ABSTRACT

An exact analytical expression for the specific heat jump $\Delta C$ at the critical temperature $T_c$ has been obtained directly from the BCS gap equation for any shape of the energy dependent electronic density of states (DOS). We consider a model which takes into consideration electron-electron repulsion, formulated in the Hubbard model along with the electron-electron attraction due to electron-phonon interaction in the BCS formalism. We have analyzed this expression for constant as well as for the Lorentzian forms of DOS. It is shown that the constant DOS in the simple BCS theory cannot explain the large values of $\Delta C/T_c$, found in some superconductors. The specific heat versus temperature curve has been found to have a peak, similar to that of Eliashberg theory of superconductivity. The influence of repulsive interaction is very small and occurs mainly at higher temperatures.
The specific heat is an important tool to investigate the excitation spectrum in the superconducting state\(^1\). It also informs us about the nature of phase transition\(^2\) and the symmetry of the pairing state\(^3\). The specific heat is specially suitable to study the BCS superconductors\(^2\). For example all the parameters in the BCS formula \(T_c = 1.14 \theta_D e^{-1/\lambda}\) can in principle be determined by a single specific heat measurement. It gives the critical temperature, \(T_c\), from the position of the jump, the Debye temperature, \(\theta_D\), from the slope of the specific heat versus \(T^3\) in the limit \(T_c \to 0\), and \(\lambda\) from the ratio of high and low temperature values of the Sommerfeld constant.

In BCS theory the ratio \(\frac{\Delta C}{T_c}\), is a constant quantity. In many conventional superconductors like Pb and \(Nb_3Sn\)\(^4\), in alkali doped fullerenes\(^5\) and also in high temperature cuprates superconductors\(^2\) this ratio has been found to be greater than the BCS value. Recently the explanation of this discrepancy has been attributed to the logarithmic van-Hove singularity in the normal state electronic density of states (DOS) in the BCS theory with s wave symmetry of the gap parameter\(^6\), using electron-phonon mechanism of superconductivity and also with the gap parameter of d wave symmetry\(^7\), based on purely electronic mechanism of superconductivity. However, the present experimental scenario of high \(T_c\) materials\(^8\) cannot be described simply either by s-wave symmetric order parameter with electron-phonon interaction mechanism or d-wave symmetric order parameter with purely electronic mechanism. A more reasonable scenario should take into account both electron-electron repulsion and electron-phonon interaction.

Keeping this view in mind, we consider a model which takes into account both an electron-phonon induced attractive interaction between electrons and a repulsive Coulomb interaction, formulated in the Hubbard model. This model has recently been considered by Hocquet et al.\(^9\) to study the critical temperature and the isotope effect in high \(T_c\) superconductors. Within the Bogoliubov-Valatin\(^10\) approximation for the above model, one obtains the BCS gap equation as

\[
\Delta_k = -\frac{1}{2} \sum_{k'} \frac{(V_{kk'} + \frac{U}{N})\Delta_{k'}}{\sqrt{E_{k'}^2 + \Delta_{k'}^2}} \tanh \left( \frac{\sqrt{E_{k'}^2 + \Delta_{k'}^2}}{2kT} \right),
\]

where, \(E_k = \epsilon_k + \frac{U_n}{2} - \epsilon_f\) is the Hartree Fock one particle energy, \(U\) is the repulsive intraatomic interaction of the Hubbard model, \(N\) is the total number of sites, \(n\) is the average number of electrons per site, \(\epsilon_k\) is the bare particle energy in the band, and \(\epsilon_f\) is the Fermi energy. We shall measure the energy such that the sum of the Hartree-Fock shift \(\frac{U_n}{2}\) and the energy of the middle of the band is equal to zero. The width of the band is taken equal to
2W. Following BCS the scattering matrix element $V_{kk'}$ due to phonon mediated interaction is assumed to have a nonvanishing value $-\frac{V}{N}$ with $V > 0$ only if both $|E_k|$ and $|E_{k'}|$ are smaller than the Debye energy $\hbar \omega_D$.

