(1-\frac{T}{T_c}\right)^2\right\}. \tag{27}$$

Combining Eqs. (26) and (27), we arrive at the following equation

$$\frac{H_c(T)}{H_{c,BCS}(T)} = \langle g^2(\phi)\rangle \sqrt{\frac{7\zeta(3)}{\pi^2\langle g^4(\phi)\rangle\left[I_3+\frac{1}{y_c}-\frac{\tanh y_c}{y_c^2}\right]}}\tanh y_c$$
$$\times\left\{\frac{1-\frac{1}{2}\left(\alpha+\frac{\beta}{3}\right)\left(1-\frac{T}{T_c}\right)-\frac{\beta}{3}\left(\alpha+\frac{7}{6}\beta\right)\left(1-\frac{T}{T_c}\right)^2}{1-\frac{1}{2}\left(3-\frac{31\zeta(5)}{(7\zeta(3))^2}\right)\left(1-\frac{T}{T_c}\right)+\frac{31\zeta(5)}{(7\zeta(3))^2}\left(3-\frac{31\zeta(5)}{14(\zeta(3))^2}\right)\left(1-\frac{T}{T_c}\right)^2}\right\}. \tag{28}$$

When $g(\phi)=1$, (s-wave case)

$$\frac{H_{c,s}(T)}{H_{c,BCS}(T)} = \sqrt{\frac{7\zeta(3)}{\pi^2\left[I_3+\frac{1}{y_c}-\frac{\tanh y_c}{y_c^2}\right]}}\tanh y_c$$
$$\times\left\{\frac{1-\frac{1}{2}\left(\alpha+\frac{\beta_s}{3}\right)\left(1-\frac{T}{T_c}\right)-\frac{\beta_s}{3}\left(\alpha+\frac{7}{6}\beta_s\right)\left(1-\frac{T}{T_c}\right)^2}{1-\frac{1}{2}\left(3-\frac{31\zeta(5)}{(7\zeta(3))^2}\right)\left(1-\frac{T}{T_c}\right)+\frac{31\zeta(5)}{(7\zeta(3))^2}\left(3-\frac{31\zeta(5)}{14(\zeta(3))^2}\right)\left(1-\frac{T}{T_c}\right)^2}\right\} \tag{29}$$

and when $g(\phi)=\cos 2\phi$ (d-wave case)

$$\frac{H_{c,d}(T)}{H_{c,BCS}(T)} = \sqrt{\frac{14\zeta(3)}{3\pi^2\left[I_3+\frac{1}{y_c}-\frac{\tanh y_c}{y_c^2}\right]}}\tanh y_c$$
$$\times\left\{\frac{1-\frac{1}{2}\left(\alpha+\frac{\beta_d}{3}\right)\left(1-\frac{T}{T_c}\right)-\frac{\beta_d}{3}\left(\alpha+\frac{7}{6}\beta_d\right)\left(1-\frac{T}{T_c}\right)^2}{1-\frac{1}{2}\left(3-\frac{31\zeta(5)}{(7\zeta(3))^2}\right)\left(1-\frac{T}{T_c}\right)+\frac{31\zeta(5)}{(7\zeta(3))^2}\left(3-\frac{31\zeta(5)}{14(\zeta(3))^2}\right)\left(1-\frac{T}{T_c}\right)^2}\right\}. \tag{30}$$

Fig. 2 shows the $H_{c,(s,d)}(T)/H_{c,BCS}(T)$ ratio results as functions of increasing ω_D/T_c for various $T=T_c$ values and different pairing symmetries. We can see from the graphs that curves $H_{c,s}(T)/H_{c,BCS}(T)$ and $H_{c,d}(T)/H_{c,BCS}(T)$ follow similar trend, with $H_{c,s}(T)>H_{c,d}(T)$ for all ω_D/T_c values. Both $H_{c,s}(T)$ and $H_{c,d}(T)$ reach their peak values at $\omega_D/T_c \approx 4$, and remain constant when $\omega_D/T_c > 10$.

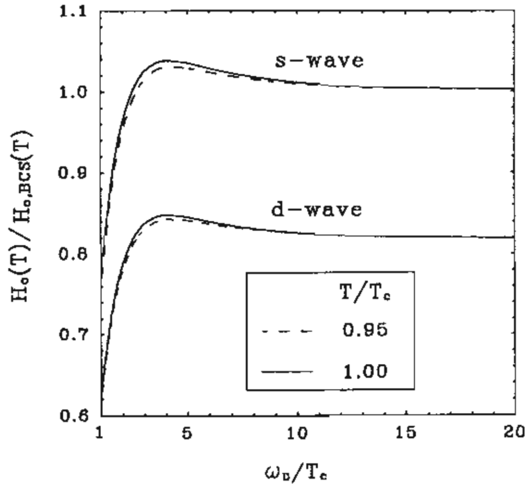

Fig. 2. Comparision of the normalized critical field, $H_c(T)/H_{c,\mathrm{BCS}}(T)$, as a function of ω_D/T_c for s- and d-wave superconductors at two reduced temperatures $T/T_c = 1.00$ and 0.95.

If we take the limit $y_c = \omega_D/2T_c \to \infty$ and $T = T_c$, then $H_{c,s}(T_c)/H_{c,\mathrm{BCS}}(T_c) = 1$ and $H_{c,d}(T_c)/H_{c,\mathrm{BCS}}(T_c) = \sqrt{2/3}$.

The specific heat jump is related to the thermodynamic potential difference by the general relation $C_S - C_N = \Delta C = -T(\partial^2 \Delta F/\partial T^2)$ which gives

$$\Delta C(T) = \frac{8N(0)T_c\langle g^2(\phi)\rangle^2 \tanh y_c}{\langle g^4(\phi)\rangle\left[I_3 + \dfrac{1}{y_c} - \dfrac{\tanh y_c}{y_c^2}\right]}\left\{1 - (3\alpha+\beta)\left(1 - \frac{T}{T_c}\right) + \frac{3}{2}(\alpha - 3\beta)(\alpha+\beta)\left(1 - \frac{T}{T_c}\right)^2\right\}. \tag{31}$$

The normalized specific heat jump ratio

$$\frac{\Delta C(T)}{C_N(T_c)} = \frac{\Delta C(T)}{\dfrac{2}{3}\pi^2 N(0)\mathrm{T}_c} = \frac{12\langle g^2(\phi)\rangle^2 \tanh^2 y_c}{\pi^2\langle g^4(\phi)\rangle\left[I_3 + \dfrac{1}{y_c} - \dfrac{\tanh y_c}{y_c^2}\right]}\left\{1 - (3\alpha+\beta)\left(1 - \frac{T}{T_c}\right)\right.$$
$$\left. + \frac{3}{2}(\alpha - 3\beta)(\alpha+\beta)\left(1 - \frac{T}{T_c}\right)^2\right\}. \tag{32}$$

When $g(\phi) = 1$, as for the s-wave case

$$\frac{\Delta C_s(T)}{C_N(T_c)} = \frac{12\tanh^2 y_c}{\pi^2\left[I_3 + \dfrac{1}{y_c} - \dfrac{\tanh y_c}{y_c^2}\right]}\left\{1 - (3\alpha+\beta_s)\left(1 - \frac{T}{T_c}\right) + \frac{3}{2}(\alpha - 3\beta_s)(\alpha+\beta_s)\left(1 - \frac{T}{T_c}\right)^2\right\}, \tag{33}$$

and as $y_c = \omega_D/2T_c \to \infty$ we find

$$\frac{\Delta C_{s,BCS}(T)}{C_N(T_c)} = \frac{12}{7\zeta(3)}\left\{1 - 3\left(3 - \frac{31\zeta(5)}{(7\zeta(3))^2}\right)\left(1 - \frac{T}{T_c}\right) + \frac{27}{2}\left(1 + \frac{93\zeta(5)}{(7\zeta(3))^2}\right)\left(1 - \frac{31\zeta(5)}{(7\zeta(3))^2}\right)\left(1 - \frac{T}{T_c}\right)^2\right\} \tag{34}$$

and when $g(\phi) = \cos 2\phi$, as for the d-wave case

$$\frac{\Delta C_d(T)}{C_N(T_c)} = \frac{8\tanh^2 y_c}{\pi^2\left[I_3 + \frac{1}{y_c} - \frac{\tanh y_c}{y_c^2}\right]}\left\{1 - (3\alpha + \beta_d)\left(1 - \frac{T}{T_c}\right) + \frac{3}{2}(\alpha - 3\beta_d)(\alpha + \beta_d)\left(1 - \frac{T}{T_c}\right)^2\right\}. \tag{35}$$

If we take $y_c = \omega_D/2T_c \to \infty$ limit, we have

$$\frac{\Delta C_{d,BCS}(T)}{C_N(T_c)} = \frac{8}{7\zeta(3)}\left\{1 - 3\left(3 - \frac{310\zeta(5)}{9(7\zeta(3))^2}\right)\left(1 - \frac{T}{T_c}\right) + \frac{27}{2}\left(1 + \frac{310\zeta(5)}{3(7\zeta(3))^2}\right)\left(1 - \frac{310\zeta(5)}{9(7\zeta(3))^2}\right)\left(1 - \frac{T}{T_c}\right)^2\right\}. \tag{36}$$

Eqs. (33) and (35) are analytical expressions for the normalized specific heat jump $\Delta C_s(T)/C_N(T_c)$ and $\Delta C_d(T)/C_N(T_c)$ within the BCS framework for the constant density of states near the Fermi energy. The ratios are plotted as functions of ω_D/T_c and pairing symmetries in Figs. 3 and 4. We can see from the curves that the ratios first increase for low ω_D/T_c values, produce a peak at $\omega_D/T_c \approx 4$ and reach constant value for large

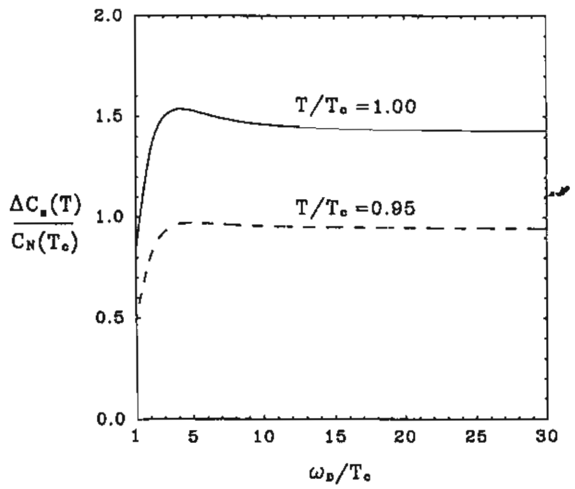

Fig. 3. The normalized specific heat jump of an s-wave superconductor $\Delta C_s(T)/C_N(T_c)$ versus ω_D/T_c for various values of T/T_c. The solid line corresponds to $T/T_c = 1.00$, the dashed line corresponds to $T/T_c = 0.95$.

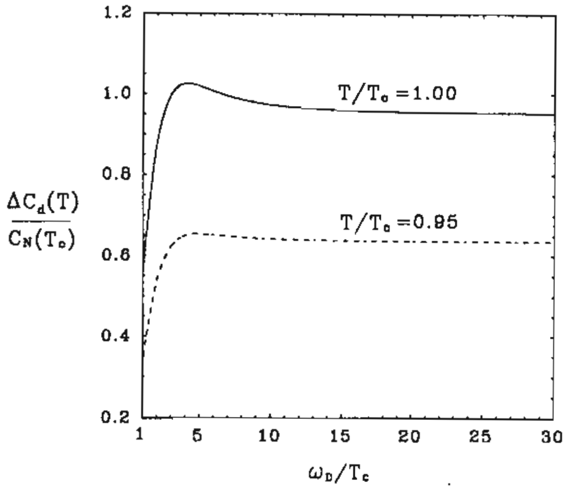

Fig. 4. $\Delta C_d(T)/C_N(T_c)$, the normalized specific heat jumps of a d-wave superconductor, versus ω_D/T_c for various values of T/T_c. The solid and dashed lines corresponds to $T/T_c = 1.00$ and 0.95, respectively.

ω_D/T_c. For the s-wave superconductor, the ratio is found to be generally larger than the d-wave superconductor and it reaches the BCS limit, 1.43, when $\omega_D/T_c > 10$. We note also from the graphs that as the reduced temperature decreases, the normalized specific heat jump ratio also decreases.

5. Conclusions

In the present work, the BCS model of superconductivity is used to derive formulas for the temperature dependence of the order parameter, the critical field and the specific heat jump at T_c and temperature near T_c. We follow the BCS formalism with the important difference that we calculate all thermodynamic quantities exactly.

We first investigate the temperature dependence of the order parameter and use it to derive an exact expression for the free energy difference between the two phases. The critical field and the specific heat expression are then obtained from the free energy difference.

Our results show that the newly calculated quantities such as $\Delta^2(T)$, $H_{c,(s,d)}(T)$ and $\Delta C_{s,d}(T)$ are generally dependent on the ratio of T_c and the Debye temperature ω_D as well as on the type of pairing. We have also shown that the relative quantities such as $\Delta^2_{s,d}(T)/\Delta^2_{BCS}$, $H_{c,(s,d)}(T)/H_{c,BCS}(T)$ and $\Delta C_{s,d}(T)/C_N(T_c)$ can differ significantly from 1, 1, and 1.43, respectively and that these quantities are very sensitive to low ω_D/T_c values but independent for large ω_D/T_c. The difference between BCS calculations and ours are most pronounced as $\omega_D/T_c \to 4$. Nevertheless, our new formulas for the critical field and the specific heat jump of the s-wave superconductor, which are one of the cornerstones of the work, properly reduces to the BCS limit as $\omega_D/T_c \to \infty$. Our analysis shows that the constant density of states in the conventional BCS theory cannot explain the large values of $\Delta C(T_c)/T_c$ found in many high temperature superconductors [6,7]. Also the s pairing symmetry consideration does not give any appreciable enhancement of $\Delta C(T)$ or $H_c(T)$ over BCS value but the d pairing symmetry decreases $\Delta C(T)$ and $H_c(T)$ considerably. We conclude that to explain the higher values of $\Delta C(T)/C_N(T_c)$ and $H_c(T)/H_{c,BCS}(T)$ over BCS value within the BCS formalism, one may need to take into account the energy dependent density of states with sharper peak at the Fermi level.

Acknowledgements

We thank the National Science and Technology Development Agency of Thailand and the Thailand Research Fund for the partial financial support of this work.

References

[1] J.R. Schrieffer, Theory of Superconductivity, Benjamin, New York, 1964.
[2] B. Allen, B. Mitrovic, in: H. Ehrenreich, F. Seitz, D. Turnbull (Eds.), Solid State Physics vol. 37 Academic Press, New York, 1982, p. 1.
[3] R. Mersevey, B. Schwartz, in: R.D. Parks (Ed.), Superconductivity vol. 1 Dekker, New York, 1969, p. 117.
[4] S.B. Nam, Phys. Lett. A 193 (1994) 111.
[5] L. Xu, Z. Shu, S. Wang, Phys. Rev. B 57 (1998) 11654.
[6] E.S.R. Gopal, Specific Heat at Low Temperature, Heywood, London, 1996.
[7] A. Junod, in: D.M. Ginsberg (Ed.), Physical Properties of High Temperature Superconductors II World Scientific, Singapore, 1990, p. 13.

Journal of Superconductivity: Incorporating Novel Magnetism, Vol. 13, No. 1, 2000

Specific Heat Jump at T_c of High T_c Superconductors: Effect of Van Hove Singularity

B. Krunavakarn,[1] S. Kaskamalas,[1] N. Jinuntuya,[2] and S. Yoksan[3]

Received 15 January 1999

In the BCS framework, exact expressions for the ratio between the jump in the specific heat at T_c and the normal phase specific heat are derived within the Van Hove singularity scenario. Analytical results are obtained for an isotropic s-wave and anisotropic d-wave pairing symmetries. Graphical solutions of the ratio as functions of ω_D/T_c and E_f/T_c, where ω_D is the cutoff energy and E_f is the Fermi energy, show significant deviations from the BCS value of 1.43.

KEY WORDS: Specific heat jump; s, d pairing symmetry; Van Hove superconductor.

1. INTRODUCTION

To understand the origin of high-temperature superconductivity, a model based on the close proximity of the Fermi level to a quasi-two-dimensional Van Hove singularity (VHS) in the density of states $N(\varepsilon)$ has been suggested [1–3]. Recent high-resolution angle-resolved photoemission spectroscopy measurements on high T_c superconductors [4–6] have identified the presence of saddle points in the band structure of these materials and these saddle points are shown to correspond to logarithmic VHS in the density of states. The influence of VHS on several properties of cuprate superconductors have been studied [7–9].

Specific heat is an important property of a superconductor. It can inform us about the nature of phase transition and the symmetry of the pairing state [10,11]. The jump in the specific heat, ΔC, at the critical temperature provides a relative measure of the superconducting volume, showing the fraction that undergoes the superconducting transition. In BCS theory the ratio $\Delta C(T_c)/C_N(T_c)$ is a universal constant, 1.43. In many high-temperature cuprate superconductors this ratio has been found to be greater than the BCS value [10,11]. The explanation of this discrepancy has been attributed to the logarithmic VHS in the normal state density of states with s-wave order parameter [12,13], and also with the d-wave order parameter [14,15]. Sarkar and Das [16] studied the specific heat jump of s-wave cuprates and found that an extended VHS can account for some of the experimental results reasonably well. In their investigation of the specific heat jump, Newns *et al.* [17] showed that the d-wave version of the Van Hove scenario at the BCS level of approximation is viable. Recently Dagotto *et al.* [18] proposed a theoretical model including both the VHS and antiferromagnetic fluctuation effect. Their model explains many features of high T_c materials and predicts a gap parameter of $d_{x^2-y^2}$ wave type [19].

Now in the BCS framework, the specific heat jump is usually calculated from the temperature derivative of the square of the gap parameter and the reduced gap ratio (R). Refs. [12], [13], and [16] defined $A^2 = -d[\Delta(T)/\Delta(0)]^2/d(T/T_c)$ and $B^2 = [\Delta(0)/T_c]^2$. $\Delta(T)$ is the temperature-dependent energy gap function, and obtained $A = 1.74$, $B = 1.76$. As is well known these quantities having such values when the condition $\omega_D/T_c \rightarrow \infty$ is considered. In conventional superconductors this restriction is valid because the cutoff energy ω_D is much greater than T_c.

[1] Department of Physics, Chulalongkorn University, Bangkok 10330, Thailand.
[2] Department of Physics, Kasetsart University, Bangkok 10900, Thailand.
[3] Department of Physics, Srinakharinwirot University, Bangkok 10110, Thailand.

With the discovery of high-temperature oxides the Debye cutoff ω_D is not that much greater than T_c, the dimensionless ratio ω_D/T_c is finite. Therefore new calculations of A and B are needed [20].

It is, therefore of great interest to obtain exact analytical expressions for $\Delta C(T_c)/C_N(T_c)$ without making any approximation concerning ω_D/T_c, to know what the BCS theory predicts for A, B, and $\Delta C(T_c)/C_N(T_c)$ when ω_D/T_c is beyond its restricted value. The purpose of this paper is to investigate the specific heat jump of isotropic s-wave and anisotropic d-wave superconductors within the BCS framework for a constant density of states and for a VHS density of states.

Section 2 deals with the thermodynamic property of a superconductor. It starts with the gap equation from which we derive a formal but completely general formula for the temperature dependence of the order parameter and the normalized specific heat jump. Effects of constant and VHS density of states on the specific heat difference are presented analytically and graphically in Section 3. Finally, discussions and conclusions are drawn in Section 4.

2. TEMPERATURE DEPENDENCE OF THE ORDER PARAMETER AND SPECIFIC HEAT JUMP AT T_c

Within the BCS framework, the gap equation is given by the equation

$$\Delta_{\bar{k}} = \sum_{\bar{k}'} \frac{V_{\bar{k}\bar{k}'}\Delta_{\bar{k}'}\tanh\left(\frac{E_{\bar{k}'}}{2T}\right)}{2E_{\bar{k}'}} \qquad (1)$$

where $E_{\bar{k}}^2 = (\varepsilon_{\bar{k}} - E_f)^2 + \Delta_{\bar{k}}^2$, ε_k is the quasiparticle energy, E_f is the Fermi energy, $\Delta_{\bar{k}}$ is the order parameter, $V_{\bar{k}\bar{k}'}$ is the positive phonon mediated interaction, which is finite within the energy range of $\hbar\omega_D$ around E_f, and ω_D is the Debye frequency. For the sake of simplicity we assume that

$$V_{\bar{k}\bar{k}'} = Vg(\phi)g(\phi'), \quad \text{if } E_f - \hbar\omega_D \le \varepsilon_{\bar{k}}, \varepsilon_{\bar{k}'} \le E_f + \hbar\omega_D \qquad (2)$$

and $g(\phi) = 1$ or $\cos 2\phi$ depending on whether the superconductor is an s- or d-wave one, here ϕ is the angle between the momentum $\bar{k}$ of the pair electrons and the a-axis of a CuO_2 plane, i.e., $\phi = \tan^{-1}(k_y/k_x)$, and V represents the constant electron-phonon interaction strength.

For the form of the scattering matrix element given by Eq. (2), the solution of the gap equation has the structure

$$\Delta_{\bar{k}} = \Delta(T)g(\phi) \qquad (3)$$

where $\Delta(T)$ is the temperature-dependent energy gap function. Upon substituting Eqs. (2) and (3) in Eq. (1), one obtains the equation

$$\frac{1}{V} = \int_0^{2\pi}\frac{d\phi}{2\pi}g^2(\phi)\int_{-\omega_D}^{\omega_D}\frac{d\varepsilon}{2E}N(\varepsilon)\tanh\left(\frac{E}{2T}\right) \qquad (4)$$

where $N(\varepsilon)$ is the electronic density of states per spin. By differentiating Eq. (4) with respect to T, the temperature gradient of $\Delta^2(T)$ at $T = T_c$ is given by the expression

$$\frac{1}{T_c}\frac{d\Delta^2(T)}{dT}\Big|_{T=T_c} = \frac{8\int_0^{2\pi}\frac{d\phi}{2\pi}g^2(\phi)\int_0^{\omega_D/2T_c}dx\,N(2T_cx)\,\mathrm{sech}^2(x)}{\int_0^{2\pi}\frac{d\phi}{2\pi}g^4(\phi)\int_0^{\omega_D/2T_c}dx\,N(2T_cx)\left[\frac{\mathrm{sech}^2(x)}{x^2}-\frac{\tanh(x)}{x^3}\right]} \qquad (5)$$

The jump in the specific heat T_c within the framework of the BCS formalism is calculated from the usual expressions for specific heat of the normal and superconducting phases given by

$$C_N = 2\sum_{\bar{k}}\varepsilon_{\bar{k}}\frac{\partial f(\varepsilon_{\bar{k}})}{\partial T} \qquad (6)$$

$$C_S = 2\sum_{\bar{k}}E_{\bar{k}}\frac{\partial f(E_{\bar{k}})}{\partial T}. \qquad (7)$$

Here the indices N and S denote the normal and superconducting states, respectively. $f(\varepsilon_{\bar{k}})$ is the usual Fermi distribution function for electron with vector $\bar{k}$. The factor 2 arises for the sum overspins of the Cooper pair. We finally obtain the ratio between the jump in the specific heat at a transition from the normal to the superconducting states and the normal specific heat as

$$\frac{\Delta C(T_c)}{C_N(T_c)} = \frac{1}{\int_0^\infty dx N(2T_c x) x^2 \operatorname{sech}^2(x)} \left\{ \frac{\int_0^{\omega_D/2T_c} dx N(2T_c x) x^2 \operatorname{sech}^2(x) - \left[\int_0^{2\pi} \frac{d\phi}{2\pi} g^2(\phi) \int_0^{\omega_D/2T_c} dx N(2T_c x) \operatorname{sech}^2(x) \right]^2}{\int_0^{2\pi} \frac{d\phi}{2\pi} g^4(\phi) \int_0^{\omega_D/2T_c} dx N(2T_c x) \left| \frac{\operatorname{sech}^2(x)}{x^2} - \frac{\tanh(x)}{x^3} \right|} \right\} - 1 \tag{8}$$

3.1. Effect of Constant Density of States

We note that Eqs. (5) and (8) are exact analytical expressions for the temperature gradient of $\Delta^2(T)$ and the normalized specific heat jump $\Delta C(T_c)/C_N(T_c)$. In the standard BCS treatment, $N(\varepsilon)$ is assumed to be constant, independent of energy, i.e., $N(\varepsilon) = N(0)$. if we take $g(\phi) = 1$ which is the s-wave case, then $\Delta C(T_c)/C_N(T_c)$ simplifies to

$$\frac{\Delta C(T_c)}{C_N(T_c)} = \frac{12}{\pi^2} \left\{ \left(\frac{\omega_D}{2T_c}\right)^2 \left[1 + \tanh\left(\frac{\omega_D}{2T_c}\right)\right] - \left(\frac{\omega_D}{T_c}\right) \ln\left[2\cosh\left(\frac{\omega_D}{2T_c}\right)\right] + Li_2[-e^{-\omega_D/T_c}] - \frac{\tanh^2(\omega_D/T_c)}{\frac{\tanh(\omega_D/2T_c)}{(\omega_D/2T_c)^2} - \frac{1}{(\omega_D/2T_c)} - \frac{2}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(n+\frac{1}{2})^3} \tan^{-1}\left(\frac{\omega_D/T_c}{(2n+1)\pi}\right)} \right\}, \tag{9}$$

where $Li_2(x) = \sum_{k=1}^{\infty} x^k/k^2$ is the dilogarithmic function [22]. In the limit $\omega_D/T_c \to \infty$, Eq. (9) reduces to $\Delta C(T_c)/C_N(T_c) = 12/7\zeta(3) = 1.43$, which is identical to the standard classical BCS value, here $\zeta(3)$ is the Riemann zeta function and $C_N(T_c) = 2/3\, \pi^2 N(0) T_c$.

Our exact result shows that $\Delta C(T_c)/C_N(T_c)$ is material dependent and depends only on the ratio ω_D/T_c. Graphical computation of Eq. (9) shows that the curve of $\Delta C(T_c)/C_N(T_c)$ versus ω_D/T_c increases monotonically as ω_D/T_c increases and reaches its constant value of 1.43 when ω_D/T_c is greater than 7.