The specific heat jump, $\Delta C$, at the critical temperature $T_c$ is related to the temperature derivative of the square of the gap parameter by the expression\(^\text{11}\),

$$\Delta C = -\sum_k \left( -\frac{\partial f_k}{\partial \epsilon_k} \right) \left[ \frac{d\Delta_k^2}{dT} \right]_{T=T_c},$$

where $f_k$ is the Fermi distribution function for electrons of wave vector $k$ at the critical temperature $T_c$. The temperature derivative of the square of the gap parameter, can be obtained from the numerical solutions of the BCS gap equation. However, usually this derivative is obtained from the approximate analytical expression for the gap parameter near $T_c$. In this paper, we show that it is not necessary to have an explicit expression of the gap parameter near $T_c$ to obtain its derivative at $T_c$.

For the simple BCS form of the scattering matrix element, as described above, the solutions of the BCS gap Eq. (1) have the following structure

$$\Delta_k = \Delta_1 \quad \text{if} \quad |E_k| < \hbar \omega_D$$

$$= \Delta_2 \quad \text{if} \quad |E_k| > \hbar \omega_D$$

Upon substituting the solutions (3) in Eqs. (1) and (2), one obtains the equations for $\Delta C$, $\Delta_1$ and $\Delta_2$ as

$$\Delta C = \left[ \frac{d\Delta_1^2}{dT} \right]_{T=T_c} \langle \eta(\epsilon) \rangle_D + \left[ \frac{d\Delta_2^2}{dT} \right]_{T=T_c} (\langle \eta(\epsilon) \rangle_W - \langle \eta(\epsilon) \rangle_D),$$

$$\Delta_1 = (V - U)\Delta_1 F_{1}^D - U\Delta_2 (F_{2}^W - F_{2}^D)$$

$$\Delta_2 = -U\Delta_1 F_{1}^D - U\Delta_2 (F_{2}^W - F_{2}^D)$$

where

$$F_{1}^D = \int_{-\hbar \omega_D}^{\hbar \omega_D} d\epsilon \frac{\eta(\epsilon+\epsilon_f) \tanh \left( \frac{\sqrt{\epsilon^2+\Delta_1^2}}{2} \right)}{2\sqrt{\epsilon^2+\Delta_1^2}},$$

$$F_{2}^W = \int_{-W-\epsilon_f}^{W-\epsilon_f} d\epsilon \frac{\eta(\epsilon+\epsilon_f) \tanh \left( \frac{\sqrt{\epsilon^2+\Delta_2^2}}{2} \right)}{2\sqrt{\epsilon^2+\Delta_2^2}}.$$
\( \eta(\epsilon) \) is the electronic density of states (DOS) per spin, \( \alpha = 1,2 \), and \( \langle \eta(\epsilon) \rangle_D \) and \( \langle \eta(\epsilon) \rangle_W \) are the thermally averaged DOS, given as

\[
\langle \eta(\epsilon) \rangle_D = \int_{-\hbar \omega_D + \epsilon_j}^{\hbar \omega_D + \epsilon_j} d\epsilon \eta(\epsilon)(-\frac{\partial f}{\partial \epsilon})
\]

(7)

\[
\langle \eta(\epsilon) \rangle_W = \int_{-W}^{W} d\epsilon \eta(\epsilon)(-\frac{\partial f}{\partial \epsilon})
\]

A simple algebraic manipulation of the set of Eqs. (5) shows that

\[
\Delta_2 = (1 - V F_1^D) \Delta_1.
\]

(8)

Upon substituting the expression (8) for \( \Delta_2 \) in Eqs. (5), we get

\[
1 = (V - \frac{U}{1 + U(F_2^W - F_2^D)}) F_1^D.
\]

(9)

We shall use Eqs. (8) and (9) to calculate the temperature derivative of the square of the gap parameters \( \Delta_1 \) and \( \Delta_2 \) at the critical temperature \( T_c \) in order to obtain the specific heat jump \( \Delta C \). Differentiating Eq. (8) with respect to \( T \) and taking the limit \( \Delta_1 \to 0 \) as \( T \to T_c \) we get

\[
\left[ \frac{d\Delta_2^2}{dT} \right]_{T=T_c} = (1 - V F_1^D)^2 \left[ \frac{d\Delta_1^2}{dT} \right]_{T=T_c},
\]

(10)

Similarly differentiating Eq. (9) with respect to \( T \) and taking the limits \( \Delta_1, \Delta_2 \to 0 \) as \( T \to T_c \) we get

\[
F_D U^* (G_W - G_D) \left[ \frac{d\Delta_2^2}{dT} \right]_{T=T_c} + (V - U^*) \frac{\partial F_1^D}{\partial T_c} +
\]

\[
(V - U^*) G_D \left[ \frac{d\Delta_1^2}{dT} \right]_{T=T_c} + F_D U^* \frac{\partial (F_W - F_D)}{\partial T_c} = 0
\]