As a matter of interest we also compute the jump in the specific heat for the d-wave superconductor. Taking $g(\phi) = \cos 2\phi$ and $N(\varepsilon) = N(0)$ in Eq. (8), we find that the normalized jump is given by

$$\frac{\Delta C(T_c)}{C_N(T_c)} = \frac{12}{\pi^2} \left\{ \left(\frac{\omega_D}{2T_c}\right)^2 \left[1 + \tanh\left(\frac{\omega_D}{2T_c}\right)\right] - \left(\frac{\omega_D}{T_c}\right) \ln\left[2\cosh\left(\frac{\omega_D}{2T_c}\right)\right] + Li_2[-e^{-\omega_D/T_c}] - \frac{\frac{2}{3}\tanh^2(\omega_D/2T_c)}{\frac{\tanh(\omega_D/2T_c)}{(\omega_D/2T_c)^2} - \frac{1}{(\omega_D/2T_c)} - \frac{2}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(n+\frac{1}{2})^3} \tan^{-1}\left(\frac{\omega_D/T_c}{(2n+1)\pi}\right)} \right\} \tag{10}$$

This equation gives $\Delta C(T_c)/C_N(T_c) = 0.95$ in the limit $\omega_D/T_c \to \infty$. Graphical solutions of $\Delta C(T_c)/C_N(T_c)$ vs. ω_D/T_c are plotted in Fig. 1. Again we can see that the deviation of the ratio from the BCS result is significantly for all ω_D/T_c values.

3.2. Effect of VHS Density of States

However, if the density of states is energy dependent such as in the case of VHS, by taking $g(\phi) = 1$ for the s-wave case and $N(\varepsilon) = N(0) \ln|E_1/\varepsilon|$ in Eqs. (6) and (8), we obtain the normal phase specific heat and the ratio between the specific heat jump and the normal phase specific heat of an s-wave Van Hove superconductor as

$$C_N(T_c) = \frac{2}{3}\pi^2 N(0) T_c \left[\ln\left(\frac{E_1}{T_c}\right) - 1.0458\right] \tag{11}$$

and

$$\frac{\Delta C(T_c)}{C_N(T_c)} = \frac{P(\omega_D, T_c, E_1) - Q(\omega_D, T_c, E_1)}{\frac{\pi^2}{12} \ln\left(\frac{E_1}{2T_c}\right) - 0.2902} - 1 \tag{12}$$

where

$P(\omega_D, T_c, E_f)$

$$= \ln\left(\frac{E_F}{2T_c}\right)\left\{\left(\frac{\omega_D}{2T_c}\right)^2\left[1 + \tanh\left(\frac{\omega_D}{2T_c}\right)\right]\right.$$

$$- \left(\frac{\omega_D}{T_c}\right)\ln\left[2\cosh\left(\frac{\omega_D}{2T_c}\right)\right]$$

$$\left. + \frac{\pi^2}{12} + Li_2\left[-e^{-\omega_D/T_c}\right]\right\}$$

$$-2\sum_{k}(-1)^k$$

$$\left\{\begin{array}{l} e^{-k\omega_D/T_c}\left[\frac{3}{4k^2} - \frac{\omega_D}{4kT_c} - \left(\frac{\omega_D}{2T_c}\right)\ln\left(\frac{\omega_D}{2T_c}\right)\right. \\ \left. - \frac{1}{k}\left(\frac{\omega_D}{2T_c}\right)\ln\left(\frac{\omega_D}{2T_c}\right)\right] + \frac{3}{4k^2} \\ + \sum_{n=0}^{\infty}\frac{(-1)^n(2k)^n}{k(n+1)!}\left(\frac{\omega_D}{2T_c}\right)^{n+1}\left[\ln\left(\frac{\omega_D}{2T_c}\right) - \frac{1}{n+1}\right] \end{array}\right\} \tag{13}$$

and

$Q(\omega_D, T_c, E_f)$

$$= \frac{\left(\ln\left(\frac{E_f}{\omega_D}\right)\tanh\left(\frac{\omega_D}{2T_c}\right) + 2\sum_{n}\frac{1}{(n+\frac{1}{2})\pi}\tan^{-1}\left(\frac{\omega_D/T_c}{(2n+1)\pi}\right)\right)^2}{\left\{\begin{array}{l} \ln\left(\frac{E_f}{\omega_D}\right)\left[\frac{\tanh(\omega_D/2T_c)}{(\omega_D/2T_c)^2} - \frac{1}{(\omega_D/2T_c)}\right) \\ - 2\sum_{n=0}^{\infty}\frac{1}{((n+\frac{1}{2})\pi)^2}\tan^{-1}\left(\frac{\omega_D/T_c}{(2n+1)\pi}\right)\left[\ln\left(\frac{E_f}{\omega_D}\right) + 1\right] \\ - \pi\sum_{n=0}^{\infty}\frac{1}{((n+\frac{1}{2})\pi)^3}\sinh^{-1}\left(\frac{\omega_D/T_c}{(2n+1)\pi}\right) \\ + 2\sum_{n=0}^{\infty}\sum_{k}\sum_{m=1}\frac{1}{((n+\frac{1}{2})\pi)^2}\frac{(2k)!}{2^{2k}(k!)^2(2k+1)(2k-2m+1)} \\ \tanh^{2k-2m+1}\left(\sinh^{-1}\left(\frac{\omega_D/T_c}{(2n+1)\pi}\right)\right) \end{array}\right\}} \tag{14}$$

In the limit $\omega_D/T_c \to \infty$ and $E_f/T_c = 200$, Eqs. (12)–(14) gives $\Delta C(T_c)/C_N(T_c) = 1.94$.

By taking $g(\phi) = \cos 2\phi$ in Eq. (8), the normalized specific heat jump $\Delta C(T_c)/C_N(T_c)$ for a d-wave superconductor is calculated, and one obtains

$$\frac{\Delta C(T_c)}{C_N(T_c)} = \frac{6/\pi^2}{\ln\left(\frac{E_f}{T_c}\right) - 1.0458}$$

$$\left\{P(\omega_D, T_c, E_f) - \frac{2}{3}Q(\omega_D, T_c, E_f)\right\} - 1 \tag{15}$$

with $P(\omega_D, T_c, E_f)$ and $Q(\omega_D, T_c, E_F)$ as defined in Eqs (13) and (14), respectively. Results are presented in Fig. 2 for values of ω_D/T_c up to 25. In the limit $\omega_D/T_c \to \infty$ and $E_f/T_c = 200$, Eq. (15) gives $\Delta C(T_c)/C_N(T_c) = 1.29$. In general, we can see that the normalized specific heat jump for a d-wave superconductor is predicted to be much smaller than the BCS value of 1.43. However, for an s-wave Van Hove superconductor, the jump is significantly higher.

4. DISCUSSIONS AND CONCLUSIONS

Our graphical solutions for the normalized specific heat jump help clarify how the jump is affected by the electronic density of states at the Fermi level, the symmetry of order parameters, and material parameters. We can see that the deviations of the ratio $\Delta C(T_c)/C_N(T_c)$ from the canonical BCS value in high T_c superconductors can be accounted for by considering either the symmetry of the gap or the VHS or the values of the parameters such as ω_D, T_c, and E_f.

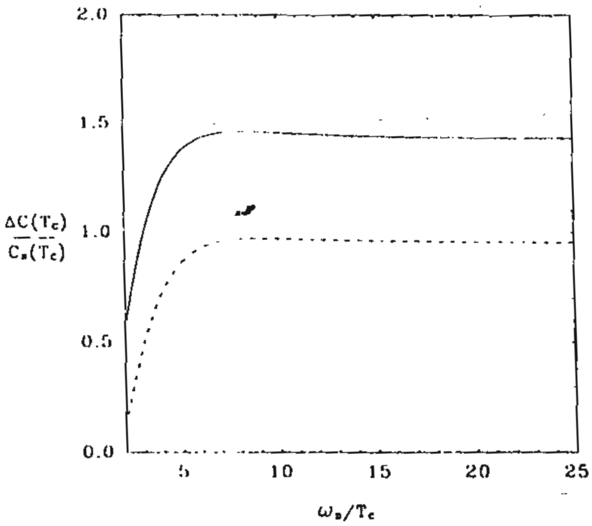

Fig. 1. Jumps in specific heat, in units of the normal state specific heat at the transition, versus ratio ω_D/T_c for the constant density of states at the Fermi level. The solid and dashed curves show results of calculations based on s and d gaps, respectively.

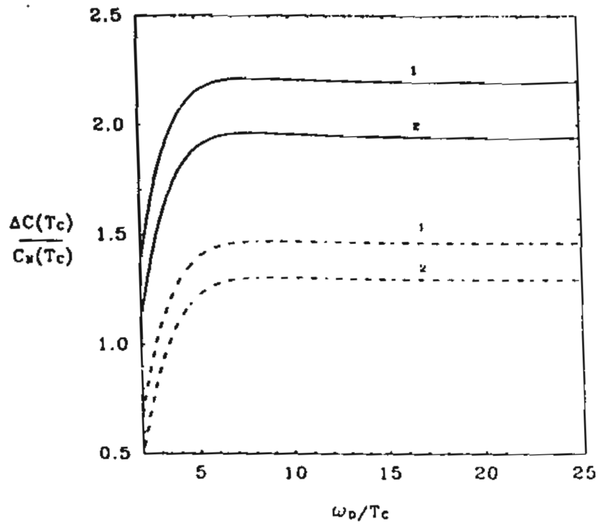

Fig. 2. Normalized electronic specific heat jump $\Delta C(T_c)/C_N(T_c)$ versus ratio ω_D/T_c of a Van Hove superconductor. The solid and dashed curves correspond to an s- and d-wave gap symmetry, respectively. Curves 1 and 2 correspond to E_F/T_c = 50 and 200, respectively.

As shown in Fig. 1 for the s-wave superconductors with the constant density of states, our formula recovers the usual BCS result (1.43) by putting $\omega_D/T_c \rightarrow \infty$ in Eq. (9). The fall of $\Delta C(T_c)/C_N(T_c)$ with decreasing ω_D/T_c is predicted when ω_D/T_c is less than or 7.

Recently Bandyopadhyay *et al.* [23] reported the results of specific heat results of specific heat measurements carried out on samples of Tl-based 2-2-2-3 compounds. their data for the average Debye temperature for 2-2-2-3 is 480 K. The T_c values of the 2-2-2-3 system are 107 and 125 K. They evaluated the BCS ratio $\Delta C(T_c)/C_N(T_c)$ for the system and found the ratios to be 1.45. This value is greater than our for the s-wave superconductor. Hence the Tl-system is not a simple BCS superconductor.

We have also studied $\Delta C(T_c)/C_N(T_c)$ as a function of ω_D/T_c for a d-wave superconductor having the constant density of states at the Fermi level. $\Delta C(T_c)$ and $C_N(T_c)$ are calculated using the exact expressions (6) and (8). It is found that the d-wave symmetry shifts $\Delta C(T_c)$ lower, hence the smaller value of the ratio $\Delta C(T_c)/C_N(T_c)$. this is probably due to the fact that there are a few more non-superconducting particles when a d-wave gap parameters opens compared to an s-wave gap. The limiting values of $\Delta C(T_c)/C_N(T_c)$ is 1.29, which is considerably lower than the BCS value of 1.43. The ratio of the specific heat jump $\Delta C(T_c)/C_N(T_c)$ versus ω_D/T_c for the d-wave gap parameter case is also presented in Fig. 1. Our formula also predicts that the jump at T_c decrease when $\omega_D/T_c \leq 6$.

As for the VHS superconductor, we find that the effect of VHS on the electronic-specific heat jump of an s-wave superconductor is to increase the value of the jump at T_c considerably over the BCS values. The limiting value of $\Delta C(T_c)/C_N(T_c)$ with $\omega_D/T_c \rightarrow \infty$ is found to be 1.94 in fine agreement with Sarkar and Das [16] who found the numerical value of the ratio at T_c to be 2.13 by using a more realistic density of states. Our results is also in agreement with Dorbolo *et al.* [14, 15] who in their study of the influence of a VHS on the ratio found the ratio at T_c to be 2, when they took $\Delta(0)$ to be 20 meV. We also found that the normalized ratio increases rapidly as ω_D/T_c increase from 2, reaches a maximum at ω_D/T_c = 7 and as ω_D/T_c increase further, the normalized specific-heat jump remains unchanged. In addition our calculations show unambiguously that when the ratio E_F/T_c decreases, the jump ratio increases.

Finally the normalized specific heat difference for the d-wave VHS case is presented in Fig. 2. The graph shows that the normalized jump at T_c is much lower than the BCS values and that the magnitude of the jump is almost the same as that of the constant density of states case. Dorbolo *et al.* [14, 15] found that the ratio $C_s(T_c)/C_N(T_c)$ in a zero magnetic field in a d-wave superconductor with typical values of physical parameters in high T_c superconductor is 1.4, which agrees well with our calculation here. We found that as E_F/T_c decreases, the ratio $\Delta C(T_c)/C_N(T_c)$ increases. But for experimental data on $YBa_2Cu_3O_{7-\delta}$, for which [26] obtained $\Delta C(T_c)/C_N(T_c) \approx 4.8$, our theory cannot explain the result; this may be due to the fact that the high-T_c superconductor is not quite two-dimensional.

In conclusion, we would like to stress here that our calculation is strictly two-dimensional. A test of the quantitative finding presented in this paper with respect to parameter changes can be made by varying the ratio ω_D/T_c and E_F/T_c. Should the test fail, we would need to conclude that the BCS theory that incorporates the VHS density of states is inapplicable to the material and that a new or modified density of states and theory are required.