(11)

where
\[ F_D = \int_{-\hbar \omega_D/2kT_c}^{\hbar \omega_D/2kT_c} d\epsilon \frac{\eta(2kT_c \epsilon + \epsilon_f) \tanh(\epsilon)}{2\epsilon} \]

\[ F_W = \int_{-(W - \epsilon_f)/2kT_c}^{(W - \epsilon_f)/2kT_c} d\epsilon \frac{\eta(2kT_c \epsilon + \epsilon_f) \tanh(\epsilon)}{2\epsilon} \]

\[ G_D = -\int_{-\hbar \omega_D/2kT_c}^{\hbar \omega_D/2kT_c} d\epsilon \frac{\eta(2kT_c \epsilon + \epsilon_f)}{(4kT_c)^2} Q(\epsilon) \]  

\[ G_W = -\int_{-(W - \epsilon_f)/2kT_c}^{(W - \epsilon_f)/2kT_c} d\epsilon \frac{\eta(2kT_c \epsilon + \epsilon_f)}{(4kT_c)^2} Q(\epsilon) \]

\[ Q(\epsilon) = \frac{\tanh^2 \frac{\epsilon}{2kT_c} + \tanh \frac{\epsilon - \epsilon_f}{2kT_c}}{\epsilon} \]

and

\[ U^* = \frac{U}{1 + U(F_W - F_D)}. \] (13)

Upon substituting \( \left[ \frac{d\Delta_1^2}{dT} \right]_{T=T_c} \) from Eq. (10) in Eqs. (11) and (4), we get

\[ \frac{d\Delta_1^2}{dT} \bigg|_{T=T_c} = \frac{(V^*)^2 F_D}{(V^*)^2 G_D + U^2 F_D^2 (G_W - G_D)}, \] (14)

and the jump in the specific heat at \( T_c \) as

\[ \Delta C = -\left[ \frac{d\Delta_1^2}{dT} \bigg|_{T=T_c} \right] \{ \langle \eta(\epsilon) \rangle_D + \xi^2 (\langle \eta(\epsilon) \rangle_W - \langle \eta(\epsilon) \rangle_D) \}. \] (15)

Here \( V^* = V - U^* \) and \( \xi = 1 - VF_D \). It is possible to eliminate \( V \) from Eq. (14) by using the expression for \( T_c \) which can be obtained from Eq. (9) by taking the limits \( \Delta_1 \to 0 \) and \( \Delta_2 \to 0 \). It is given as

\[ 1 - V^* F_D = 0. \] (16)

Substituting the value of \( U^* \) from Eq. (16) in Eq. (14) we get

\[ \left[ \frac{d\Delta_1^2}{dT} \bigg|_{T=T_c} \right] = \frac{(U^*)^2 F_D}{G_D + (U^* F_D)^4 (G_W - G_D)}. \] (17)

It should be noted that Eq (15), together with Eq. (17), is an exact analytical expression for the specific heat jump \( \Delta C \) within the BCS framework. It can be used to check the validity of other results of \( \Delta C \), obtained from the approximate expressions for the gap parameters.
For example, recently Nam\textsuperscript{12} has calculated the specific heat jump $\Delta C$ from the BCS gap equation in absence of short range interactions by expanding the gap parameter near $T_c$. Considering the constant DOS near the Fermi energy and replacing the thermally averaged DOS $\langle \eta(e) \rangle_D$ by $\eta(e_f)$, he showed that at $h\omega_D/2kT_c = 2$ the ratio $\Delta C/T_c$ is equal to 3.4$\gamma$ compared to the BCS value of 1.4$\gamma$. Here $\gamma$ is the Sommerfeld constant $\gamma = 2\pi^2k^2\eta(e_f)/3$. Our exact results show that his results are in error. For the constant DOS near the Fermi energy and the thermally averaged DOS $\langle \eta(e) \rangle_D = \eta(e_f)$, Eqs. (12) - (17) show that in absence of repulsive interaction $U$
olinkurl{Hej})$kTtanh(h\omega_D/2kTc)/2kTc1 tanh$eJ\gamma_2kTc$ae[e2]tanhe-e
d\eta(e)
olinkurl{ET}^\infty de \left[\tanh^2e + \tanh^2 e'\right] = \frac{1}{1.43\gamma} $C/T_c$ \rightarrow \frac{18\gamma}{\pi^2} = 1.82$\gamma$
olinkurl{ET}^\infty de \left[\tanh^2 e + \tanh^2 e'\right] = \frac{1}{1.43\gamma} $C/T_c$ \rightarrow \frac{18\gamma}{\pi^2} = 1.82$\gamma$
olinkurl{ET}^\infty de \left[\tanh^2 e + \tanh^2 e'\right] = \frac{1}{1.43\gamma} $C/T_c$ \rightarrow \frac{18\gamma}{\pi^2} = 1.82$\gamma$
olinkurl{ET}^\infty de \left[\tanh^2 e + \tanh^2 e'\right] = \frac{1}{1.43\gamma} $C/T_c$ \rightarrow \frac{18\gamma}{\pi^2} = 1.82$\gamma$}