ACKNOWLEDGMENTS

This work has been partially supported by the National Science and Technology Development

Agency of Thailand and the Thailand Research Fund.

REFERENCES

1. J. Labbe and J. Bok. *Europhys. Lett* **3**, 1225 (1987)
2. J. Friedel, *J. Phys. (Paris)* **48**, 1787 (1987).
3. D. M. Newns, P. C. Pattnaik, and C. C. Tsuei, *Phys. Rev. B* **43**, 3075 (1991).
4. D. S. Dessau, *et al., Phys. Rev. Lett.* **71**, 2781 (1993).
5. K. Gofron, *et al., Phys. Rev. Lett.* **73**, 3302 (1994).
6. J. Ma, *et al., Phys. Rev. B* **51**, 3832 (1995).
7. D. M. Newns, *et al., Comments Condens. Matter Phys.* **15**, 273 (1992).
8. D. M. Newns, *et al., Phys. Rev. Lett.* **73**, 1695 (1994).
9. M. Houssa, *et al., Phys. Rev. B* **56**, 6226 (1997).
10. E.S.R. Gopal, *Specific Heat at Low Temperatures* (Heywood. London, 1996.)
11. A. Junod. in *Physical Properties of High Temperature Super- conductors II*, Ed. D. M. Ginsberg (World Scientific, Singa-pore. 1990). p. 13.
12. C. C. Tsuei. *et al., Phys. Rev. Lett.* **69**, 2134 (1992).
13. A. Gama Goigochea, *Phys. Rev. B* **49**, 6864 (1994).
14. S. Dorbolo, *et al., Physica C* **267**, 175 (1997)
15. S. Dorbolo, *Physica C* **276**, 175 (1997)
16. S. Sarkar, and A. N. Das, *Phys. Rev. B* **54**, 14974 (1996).
17. D. M. Newns, *et al., Phys. Rev. B* **52**, 13611 (1995).
18. E. Dagotto, *et al., Phys. Rev. Lett.* **74**, 310 (1995).
19. C. C. Tsuei, and J. R. Kirtley, *Physica (Amsterdam)* 282C, **4** (1997).
20. B. Krunavakarn, *et al., J. Superconduct.* **11**, 271 (1998).
21. C. Pakokthom, *et al., J. Superconduct.* **11**, 429 (1998).
22. M. Abramowitz, and I.A.Stegun, in *Handbook of Mathematical Functions* (Dover, New York, 1972). pp. 67, 1004.
23. A. K. Bandyopadhyay. *et al., Physica C* **165**, 29 (1990).
24. E. Braun. *et al., Z. Phys. B* **84**, 333 (1991).
25. W. Schnelle. *et al., Physica C* **209**, 456 (1993).
26. A. Junod. *et al., Physica C* **152**, 495 (1998).
27. N. Philips. *et al., Phys. Rev. Lett.* **65**, 357 (1990)

phys. stat. sol. (b) **226**, No. 2, 315–321 (2001)

Effect of Pseudogap on the Isotope Exponent of High-T_c Superconductors

P. UDOMSAMUTHIRUN[1]) (a, b)

(a) Department of Physics, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand

(b) School of Physics, Institute of Science, Suranaree University of Technology, Nakorn Ratchasima 30000, Thailand

(Received by P. Deak April 5, 2001; accepted May 14, 2001)

Subject classification: 74.20.Fg; 74.72.-h; S10.15

The purpose of this paper is to explain the unusual isotope coefficients of cuprates by considering the influence of a pseudogap and phononic and electronic interactions in weak-coupling limit. Exact analytic expressions of the isotope exponent (α) for the s- and d-wave pairing symmetry are derived. It is found that α can fit the experimental data well and that the presence of the pseudogap increases α in the low-T_c region, but has no effect in the high-T_c region.

1. Introduction

The explanation of the isotope effect in high-T_c cuprate superconductors remains obscure through there are many possible explanations for its unusual doping dependence [1]. Experimantally it is found that optimally doped samples show a very small isotope exponent α of the order 0.05 or even smaller [2], while in the simplest scenario for phonon-induced pairing, $\alpha = 0.05$. This unusually small value in connection with high-T_c values leads to the early suggestion that the pairing interaction in high-T_c cuprates might be predominantly of electronic origin with a possible small phononic contribution [3]. This scenario is difficult to reconcile with the fact that some isotope exponents also show unusually high values, reaching values of 0.5 or even higher in some doped superconductors.

In recent years, the existence of a pseudogap in the normal state of underdoped high-T_c cuprate superconductors is considered to be among the most important features of cuprates. The evidence of a gap-like structure in the normal state at $T^* > T_c$ was provided by a variety of experimental methods [4–9]. Suzuki and Watanabe [10] have shown that the magnitude of a pseudogap at T_c is much larger than the superconducting gap at $T = 0$ K in the underdoped region and smaller in the near optimum doping and overdoped regions.

To explain the unusual isotope effect of cuprates being smaller, almost absence, than the conventional value 0.5, many models have been proposed such as the van Hove singularity [11–13], anharmonic phonon [14, 15], and pair-breaking effects [16]. Recently, Dahm [17] studied the influence of the pseudogap on the isotope exponent showing an electronic pairing interaction with a subdominant electron-phonon interaction. In the weak-coupling limit, he found that the introduction of a pseudogap leads to a strong increase of the isotope exponent, higher than its values in the absence of a pseudogap. He performs his study numerically.

[1]) e-mail: pongkaew@psm.swu.ac.th

 0370-1972/01/22608-0315 $ 17.50+.50/0

The purpose of this paper is to explain the unusual isotope effect of cuprates being smaller and higher than 0.5 by considering the influence of a pseudogap and subdominant electron–phonon interaction in the weak-coupling limit. We will derive exact formulas of the isotope exponent for superconductors having a constant density of states.

2. Formulation

Within the simple model of Loram et al. [18] superconductivity and normal-state pseudogaps are assumed to arise from independent and competing correlations and hence the superconducting gap can be written as

$$\Delta^2(T) = \Delta'^2(T) + E_g^2\,, \tag{1}$$

where $\Delta'(k)$ is the superconducting order parameter and E_g is the normal-state pseudogap. Therefore, at $T = T_c$, $\Delta(T_c) = E_g$ and the linearized gap equation in the weak-coupling limit for an anisotropic pairing interaction $V(k, k')$ reads as

$$\Delta'(k) = \sum_{k'} V(k, k')\,\frac{\tanh\sqrt{\varepsilon_{k'}^2 + E_g^2}/2T_c}{2\sqrt{\varepsilon_{k'}^2 + E_g^2}}\,\Delta'(k')\,. \tag{2}$$

Here ε_k is the band dispersion and $V(k, k')$ is the pairing interaction.

Following closely the work of Dahm [17], we assume that the pairing interaction consists of two parts: a phononic part $V_p(k, k')$ and the electronic part $V_e(k, k')$, such that the pairing interaction

$$V(k, k') = V_p(k, k') + V_e(k, k')\,. \tag{3}$$

The dominant contribution should be V_e. We have

$$V_{e,p}(k, k') = \begin{cases} V_{e0,p0}\Psi_\eta(k)\Psi_\eta(k') & \text{if} \quad |\varepsilon_k|, |\varepsilon_{k'}| \le \omega_{e,p} \\ 0 & \text{else} \end{cases}, \tag{4}$$

here ω_e and ω_p is the characteristic energy cutoff of the electronic and phononic part, respectively. ω_e is assumed to be independent of the isotopic mass and ω_p varies with the isotopic mass M like $1/\sqrt{M}$ as in the harmonic approximation. $\Psi_\eta(k)$ is the basis function for the pairing symmetry considered and

$$\begin{aligned} \Psi_\eta(k) &= 1 && \text{for s-wave pairing}\,, \\ &= \cos 2\theta_k && \text{for } d_{x^2-y^2} \text{ wave pairing}\,, \end{aligned} \tag{5}$$

where $\theta = \tan^{-1}(k_y/k_x)$ is the angular direction of the momentum k in the ab plane.

For such an interaction the superconducting order parameter can be separated into two parts: $\Delta(k) = \Delta_e(k) + \Delta_p(k)$ with

$$\Delta_{e,p}(k) = \begin{cases} \Delta_{e0,p0}\Psi_\eta(k) & \text{if} \quad |\varepsilon_k| \le \omega_{e,p} \\ 0 & \text{else}\,. \end{cases}, \tag{6}$$

Because it is widely accepted that the pseudogap in cuprates occurs below a certain temperature T^*, which is much higher than T_c [19], we can assume that $T^* > \omega_p > \omega_e$.

We also assume that $\Delta(k)$ and $E_g(k)$ have the same symmetry [20–22], so we choose $E_g(k)$ to be

$$E_g(k) = \begin{cases} E_{g0} & \text{for s-wave pairing}\,, \\ E_{g0}\cos(2\theta) & \text{for } d_{x^2-y^2} \text{ wave pairing}\,, \end{cases} \tag{7}$$

where E_{g0} is constant.

If we substitute Eqs. (3–7) into Eq. (2) and using the condition $\omega_p > \omega_e$, we arrive at the following equation:

$$\lambda(\omega_e,\,\omega_p,\,T_c) = \frac{V_{e0}L_e + V_{p0}L_p}{2} + \frac{1}{2}\sqrt{(V_{e0}L_e - V_{p0}L_p)^2 + 4V_{e0}V_{p0}L_e^2}\,, \tag{8}$$

where $L_e = L(\omega_e,\,T_c)$ and $L_p = L(\omega_p,\,T_c)$ and

$$L(\omega,\,T_c) = \frac{1}{2\pi}\int_0^{2\pi} d\theta\,\psi_\eta^2(\theta)\int_0^{\omega} d\varepsilon\,\frac{N(\varepsilon)}{\sqrt{\varepsilon^2+E_g^2}}\tanh\left(\frac{\sqrt{\varepsilon^2+E_g^2}}{2T_c}\right) \tag{9}$$

and T_c is determined from the implicit equation

$$\lambda(\omega_e,\,\omega_p,\,T_c) = 1\,. \tag{10}$$

From the isotope exponent α can be calculated as

$$\alpha = \frac{1}{2}\frac{d\,\ln T_c}{d\,\ln\omega_p} = -\frac{1}{2}\frac{\omega_p}{T_c}\frac{\dfrac{\partial\lambda}{\partial L_p}\dfrac{\partial L_p}{\partial\omega_p}}{\dfrac{\partial\lambda}{\partial L_p}\dfrac{\partial L_p}{\partial T_c} + \dfrac{\partial\lambda}{\partial L_e}\dfrac{\partial L_e}{\partial T_c}}$$
$$= \frac{-\dfrac{1}{2}\dfrac{\omega_p}{T_c}\dfrac{\partial L_p}{\partial\omega_p}}{\dfrac{\partial L_p}{\partial T_c} + \dfrac{V_{e0}}{V_{p0}}\left(\dfrac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e}\right)\dfrac{\partial L_e}{\partial T_c}}\,. \tag{11}$$

For a superconductor with a constant density of states, $N(E) = N_0$ through out the Fermi energy. It is a basic DOS consideration. By inserting this DOS in Eq. (9), we calculate the isotope exponent in Eq. (11), and find the s-wave isotope exponent as

$$\alpha_s = \frac{1}{2}\frac{\dfrac{\omega_p}{\sqrt{\omega_p^2+E_{g0}^2}}\tanh\left(\dfrac{\sqrt{\omega_p^2+E_{g0}^2}}{2T_c}\right)}{\left(f_s(\omega_p) + \dfrac{V_{e0}}{V_{p0}}\left[\dfrac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e}\right]f_s(\omega_e)\right)}\,, \tag{12}$$

where

$$f_s(\omega) = \frac{\sqrt{\omega^2+E_{g0}^2}}{\omega}\tanh\left(\frac{\sqrt{\omega^2+E_{g0}^2}}{2T_c}\right) - \frac{E_{g0}}{\omega}\tanh\left(\frac{E_{g0}}{2T_c}\right)$$
$$- \sum_{n=0}^{\infty}\frac{4T_cE_{g0}^2}{(E_{g0}^2+a^2)^{3/2}}\tan^{-1}\left[\frac{\omega}{\sqrt{E_{g0}^2+a^2}}\right]\,. \tag{13}$$

and

$$L(\omega, T_c) = N_0 \int_0^{\omega} d\varepsilon \frac{1}{\sqrt{\varepsilon^2 + E_{g0}^2}} \tanh\left(\frac{\sqrt{\varepsilon^2 + E_{g0}^2}}{2T_c}\right)$$
$$= 4N_0 T_c \sum_{n=0}^{\infty} \frac{1}{\sqrt{E_{g0}^2 + a^2}} \tan^{-1}\left(\frac{\omega}{\sqrt{E_{g0}^2 + a^2}}\right) \tag{14}$$

here $a = 2\pi T_c(n + 1/2)$.

In the case $E_{g0} = 0$, Eq. (12) becomes

$$\alpha_{so} = \frac{1}{2} \frac{1}{\left(1 + \frac{V_{e0}}{V_{p0}} \left[\frac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e}\right] \frac{\tanh(\omega_e/2T_c)}{\tanh(\omega_p/2T_c)}\right)}, \tag{15}$$

where

$$L(\omega, T_c) = N_0 \int_0^{\omega} d\varepsilon \frac{\tanh(\varepsilon/2T_c)}{\varepsilon}$$
$$= \frac{N_0}{\pi} \sum_{n=0}^{\infty} \frac{4}{2n+1} \tan^{-1}\left(\frac{\omega}{2\pi T_c(n + 1/2)}\right). \tag{16}$$

Equation (15) gives α for the s-wave superconductor without a pseudogap. For a purely electronic interaction, $V_{p0} = 0$, Eq. (15) gives $\alpha = 0$ and for a purely phononic interaction, $V_{e0} = 0$, it gives $\alpha = 1/2$ that is the BCS result, and also agrees with Dahm [17] s' result.

For a $d_{x^2-y^2}$ wave pairing, we get

$$\alpha_d = \frac{\omega_p \sum_{n=0}^{\infty} \left(\sqrt{\frac{\omega_p^2 + a^2}{\omega_p^2 + E_{g0}^2 + a^2}} - 1\right)}{\left\{f_d(\omega_p) + \frac{V_{e0}}{V_{p0}} \left(\frac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e}\right) f_d(\omega_e)\right\}}, \tag{17}$$

where

$$f_d(\omega) = \frac{L(\omega, T_c) E_{g0}^2}{N_0}$$
$$+ \sum_{n=0}^{\infty} \frac{2a^2}{\sqrt{E_{g0}^2 + a^2}} \left\{E(\beta, q) - F(\beta, q) - \frac{\omega E_{g0}^2}{\sqrt{(E_{g0}^2 + a^2)(\omega^2 + a^2)(\omega^2 + E_{g0}^2 + a^2)}}\right\},$$

$$L(\omega, T_c) = \frac{4N_0 T_c}{E_{g0}^2} \sum_{n=0}^{\infty} \left\{\omega - \frac{a^2}{\sqrt{E_{g0}^2 + a^2}} F(\beta, q) + \sqrt{E_{g0}^2 + a^2}\, E(\beta, q) - \omega \sqrt{\frac{\omega^2 + E_{g0}^2 + a^2}{\omega^2 + a^2}}\right\},$$

here

$$a = 2\pi T_c(n + 1/2), \quad \beta = \tan^{-1}\left(\frac{\omega}{2\pi T_c(n + 1/2)}\right), \quad q = \frac{E_{g0}}{\sqrt{E_{g0}^2 + a^2}}$$

and, here $F(\beta, q)$ and $E(\beta, q)$ are the elliptic integral of first and second kind, respectively.

In the case $E_{g0} = 0$, Eq. (17) gives α_{d0} of a d-wave superconductor without pseudogap. This equation has the same form as α_{s0}, the s-wave superconductor equation without a pseudogap, but $L(\omega, T_c)$ of d-wave = (1/2) $L(\omega, T_c)$ of s-wave.

3. Discussion

By using Eqs. (10), (12) and (17), we plot the isotope exponent α versus T_c for the s- and d-wave cases. The influence of pseudogap on the isotope exponent for the s-wave pairing is shown in Fig. 1 and that for d-wave pairing in Fig. 2. We compare our calculations with the experimental data of $La_{2-x}Ba_xCuO_4$, $La_{2-x}Sr_xCuO_4$ [23], and $(Y_{1-x-y}Pr_xCa_y)Ba_2Cu_3O_{7-\delta}$, $(Y_{1-x}Pr_x)Ba_2Cu_3O_{7-\delta}$, $YBa_2(Cu_{1-z}Zn_z)_3O_{7-\delta}$ [24], and $(Y_{1-x}Pr_x)Ba_2Cu_3O_{7-\delta}$ [25], and $YBa_{2-x}La_xCu_3O_{7-\delta}$ [26]. With various values of ω_p, ω_e, λ_p and E_{g0}, the curve fit the experimental data both for the s- and d-wave case so that the isotope exponent will decrease when T_c of doped cuprate increases. Here we define that $\lambda_p = N_0V_{p0}$ and $\lambda_e = N_0V_{e0}$. Although, we cannot fit all points using one set of parameters, we are sure that every point can be fitted with an appropriate set of parameters. We can predict the trend of isotope exponent by using this model. The isotope exponent of a high-T_c superconductor should decrease and be almost absent in the high-T_c region, and in the low-T_c region it depends on the magnitude of the pseudogap. In the low-T_c region, higher values of the pseudogap give higher values of the isotope exponent. In the high-T_c region, the pseudogap has no effect on the isotope exponent.

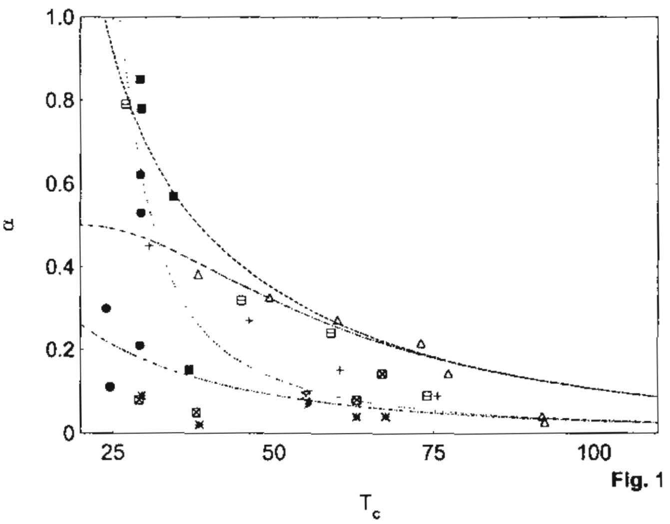

Fig. 1. Plot of the isotope exponent α versus T_c (in K) for the s-wave pairing and various values of ω_p, ω_e, λ_p and E_{g0}: (– – – –) $\lambda_p = 0.3$, $\omega_p = 500$ K, $\omega_e = 400$ K, $E_{g0} = 50$ K; (– · — · –) $\lambda_p = 0.3$, $\omega_p = 500$ K, $\omega_e = 400$ K, $E_{g0} = 0$ K; (··· ···) $\lambda_p = 0.2$, $\omega_p = 500$ K, $\omega_e = 400$ K, $E_{g0} = 120$ K; and (– · · –) $\lambda_p = 0.2$, $\omega_p = 500$ K, $\omega_e = 400$ K, $E_{g0} = 0$ K. We compare our calculation with the experimental data of $La_{2-x}Sr_xCuO_4$ (■), $La_{2-x}Ba_xCuO_4$ [23] (●), and $(Y_{1-x-y}Pr_xCa_y)Ba_2Cu_3O_{7-\delta}$ (⊠), $(Y_{1-x}Pr_x)Ba_2Cu_3O_{7-\delta}$ (⊟), $YBa_2(Cu_{1-z}Zn_z)_3O_{7-\delta}$ [24] (∗), $(Y_{1-x}Pr_x)Ba_2Cu_3O_{7-\delta}$ [25] (+), and $YBa_{2-x}La_xCu_3O_{7-\delta}$ [26] (△)

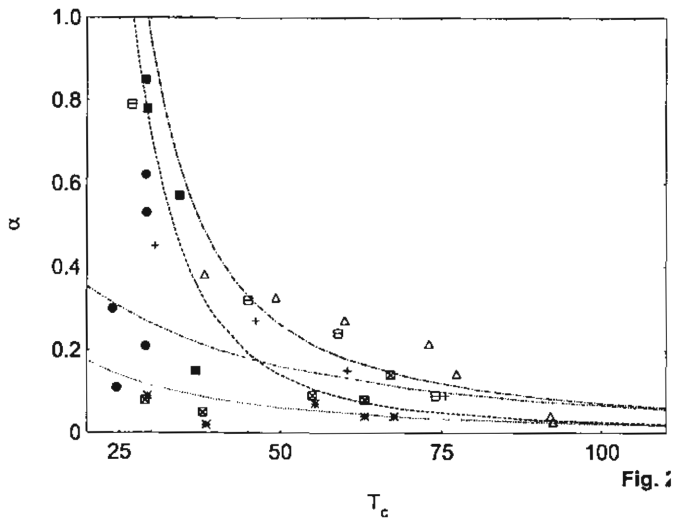

Fig. 2. Plot of the isotope exponent α against T_c (in K) for d-wave pairing and various values of ω_p, ω_e, λ_p and E_{g0}: (– – – –) $\lambda_p = 0.35$, $\omega_p = 500$ K, $\omega_e = 400$ K, $E_{g0} = 0$ K; (– · · –) $\lambda_p = 0.4$, $\omega_p = 700$ K, $\omega_e = 650$ K, $E_{g0} = 0$ K; (–·–) $\lambda_p = 0.4$, $\omega_p = 700$ K, $\omega_e = 650$ K, $E_{g0} = 150$ K and (– – –) $\lambda_p = 0.35$, $\omega_p = 500$ K, $\omega_e = 400$ K, $E_{g0} = 250$ K. We also compare our calculations with the same set of experimental data as in Fig. 1

In our model, the values of the parameters in the d-wave case are higher than in the s-wave case, yet for both cases our α can fit the experimental data well. So we need more experimental data to confirm our prediction for α.

4. Conclusion

We have investigated the effect of pseudogap on the isotope exponent in s- and d-wave pairing states in the weak-coupling limit. We can explain the unusual isotope effect of cuprates both smaller and higher than 0.5. The magnitude of the isotope exponent is proportional to the magnitude of the pseudogap in the low-T_c regions but there is no effect of pseudogap in the higher-T_c region.

Acknowledgements The author would like to thank Prof. Dr. S. Yoksan for useful discussion and encouragement. Partial financial support by the Thailand Research Fund and RGJ grant No. 3.F.TS/42/G1 is gratefully acknowledged.

References

[1] J. P. FRANCK, in: Physical Properties of High-Temperature Superconductors, Vol. 4, Ed. D. M. GINSBERG, World Scientific Publ. Co., Singapore 1994 (p. 184).
[2] B. BATLOGG et al., Phys. Rev. Lett. **58**, 2333 (1987).
[3] F. MARSIGLIO, R. AKIS, and J. P. CARBOTTLE, Solid State Commun. **64**, 905 (1987).
[4] D. S. MARSHALL et al., Phys. Rev. Lett. **76**, 4841 (1996).
[5] G. V. M. WILLIAMS et al. Phys. Rev. Lett. **80**, 377 (1998).
[6] F. RAFFA et al., Phys. Rev. Lett. **81**, 5912 (1998).
[7] R. OSBORN and E. A. GOREMYEHKIN, Physica C **185–189**, 1179 (1991).

[8] J. Mesot et al., Europhys. Lett. **44**, 498 (1998).
[9] D. Rubio Temporano et al., Phys. Rev. Lett. **84**, 1990 (2000).
[10] M. Suzuki and T. Watanabe, Phys. Rev. Lett. **85**, 4787 (2000).
[11] J. Labbe and J. Bok, Europhys. Lett. **3**, 1225 (1987).
[12] C. C. Tsuei, D. M. Newns, C. C. Chi, and P. C. Pattnaik, Phys. Rev. Lett. **65**, 2724 (1990).
[13] R. J. Radtke and M. R. Norman, Phys. Rev. B **50**, 9554 (1994).
[14] H. B. Schuttler and C. H. Pao, Phys. Rev. Lett. **75**, 4504 (1995).
[15] L. Pietronero and S. Strassler, Europhys. Lett. **18**, 627 (1992).
[16] J. P. Carbotte, M. Greeson, and A. Perez-Gonzalez, Phys. Rev. Lett. **66**, 1789 (1991).
[17] T. Dahm, Phys. Rev. B **61**, 6381 (2000).
[18] J. W. Loram, K. A. Mitza, J. R. Cooper, and W. Y. Liang, J. Supercond. **7**, 243 (1994).
[19] T. Timusk and B. Statt, Rep. Prog. Phys. **62**, 61 (1999).
[20] H. Ding et al., Nature **382**, 51 (1996).
[21] G. V. M. Williams et al., Phys. Rev. Lett. **78**, 721 (1997).
[22] A. G. Loeser et al., Science **273**, 325 (1996).
[23] M. K. Crawford et al., Science **250**, 1390 (1990).
[24] G. Soerensen and S. Gygax, Phys. Rev. B **51**, 11848 (1995).
[25] J. P. Franck et al., Phys. Rev. B **44**, 5318 (1991).
[26] H. J. Bornemann and D. E. Morris, Phys. Rev. B **44**, 5322 (1991).

ELSEVIER

Physica B 321 (2002) 353–355

PHYSICA B

www.elsevier.com/locate/physb

Free-energy formula for a BCS superconductor near zero temperature

B. Krunavakarn[a], S. Kaskamalas[a], P. Rungruang[b], S. Yoksan[b,*]

[a] Department of Physics, Chulalongkorn University, Bangkok 10330, Thailand
[b] Department of Physics, Srinakharinwirot University, Sukhumvit 23, Bangkok 10110, Thailand

Abstract

We derive the exact formula for the free-energy difference between the superconducting and the normal state of a weak-coupling superconductor at temperature close to zero as a function of temperature T, order paramete $\Delta(T)$, and cut-off temperature ω_D. Corrections to the BCS's result are found and the variation of the free-energ difference with the reduced temperature $T/\Delta(T)$ is presented in analytical form.