At intermediate temperatures $\frac{\Delta C}{T_c}$ increases monotonically with temperature as shown in Fig. 1. Thus for the constant DOS $\frac{\Delta C}{T_c}$ cannot reach the value of 3.4$\gamma$ as obtained by Nam\textsuperscript{12}.

The temperature dependence of thermal DOS $\langle \eta(e) \rangle_D$ and $\langle \eta(e) \rangle_W$, neglected in obtaining Eq. (18), is to reduce $\frac{\Delta C}{T_c}$ and produce a peak at $\frac{kT}{h\omega_D} = 0.24$ in absence of repulsive interaction $U$. As shown in Fig. 1 this behavior of $\frac{\Delta C}{T_c}$ is very similar to that of Marsiglio et al.\textsuperscript{13} and Carbotte\textsuperscript{14}, obtained by using Eliashberg theory of superconductivity. In presence of the repulsive interaction $U$, $\frac{\Delta C}{T_c}$ depends upon the position of the Fermi energy. We have performed out calculations for the Fermi energy located at zero of our energy scale. As shown in Fig.1, the effect of repulsive interaction $U$ on $\frac{\Delta C}{T_c}$ is very small. Visible effect occurs only at higher temperatures where it increases $\frac{\Delta C}{T_c}$. In Fig. 2 we have plotted $\frac{\Delta C}{T_c}$ versus $\frac{kTc}{h\omega_D}$ for normalized Lorentzian DOS. It is found that $\frac{\Delta C}{T_c}$ increases as the width of the peak of the Lorentzian DOS decreases. Similar result was found by Tsuei et al\textsuperscript{6}. The effect of repulsive interaction $U$ is again very small and decreases as the width of the peak increases.

Thus we have shown that one can obtain an exact analytical expression for the jump in specific heat at $T_c$ directly from the BCS gap equation. The analysis of this expression shows...
that the constant DOS in the conventional BCS theory cannot explain the large values of $\Delta C/T_c$ found in many superconductors. To explain the higher values of $\frac{\Delta C}{T_c}$ within the BCS framework, one must take into account the energy dependent density of states with sharper peak at the Fermi level. The effect of repulsive interaction is quite small compared to the effect of the energy dependent density of states.

Acknowledgments

This work was done within the framework of the Associateship Scheme of the International Centre for Theoretical Physics, Trieste, Italy. One of us (S.L.) thanks Conselho Nacional de Desenvolvimento Cientifico e Technologico(CNPq), Brasil for financial assistance.
REFERENCES


FIG. 1. $\Delta C/T_c$ (in units of $\frac{k_F^2 k_F}{6W}$) versus $kT_c/\hbar \omega_D$ for constant density of states.
FIG. 2. $\Delta C/T_c$ (in units of $\frac{2\pi e^2 \omega_D}{6W}$) versus $kT_c/h\omega_D$ for the normalized Lorentzian density of states, $\rho(\epsilon) = \frac{1}{2\tan^{-1}\left(\frac{\epsilon}{b}\right)} \frac{b^2}{\epsilon^2 + b^2}$, for various values of $b/W$ and $U/2W$. The solid line corresponds to $U/2W = 0.0$, the dashed line corresponds to $U/2W = 0.2$ and the small dashed line corresponds to $U/2W = 0.4$. 