Keywords: Superconductivity; BCS; Free energy; Zero temperature

Recently, Xu et al. [1] derived a formula for calculating the free-energy difference between the superconducting and the normal states of a weak-coupling superconductor near zero temperature. Starting from the free-energy density difference

$$F_S - F_N = -\frac{1}{2}N(0)\Delta^2(T) - N(0)\Delta^2(T)\ln\left[\frac{\Delta(0)}{\Delta(T)}\right] - 4N(0)kT\int_0^{\hbar\omega_D} d\varepsilon \ln(1 + e^{-\beta\sqrt{\varepsilon^2+\Delta^2(T)}}) + \frac{1}{3}\pi^2 N(0)(kT)^2, \quad (1)$$

where F_S and F_N are the free-energy densities of the superconducting state and normal state, respectively; $\Delta(T)$ and $\Delta(0)$ are superconducting order parameters at temperature T and zer temperature, respectively; $N(0)$ is the density ‹ states at the Fermi level; ε is the electron's kinet energy measured from the Fermi surface; $\hbar\omega_D$ tl Debye cut-off energy; k the Boltzmann constan and $\beta = 1/kT$, Ref. [1] obtained the free-enerᵹ difference

$$\Delta F = F_S - F_N = -\frac{1}{2}N(0)\Delta^2(T) - N(0)\Delta^2(T)\ln\left[\frac{\Delta(0)}{\Delta(T)}\right] + \frac{1}{3}\pi^2 N(0)(kT)^2 - 4N(0)kT\left(\frac{\pi kT\Delta(T)}{2}\right) \times e^{-\Delta(T)/kT}\left(1 + \frac{3kT}{8\Delta(T)}\right).$$

This expression for ΔF is obviously incorre since it is independent of ω_D, whereas ı integration in Eq. (1) is ω_D dependent.

*Corresponding author. Tel./fax: +66-2-2584002.
E-mail address: suthat@psm.swu.ac.th (S. Yoksan).

0921-4526/02/$ - see front matter
PII: S0921-4526(02)01073-6

We start with the free-energy density difference of a BCS superconductor [2]:

$$F_S - F_N = \int_0^{\Delta(T)} d\Delta'(T)[\Delta'(T)]^2 \frac{\partial}{\partial \Delta'(T)}\left(\frac{1}{V}\right), \quad (3)$$

where V is the electron–phonon coupling constant. Together with the gap equation

$$\frac{1}{V} = N(0)\int_0^{\omega_D} \frac{d\varepsilon}{\sqrt{\varepsilon^2+\Delta^2(T)}} \times \tanh\left[\frac{\sqrt{\varepsilon^2+\Delta^2(T)}}{2T}\right], \quad (4)$$

we obtain by direct substitution of Eq. (4) in Eq. (3) the following expression:

$$\frac{F_S - F_N}{N(0)} = \Delta^2(T)\sinh^{-1}\left[\frac{\omega_D}{\Delta(0)}\right] - 4T\int_0^{\omega_D} d\varepsilon \times \ln\left[\frac{\cosh((1/2T)\sqrt{\varepsilon^2+\Delta^2(T)})}{\cosh(\varepsilon/2T)}\right]. \quad (5)$$

The expression for the zero-temperature order parameter, $\Delta(0)$ is obtained by setting $T = 0$ in Eq. (4) and one arrives at the relation

$$\frac{1}{V} = N(0)\sinh^{-1}\left[\frac{\omega_D}{\Delta(0)}\right]. \quad (6)$$

Since at $T = T_c$, $\Delta(T_c) = 0$, Eq. (4) becomes

$$\frac{1}{V} = N(0)\sum_{n=0}^{\infty} \frac{4}{(2n+1)\pi}\tan^{-1}\left[\frac{\omega_D/T_c}{(2n+1)\pi}\right]. \quad (7)$$

Eqs. (6) and (7) give us the expression for $\Delta(0)$ as

$$\Delta(0) = \frac{\omega_D}{\sinh[\sum_{n=0}^{\infty}(4/(2n+1)\pi)\tan^{-1}(\omega_D/T_c/(2n+1)\pi)]}. \quad (8)$$

After straightforward integration and lengthy algebra, Eq. (5) becomes

$$\frac{\Delta F}{N(0)} = \Delta^2(T)\left[\sinh^{-1}\left(\frac{\omega_D}{\Delta(0)}\right) - \sinh^{-1}\left(\frac{\omega_D}{\Delta(T)}\right)\right] - \left[\omega_D\sqrt{\omega_D^2+\Delta^2(T)} - \omega_D^2\right] + T^2\left[\frac{\pi^2}{3} + 4\mathrm{Li}_2(-e^{-\omega_D/T})\right] - 4\omega_D T\ln\left[1+e^{-\sqrt{\omega_D^2+\Delta^2(T)}/T}\right] - 4T\sum_{n=1}^{\infty}(-1)^{n+1}\frac{e^{-n\Delta(T)/T}}{n}\sqrt{\frac{\pi\Delta(T)T}{2n}} \times \sum_{m=0}^{\infty}\left[\frac{T}{2n\Delta(T)}\right]^m \frac{\Gamma(m+\frac{3}{2}) - \Gamma(m+\frac{3}{2}, n\phi(T))}{\Gamma(m+1)\Gamma(\frac{3}{2}-m)}, \quad (9)$$

where $\Gamma(z+1) = \int_0^{\infty} dt e^{-t}t^z$, is the well-known gamma function, $\Gamma(z+1, n\phi(T)) = \int_{n\phi(T)}^{\infty} dt e^{-t}t^z$ is the incomplete gamma function [3], $\phi(T) = [\sqrt{\omega_D^2+\Delta^2(T)} - \Delta(T)]/T$, and $\mathrm{Li}_2(x)$ is the dilogarithm function [4]. At $T = 0$, Eq. (9) reduces to $\Delta F/N(0) = \omega_D^2 - \omega_D\sqrt{\omega_D^2+\Delta^2(0)}$, and in the limit $\omega_D \gg \Delta(0)$, $\Delta F/N(0)$ is equal to $-\frac{1}{2}\Delta^2(0)$.

If we take the limit $\omega_D/T_c \to \infty$, approximation of Eq. (9) is performed to the term containing the factor $(T/\Delta(T))^2$, we have

$$F_S = F_N - \frac{1}{2}N(0)\Delta^2(T) - N(0)\Delta^2(T)\ln\left[\frac{\Delta(0)}{\Delta(T)}\right] + \frac{1}{3}\pi^2 N(0)T^2 - 4N(0)Te^{-\Delta(T)/T}\sqrt{\frac{\pi T\Delta(T)}{2}} \times \left[1 + \frac{3}{8}\left(\frac{T}{\Delta(T)}\right) - \frac{15}{128}\left(\frac{T}{\Delta(T)}\right)^2\right]. \quad (10)$$

The last term on the right-hand side of Eq. (10) is a correction to the Xu et al.'s result [1].

Acknowledgements

Financial support provided by the Thailand Research Fund is gratefully acknowledged.

References

[1] L. Xu, Z. Shu, S. Wang, Phys. Rev. B 57 (1998) 11 654.
[2] A.L. Fetter, J.D. Walecka, Quantum Theory of Many Particle Systems, McGraw-Hill, New York, 1971 (Chapter 13).
[3] M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions, Dover, New York, 1972, p. 63, 1099.
[4] I.S. Gradshteyn, I.W. Ryzhik, Tables of Integral Series and Products, Academic Press, New York, 1965.

(41)

INTERNATIONAL JOURNAL OF
MODERN PHYSICS B

Volume 16, Number 24
September 20, 2002

Thermodynamic Properties of a BCS Superconductor Near Zero Temperature

B. Krunavakarn, P. Yingpratanporn, S. Kaskamalas and S. Yoksan

Abstracts and the table of contents, as well as
sample issues in PDF are available on the
World-Wide Web at the URL:
www.worldscinet.com/ijmpb/ijmpb.shtml

World Scientific
New Jersey • London • Singapore • Hong Kong • Bangalore

International Journal of Modern Physics B, Vol. 16, No. 24 (2002) 3615–3621

THERMODYNAMIC PROPERTIES OF A BCS SUPERCONDUCTOR NEAR ZERO TEMPERATURE

B. KRUNAVAKARN*, P. YINGPRATANPORN*,
S. KASKAMALAS† and S. YOKSAN‡

*Department of Physics, Chulalongkorn University,
Bangkok 10330, Thailand
†Department of Electrical Engineering, Dhurakijpundit University,
Bangkok 10210, Thailand
‡Department of Physics, Srinakharinwirot University,
Bangkok 10110, Thailand
†suthat@psm.swu.ac.th

Received 20 May 2002

We theoretically study the thermodynamic properties of a BCS superconductor near zero temperature. Derivations of the temperature dependence of the order parameter and an exact formula for the free-energy difference between the superconducting and normal states are presented as functions of temperature and material parameters of the superconductor. Under the condition that the cut-off energy is much greater than the temperature, formulas for the critical field and specific heat in the superconducting state are presented. Our expressions for these thermodynamic quantities show new corrections to the BCS's results.

Keywords: Thermodynamic properties; BCS superconductor; zero temperature.

1. Introduction

Recently, Xu *et al.*[1] derived a formula for calculating the free-energy difference between the superconducting and normal states of a weak-coupling superconductor near zero temperature. Starting from the free-energy density difference

$$F_S - F_N = -\frac{1}{2}N(0)\Delta^2(T) - N(0)\Delta^2(T)\ln\left[\frac{\Delta(0)}{\Delta(T)}\right]$$

$$- 4N(0)kT\int_0^{\hbar\omega_D} d\epsilon \ln(1+e^{-\beta\sqrt{\epsilon^2+\Delta^2(T)}}) + \frac{1}{3}\pi^2 N(0)(kT)^2\,, \quad (1)$$

where F_S and F_N are the free-energy density of the superconducting state and normal state, respectively, $\Delta(T)$ and $\Delta(0)$ are superconducting order parameters at temperature T and zero temperature, respectively, $N(0)$ is the density of states at the Fermi level, ϵ is the kinetic energy of the electron measured from the Fermi surface, $\hbar\omega_D$ the cut-off energy, k the Boltzman constant, and $\beta = 1/kT$. Due to the difficulty in evaluating the integral term in (1), it is usually assumed that in the limit[1-3] $T \to 0K$, $\omega_D/T \to \infty$. As a consequence, in Ref. 1 the approximate free energy density difference is calculated to be

$$\Delta F = F_S - F_N = -\frac{1}{2}N(0)\Delta^2(T) - N(0)\Delta^2(T)\ln\left[\frac{\Delta(0)}{\Delta(T)}\right] + \frac{1}{3}\pi^2 N(0)(kT)^2 - 4N(0)kT\left(\frac{\pi kT\Delta(T)}{2}\right)^{1/2} \times e^{-\Delta(T)/kT}\left(1+\frac{3kT}{8\Delta(T)}\right). \quad (2)$$

Usually, it is very straightforward to obtain numerically the full temperature dependence to any desired accuracy, but it is of theoretical interest to derive this free energy difference as a function of the temperature and material parameters explicitly. The purpose of this paper is therefore to present the exact derivation of the free energy difference and use it to obtain new expressions for the critical field and specific heat of a BCS superconductor near zero temperature.

The paper is organized as follows. In Sec. 2 starting from the BCS gap equation, the temperature dependence of the order parameter is calculated and the complete expression for the free energy difference is obtained. Section 3 deals with the thermodynamic critical field and specific heat. New expressions for these quantities are presented. Finally, discussions and conclusion are presented in Sec. 4.

2. Gap and Free Energy Difference Equations

Within the BCS scheme, and assuming a constant density of states at the Fermi level, we have the following gap equation

$$\frac{1}{N(0)V} = \int_{-\omega_D}^{\omega_D} \frac{d\epsilon}{2\sqrt{\epsilon^2+\Delta^2(T)}}\tanh\left(\frac{\sqrt{\epsilon^2+\Delta^2(T)}}{2T}\right), \quad (3)$$

where the attractive constant V is finite within a strip of width $2\omega_D$ in the vicinity of the Fermi level.

At $T = 0$ K, an integration of (3) gives

$$\frac{1}{N(0)V} = \sinh^{-1}\left[\frac{\omega_D}{\Delta(0)}\right]. \quad (4)$$

When $T \to 0$ K, $\Delta(T)/T \gg 1$, the expansion

$$\tanh\left(\frac{E}{2T}\right) = 1 + 2\sum_{n=1}^{\infty}(-1)^n e^{-nE/T} \quad (5)$$

may be employed in the integral term of (3), allowing us to obtain the following equation:

$$\frac{1}{N(0)V} = \sinh^{-1}\left[\frac{\omega_D}{\Delta(T)}\right] + 2\sum_{n=1}^{\infty}(-1)^n \int_0^{\omega_D} \frac{d\epsilon e^{-\frac{n}{T}\sqrt{\epsilon^2+\Delta^2(T)}}}{\sqrt{\epsilon^2+\Delta^2(T)}}. \quad (6)$$

Putting $y+1=\sqrt{\epsilon^2+\Delta^2(T)}/\Delta(T)$, (6) can be written as

$$\frac{1}{N(0)V}=\sinh^{-1}\left[\frac{\omega_D}{\Delta(T)}\right]+2\sum_{n=1}^{\infty}(-1)^n e^{-n\Delta(T)/T}$$
$$\times\int_0^{\sqrt{[\omega_D/\Delta(T)]^2+1}-1}\frac{dye^{-n\Delta(T)y/T}}{\sqrt{y^2+2y}}\,. \tag{7}$$

Using the relation

$$\frac{1}{\sqrt{1+z}}=\sum_{m=0}^{\infty}\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma(m+1)\Gamma\left(\frac{1}{2}-m\right)}z^m\,, \tag{8}$$

where $\Gamma(n)$ is the gamma function[4,5] (7) is reduced to

$$\frac{1}{N(0)V}=\sinh^{-1}\left[\frac{\omega_D}{\Delta(T)}\right]+2\sum_{n=1}^{\infty}(-1)^n e^{-n\Delta(T)/T}$$
$$\times\sum_{m=0}^{\infty}\frac{\sqrt{\pi}}{\Gamma(m+1)\Gamma\left(\frac{1}{2}-m\right)}\left(\frac{T}{2n\Delta(T)}\right)^{m+1/2}$$
$$\times\int_0^{n\Delta(T)/T\left[\sqrt{[\omega_D/\Delta(T)]^2+1}-1\right]}dte^{-t}t^{m-1/2}\,, \tag{9}$$

$$=\sinh^{-1}\left[\frac{\omega_D}{\Delta(T)}\right]+2\sum_{n=1}^{\infty}\sum_{m=0}^{\infty}(-1)^n e^{-n\Delta(T)/T}$$
$$\times\frac{\sqrt{\pi}}{\Gamma(m+1)\Gamma\left(\frac{1}{2}-m\right)}\left(\frac{T}{2n\Delta(T)}\right)^{m+1/2}\left\{\Gamma\left(m+\frac{1}{2}\right)\right.$$
$$\left.-\Gamma\left[m+\frac{1}{2},\frac{n\Delta(T)}{T}\left(\sqrt{\frac{\omega_D^2}{\Delta^2(T)}+1}-1\right)\right]\right\}, \tag{10}$$

where $\Gamma(z,x)=\int_x^{\infty}dte^{-t}t^{z-1}$ is the incomplete gamma function.[4,5]

Combining (4) and (10), and since $\omega_D\gg\Delta(T),\Delta(0)$ one arrives at the following relation

$$\ln\left[\frac{\Delta(T)}{\Delta(0)}\right]=2\sum_{n=1}^{\infty}\sum_{m=0}^{\infty}(-1)^n e^{-n\Delta(T)/T}$$
$$\times\frac{\sqrt{\pi}\Gamma\left(m+\frac{1}{2}\right)}{\Gamma(m+1)\Gamma\left(\frac{1}{2}-m\right)}\left(\frac{T}{2n\Delta(T)}\right)^{m+1/2}\,. \tag{11}$$

In the low temperature limit, we approximate $\ln[\Delta(T)/\Delta(0)] \simeq -1 + \Delta(T)/\Delta(0)$, which leads to the expression

$$\frac{\Delta(T)}{\Delta(0)} = 1 - e^{-\Delta(0)/T}\sqrt{\frac{2\pi T}{\Delta(0)}}\left\{1 - \frac{1}{8}\left(\frac{T}{\Delta(0)}\right) + \frac{9}{128}\left(\frac{T}{\Delta(0)}\right)^2 - \frac{75}{1024}\left(\frac{T}{\Delta(0)}\right)^3\right\}. \tag{12}$$

The last three terms on the right of (12) are the corrections to the BCS's approximate result. Compared with the result of Abrikosov *et al.*[3]; $\Delta(T)/\Delta(0) = 1 - \sqrt{2\pi T/\Delta(0)}e^{-\Delta(0)/T}\{1 - [T/8\Delta(0)]\}$, (12) gives the same result as theirs. As for the result of Xu *et al.*, our formula for $\Delta(T)$ differs from that given there. This is due to the fact that they calculated the temperature dependence of the gap by minimizing ΔF with repect to $\Delta(T)$. This procedure is incorrect because the free energy obtained by the coupling constant integral is the equilibrium free-energy for a definite gap, therefore one cannot re-determine the gap from it any further.

Next we start with the free-energy density difference

$$\Delta F = F_S - F_N = \int_0^{\Delta(T)} d\Delta'(T)[\Delta'(T)]^2 \frac{\partial(1/V)}{\partial\Delta'(T)}, \tag{13}$$

and obtain by direct substitution of (3) into (13), the following expression

$$\begin{aligned}\frac{F_S - F_N}{N(0)} &= \Delta^2(T)\sinh^{-1}\left[\frac{\omega_D}{\Delta(0)}\right] - 2\int_0^{\Delta(0)} d\Delta'\Delta'(T) \\ &\quad \times \int_0^{\omega_D} \frac{d\epsilon}{\sqrt{\epsilon^2 + \Delta'^2(T)}}\tanh\left(\frac{\sqrt{\epsilon^2 + \Delta'^2(T)}}{2T}\right) \\ &= \Delta^2(T)\sinh^{-1}\left[\frac{\omega_D}{\Delta(0)}\right] - 2\int_0^{\omega_D} d\epsilon\{\sqrt{\epsilon^2 + \Delta^2(T)} - \epsilon \\ &\quad + 2T\ln[1 + e^{-\sqrt{\epsilon^2+\Delta^2(T)}/T}] - 2T\ln[1 + e^{-\beta\epsilon}]\}. \end{aligned} \tag{14}$$

After a straightforward integration and lengthy algebra, (14) becomes

$$\begin{aligned}\frac{F_S - F_N}{N(0)} &= \Delta^2(T)\left[\sinh^{-1}\left[\frac{\omega_D}{\Delta(0)}\right] - \sinh^{-1}\left[\frac{\omega_D}{\Delta(T)}\right]\right] \\ &\quad - [\omega_D\sqrt{\omega_D^2 + \Delta^2(T)} - \omega_D^2] + T^2\left[\frac{\pi^2}{3} + 4Li_2(-e^{-\omega_D/T})\right] \\ &\quad - 4\omega_D T\ln[1 + e^{-\sqrt{\omega_D^2+\Delta^2(T)}/T}] - 4\Delta^2(T)\sum_{n=1}^{\infty}(-1)^{n+1} \\ &\quad \times \int_1^{\sqrt{(\omega_D/\Delta(T))^2+1}} dx\sqrt{x^2 - 1}e^{-nx\Delta(T)/T}, \end{aligned} \tag{15}$$

where $Li_2(x)$ is the dilogarithmic function[4,5] $= \sum_{n=1}^{\infty}(x^n/n^2)$.

Introducing the variable $x = 1 + [tT/n\Delta(T)]$, the integral term in (15) can be evaluated exactly. This gives finally the explicit dependence of ΔF on $\Delta(T)$, $\Delta(0)$, T, and ω_D as

$$\begin{aligned}\frac{\Delta F}{N(0)} &= \Delta^2(T)\left[\sinh^{-1}\left(\frac{\omega_D}{\Delta(0)}\right) - \sinh^{-1}\left(\frac{\omega_D}{\Delta(T)}\right)\right] \\ &\quad - [\omega_D\sqrt{\omega_D^2+\Delta^2(T)} - \omega_D^2] + T^2\left[\frac{\pi^2}{3} + 4Li_2(-e^{-\omega_D/T})\right] \\ &\quad - 4\omega_D T\ln[1+e^{-\sqrt{\omega_D^2+\Delta^2(T)}/T}] - 4T\sum_{n=1}^{\infty}(-1)^{n+1}\frac{e^{-n\Delta(T)/T}}{n} \\ &\quad \times\sqrt{\frac{\pi\Delta(T)T}{2n}}\sum_{m=0}^{\infty}\left[\frac{T}{2n\Delta(T)}\right]^m \frac{\Gamma\left(m+\frac{3}{2}\right) - \Gamma\left(m+\frac{3}{2}, n\phi(T)\right)}{\Gamma(m+1)\Gamma\left(\frac{3}{2}-m\right)}, \end{aligned} \tag{16}$$

where $\phi(T) = [\sqrt{\omega_D^2+\Delta^2(T)} - \Delta(T)]/T$.

This formula is the central result of the present work.

At $T = 0$ K, (16) reduces to $\Delta F/N(0) = \omega_D^2 - \omega_D\sqrt{\omega_D^2+\Delta^2(0)}$, and in the limit of $\omega_D \gg \Delta(0)$, $\Delta F/N(0)$ is equal to $-(1/2)\Delta^2(0)$. Using the BCS approximation, we compute $\Delta F/N(0)$ in the limit $\omega_D/T \to \infty$, gives

$$\begin{aligned}\frac{\Delta F}{N(0)} &= -\frac{1}{2}\Delta^2(T) + \Delta^2(T)\ln\left[\frac{\Delta(T)}{\Delta(0)}\right] + \frac{\pi^2}{3}T^2 - 4T\sum_{n=1}^{\infty}(-1)^{n+1}\frac{e^{-n\Delta(T)/T}}{n} \\ &\quad \times\sqrt{\frac{\pi\Delta(T)T}{2n}}\sum_{m=0}^{\infty}\left[\frac{T}{2n\Delta(T)}\right]^m \frac{\Gamma\left(m+\frac{3}{2}\right)}{\Gamma(m+1)\Gamma\left(\frac{3}{2}-m\right)}. \end{aligned} \tag{17}$$

To obtain an explicit expression for ΔF, we neglect all terms of order $e^{-n\Delta(T)/T}$ for n greater than 1, and obtain

$$\begin{aligned}F_S &= F_N - \frac{1}{2}N(0)\Delta^2(T) - N(0)\Delta^2(T)\ln\left[\frac{\Delta(0)}{\Delta(T)}\right] + \frac{1}{3}\pi^2 N(0)T^2 \\ &\quad - 4N(0)Te^{-\Delta(T)/T}\sqrt{\frac{\pi T\Delta(T)}{2}}\left\{1 + \frac{3}{8}\frac{T}{\Delta(T)} - \frac{15}{128}\left(\frac{T}{\Delta(T)}\right)^2\right\}. \end{aligned} \tag{18}$$

Our approximate (18) gives the same result for F_S as Xu *et al.*'s (6),[1] yet it is different from (36.7) of Ref. 3. The latter is incorrect because Ref. 3 used the asymptotic expansion of the Bessel function in performing the integral evaluation. Whereas we do the integral in power series of temperature.

3. Thermodynamic Properties

3.1. *Critical field near $T = 0$*

Since the critical field $H_c(T)$ is given by

$$H_c^2(T) = -8\pi\Delta F(T)\,, \tag{19}$$

we therefore have, by (16),

$$\frac{H_c^2(T)}{8\pi N(0)} = \Delta^2(T)\left[\frac{1}{2} - \ln\left[\frac{\Delta(T)}{\Delta(0)}\right]\right] - \frac{\pi^2 T^2}{3} - e^{-\Delta(T)/T}T^{3/2}\sqrt{8\pi\Delta(T)}$$
$$\times\left\{1 + \frac{3}{8}\frac{T}{\Delta(T)} - \frac{15}{128}\left(\frac{T}{\Delta(T)}\right)^2\right\}. \tag{20}$$

Since (20) gives $H_c^2(0)/8\pi N(0) = (1/2)\Delta^2(0)$, we calculate $H_c^2(T)/H_c^2(0)$, and assume that near $T = 0$ K, $\Delta(T) \simeq \Delta(0)$, we obtain

$$\frac{H_c(T)}{H_c(0)} = 1 - \frac{1}{3}\left(\frac{\pi T}{\Delta(0)}\right)^2 - e^{-\Delta(0)/T}\sqrt{8\pi\left(\frac{T}{\Delta(0)}\right)^3}$$
$$\times\left\{1 + \left(\frac{3}{8} - \frac{\pi^2}{6}\right)\left(\frac{T}{\Delta(0)}\right)\right\}. \tag{21}$$

The last term in (21) is the correction to the BCS's result.[2]

3.2. *Specific heat near $T = 0$*

The specific heat is related to the free energy by the general relation $C_S = -T\partial^2 F_S/\partial T^2$. From (16), we evaluate the superconducting free energy $F_S(T)$ by using (12). We find

$$F_S = N(0)\left\{-\frac{\Delta^2(0)}{2} - 4e^{-\Delta(0)/T}T^{3/2}\sqrt{\frac{\pi\Delta(0)}{2}}\left(1 + \frac{3}{8}\frac{T}{\Delta(0)} - \frac{15}{128}\frac{T^2}{\Delta^2(0)}\right)\right\}. \tag{22}$$

By differentiating F_S twice with respect to T, we obtain

$$C_S(T) = 2\sqrt{2\pi}N(0)e^{-\Delta(0)/T}\Delta(0)\left(\frac{\Delta(0)}{T}\right)^{3/2}$$
$$\times\left\{1 + \frac{11}{8}\left(\frac{T}{\Delta(0)}\right) + \frac{225}{128}\left(\frac{T}{\Delta(0)}\right)^2\right\}. \tag{23}$$

Equation (23) is an analytical expression for the superconducting specific heat C_S within the BCS framework. Terms in the brackets are improvements on BCS result.[2] The specific heat result of (23) again differs from the Xu *et al.*'s. This is due to the fact that they used the incorrect formula for $\Delta(T)$ in determining the temperature dependence of C_S.

4. Discussions and Conclusion

In this paper, we have studied the thermodynamic properties of a BCS superconductor near zero temperature. Starting from the gap equation, we derive the temperature dependence of the order parameter (12). Then using the coupling constant integral, we derive the free-energy density difference exactly as a function of the temperature and material parameters.

The approximate free energy expression is then used to obtain all order temperature corrections to the thermodynamic quantities. We thereby obtain the temperature dependence of the critical field $H_c(T)$ and specific heat $C_S(T)$, [(21) and (23), respectively].

We found that we have made improvements in the calculation for ΔF in the BCS theory by evaluting the coupling constant integral exactly. We also find new expressions for $\Delta(T)$, $H_c(T)$ and $C_S(T)$ which give corrections to BCS's approximate results.

Acknowledgment

This research was supported by the Thailand Research Fund under Contract RTA/05/2542. One of us (B. K.) would like to express his gratitude for the scholarship from the Royal Golden Jubilee Program.

References

1. L. Xu, Z. Shu and S. Wang, *Phys. Rev.* **B57** 11654 (1998).
2. A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York 1971), Chapter 13.
3. A. A. Abrikosov *et al.*, *Methods of Quantum Field Theory in Statistical Physics* (Prentice Hall, Inc., New Jersey, 1963).
4. M. Abramowitz and I. A. Stegun, in *Handbook of Mathematical Functions* (Dover, New York, 1972), p. 63 (1099).
5. I. S. Gradshteyn and I. W. Ryzhik, *Tables of Integral Series and Products* (Academic, New York, 1965).

Current Folder: INBOX

Log Out

Compose Addresses Folders Options Search Help Fetch Bookmarks Filters

Message List | Delete Previous | Next | Forward | | Reply | | Reply All

View Full Header
View Printable Version

Subject: **MSM03-Acceptance notification**
From: **"abdelwahab cheikrouhou" <Abdel.Cheikhrouhou@tunet.tn>**
Date: **Mon, May 5, 2003 2:42 am**
To: **<suthat@swu.ac.th>**
Priority: **Normal**
Read receipt: **requested** [Send read receipt now]

Dear Prof.
I send on may 3rd /2003 the following mail "acceptance notification of your paper"

Dear Dr. Kaskamalas

"You submitted to the Third International Conference on Magnetic and Superconducting Materials MSM03 an abstract number MSM03/KAS/S041 entitled:

Critical Temperature of a Non-Fermi Liquid Superconductor

We are pleased to inform you that your contribution has been accepted for presentation at the Conference.

Type of presentation: Oral

Identification number: MSM03/KAS/S041

PLEASE, INDICATE THE ABSTRACT IDENTIFICATION NUMBER IN SUBMITTING THE MANUSCRIPT, IN THE CONFERENCE REGISTRATION FORM AND IN ALL FUTURE CORRESPONDENCE.

Your manuscript will be considered for publication in the MSM03 Proceedings, which will be published in an International journal.

You will be informed shortly by e-mail of the name of the journal and the guidelines for manuscript. The deadline for manuscript submission is June 30th, 2003.

I ask you kindly to acknowledge receipt of this mail."

You contribution has been considered as oral presentation. If you prefer dive it as poster, there is no problem, please inform me. Please inform me also if you need an acceptance notification by fax or by regular post to apply for financial support from your university or other institution, I will do it soon

We look forward to receiving your manuscript and to welcoming you in Tunisia next September.

Yours Sincerely

Prof. A. CHEIKHROUHOU

Critical Temperature of a Non-Fermi Liquid Superconductor

ถึง อ. สุทัศน์ ยกส้าน

P. Yingpratanporn(1), B. Krunavakarn(1), S. Kaskamalas(2), P. Boonma(3) and S. Yoksan(3)

(1)Department of Physics, Chulalongkorn University, Bangkok 10330, Thailand
(2)The Continuing Education Center, Chulalongkorn University, Bangkok 10330, Thailand
(3)Department of Physics, Srinakharinwirot University, Bangkok 10110, Thailand

Abstract

The critical temperature of a non-Fermi liquid superconductor is studied, using the model of Yin and Chakravarty. We derive an exact intrinsic equation for the critical temperature and study numerically its behavior as a function of α, the non-Fermi parameter which depends on the interaction between electrons. The critical value of the coupling constant λ is calculated. Our results give appreciable corrections to the work done by Grosu [J. Supercond. **15** 263 (2002)].

Key Words: Superconductivity; non-Fermi liquid.

The importance of non-Fermi liquid behavior in high temperature superconductors has been realized since the discovery of the anomalous behavior of many normal state properties which cannot be well explained by the standard Fermi liquid theory. The non-Fermi liquid model, for high-T_c superconductors has been used by many authers, such as Anderson [1], Varma et al. [2], and Chakravarty and Anderson [3]. The model uses α as the non-Fermi parameter, where a non-zero α implies breakdown of Fermi liquid theory.

Recently Grosu [4] applied the Yin and Chakravarty model [5] of the non-Fermi superconductor to study the critical temperature and the impurity effects. Based on the Thouless criterion and BCS approach with an infinite energy cutoff, Grosu calculated the particle-particle bubble and obtained approximate formulas for the critical temperature T_c, and critical coupling λ_{cr}.

In this paper, with a proper finite energy cutoff, we find an exact intrinsic equation for T_c. Our numerical calculations for T_c show that the T_c values of Ref. [4] as a function of the non-Fermi parameter are greatly exaggerated.

Following Ref. [4], we assume that the superconducting state appears due to an attractive interaction V, and the critical temperature T_c is obtained by using the Thouless criterion:

$$1 - V\Pi(0,0) = 0 \tag{1}$$

Here $\Pi(0,0)$ is the particle-particle bubble, which is given by

$$\Pi(0,0) = T_c \sum_n \int \frac{d^3k}{(2\pi)^3} G_0(\vec{k}, i\omega_n) G_0(-\vec{k}, -i\omega_n) \tag{2}$$

where

$$G_0(\vec{k}, i\omega_n) = g(\alpha)\left[\frac{\theta(\omega_n)e^{-\frac{i\pi\alpha}{2}} + \theta(-\omega_n)e^{\frac{i\pi\alpha}{2}}}{\omega_c^\alpha(i\omega_n - \epsilon_k)^{1-\alpha}}\right] \tag{3}$$

and

$$g(\alpha) = \frac{\pi\alpha/2}{\sin \pi\alpha/2} \tag{4}$$

here ω_c is a cutoff energy, $\theta(\omega)$ is the Heaviside function, and $\omega_n = \pi T_c(2n+1)$ is the Matsubara frequency. Using the constant density of states $N(0)$, $\Pi(0,0)$ becomes

$$\Pi(0,0) = 2N(0)\frac{T_c g^2(\alpha)}{\omega_c^{2\alpha}}\sum_{n=0}\frac{1}{\omega_n^{2(1-\alpha)}}\int_0^{\omega_D}\frac{d\epsilon}{\left[1+\left(\frac{\epsilon}{\omega_n}\right)^2\right]^{1-\alpha}} \tag{5}$$

where ω_D is the Debye energy cutoff.

The integral in Eq. (5) can be evaluated exactly, and substituted in Eq. (1), to obtain the following equation for T_c:

$$\frac{1}{N(0)V} = \frac{1}{\lambda} = \frac{g^2(\alpha)}{\pi}\left(\frac{\omega_c}{2\pi T_c}\right)^{-2\alpha}\left\{B\left(\frac{1}{2},\frac{1}{2}-\alpha\right)\sum_{n=0}^{\frac{\omega_D}{2\pi T_c}-\frac{1}{2}}\frac{1}{(n+\frac{1}{2})^{1-2\alpha}}\right.$$
$$\left.+\frac{1}{(\alpha-\frac{1}{2})}\left(\frac{\omega_D}{2\pi T_c}\right)^{2\alpha-1}\sum_{n=0}^{\frac{\omega_D}{2\pi T_c}-\frac{1}{2}}F\left[1-\alpha,\frac{1}{2}-\alpha;\frac{3}{2}-\alpha;-\left(\frac{\omega_n}{\omega_D}\right)^2\right]\right\} \tag{6}$$

here $F[\alpha,\beta;\gamma;z]$ is the hypergeometric function [6].

This intrinsic T_c formula is the central result of the present work.

In the limit $\alpha = 0$, since $F\left[1,\frac{1}{2};\frac{3}{2},-z^2\right] = \frac{\tan^{-1}z}{z}$ [6], and $g(\alpha) = 1$ we obtain

$$\frac{1}{\lambda} = \sum_{n=0}^{n_{max}}\frac{1}{(n+\frac{1}{2})} - \frac{2}{\pi}\sum_{n=0}^{n_{max}}\frac{1}{(n+\frac{1}{2})}\tan^{-1}\left(\frac{\pi T_c(2n+1)}{\omega_D}\right) \tag{7}$$

here $n_{max} = \frac{\omega_D}{2\pi T_c} - \frac{1}{2}$.

Since $\omega_D \gg T_c$, Eq. (7) can be written as

$$\frac{1}{\lambda} = \sum_{n=0}^{n_{max}}\frac{2}{(n+\frac{1}{2})\pi}\tan^{-1}\left(\frac{\omega_D}{\pi T_c(2n+1)}\right). \tag{8}$$

we reobtain the familiar BCS result

We next consider the case $\omega_D \gg T_c$ and $\alpha < \frac{1}{2}$, in this limit the second term in Eq. (6) vanishes and we reobtain Eq. (11) of Ref. [4].

Using Eq. (6), we compute T_c numerically and plot it as a function of α for given values of λ, ω_c and ω_D. From graph, we can see that, for these parameters

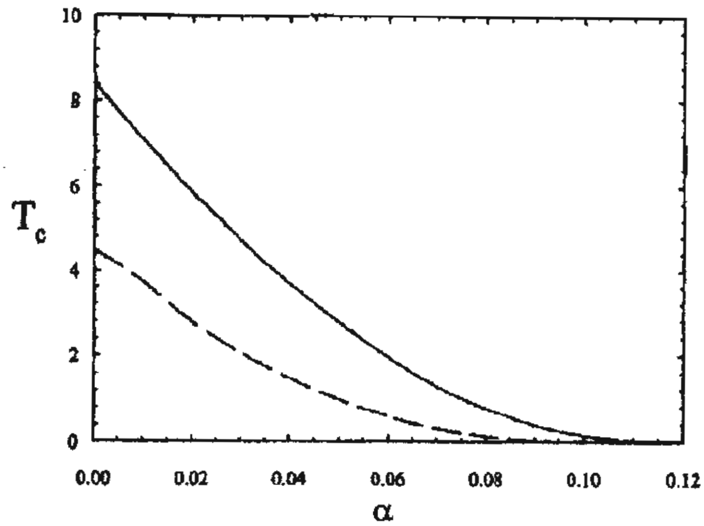

Figure 1: Plot of T_c as a function of the α parameter for $\omega_c = 1000K$, $\omega_D = 200K$ and $\lambda = 0.3$. Bottom curve is our result, and top curve is Grosu's result.

the critical temperatures have much smaller values than those obtained by taking an infinite cutoff [4].

Following closely the work of Ref. [4], we evaluate the sums in Eq. (6) and obtain the critical coupling factor

$$\lambda_{cr}(\alpha) = \left(\frac{\omega_c}{\omega_D}\right)^{2\alpha} \frac{2\pi\alpha g^{-2}(\alpha)}{\left[B\left(\frac{1}{2}, \frac{1}{2} - \alpha\right) + \frac{2\alpha}{\alpha - \frac{1}{2}}\right]} \tag{9}$$

which satisfies $\lim_{\alpha \to 0} \lambda_{cr}(\alpha) = 0$. For all $\alpha \neq 0$. our λ_{cr} is the same as λ_{cr} of Ref. [4] and λ_{cr} increases as α increases.

Finally we obtain the following equation for the critical temperature:

$$T_c = \frac{\omega_D}{\pi} \left(\frac{1 - \frac{\lambda_{cr}}{\lambda} f(\alpha)}{2^{2\alpha} - 4\alpha}\right)^{\frac{1}{2\alpha}} \tag{10}$$

where $f(\alpha) = 1 - \frac{2\alpha\Gamma(1-\alpha)}{\sqrt{\pi}\Gamma(\frac{3}{2}-\alpha)}$, here $\Gamma(x)$ is the well known gamma function [6].

When $\alpha \to 0$, the critical temperature is

$$T_c = 1.18\omega_D exp\left[-\frac{1}{\lambda}\right] \tag{11}$$

as expected.

In this paper we extended the work of Grosu [4] on the Anderson non-Fermi liquid, using the Green's function of Yin and Chakravarty [5]. By imposing a finite energy cutoff and within the BCS approach, we have derived an intrinsic exact T_c equation and found approximate formulas for T_c and critical coupling. From our study it is revealed that the variations of T_c with α is decreased considerably as compared to the Grosu's approximate results.

Acknowledgment

Partial support by the Thailand Research Fund is gratefully acknowledged.

References

[1] P. W. Anderson. *Science* **235**, 1196 (1987).

[2] C. M. Varma, P. B. Littleword, S. Schmidt-Kink, E. Abrahams, and A. E. Ruckenstein, *Phys. Rev. Lett.* **63**, 1996 (1989).

[3] S. Chakravarty and P. W. Anderson, *Phys. Rev Lett.* **72**, 3859 (1994).

[4] J. Grosu, *J. Supercond.* **15**, 263 (2002).

[5] L. Yin and S. Chakravarty, *Int. J. Mod. Phys. B* **10**, 805 (1996).

[6] I. S. Grasteyn and I. M. Ryshik, in *Tables of Integrals, Series and Products*, Academic Press, New York, 1965).