BCS Superconductivity in the Van Hove Scenario in s and d Waves

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The effect of including a van Hove singularity in the density of state of a renormalized BCS equation in s and d waves and its appropriateness in describing some properties of high-T_c cuprates in the weak-coupling region are studied in two space dimensions. The specific heat and knight shift as a function of temperature exhibit scaling below the critical temperature in d wave. We also study the jump in the specific heat at the critical temperature T_c in s and d waves, which can have values significantly higher than the standard BCS values and which increases with T_c, as experimentally observed in many d-wave high-T_c materials. The experimental results on the specific heat and knight shift of the Y-123 system are compared with the theoretical predictions.

The discovery of high-T_c cuprates [1] with many unusual properties both above and below the critical temperature T_c presents a serious question on the applicability of the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity [2, 3] at high temperatures. The high-T_c materials have many unusual properties, such as, an anomalously large ΔC and $\Delta(0)/T_c$ and small isotope effect, where ΔC is the jump in specific heat at T_c and $\Delta(0)$ is the zero-temperature BCS gap.

Despite much effort, the normal state of the high-T_c cuprates has not been satisfactorily understood yet and there are controversies about the appropriate microscopic Hamiltonian and pairing mechanism [4, 5]. The use of a van Hove singularity (vHs) in the density of states (DOS) near or at the Fermi surface makes the standard BCS model more suitable for the high-T_c cuprates [6, 7, 8]. The singularity in the density of states known as the van Hove singularity arises wherever the group velocity vanishes and where there is a locally flat region of the frequency as a function of the wavevector $\mathbf{k}$. The critical points where these singularities are observed may be saddle points. In high T_c compounds there have been evidences of saddle points which yield a logarithmic divergence. Moreover recent experiments [9, 10] have given evidences of an extended saddle point singularity which corresponds to a power law behavior [7]. The use of a vHs in the DOS can simulate different non-Fermi liquid type properties of both the normal and superconducting states [6, 7]. Some experiments also suggest a peak in the DOS associated with a vHs near the Fermi level [11, 9, 12]. There have been attempts to explain many anomalous features of the high-T_c cuprates using a vHs in the DOS [6, 7]: such as the large values of ΔC and $\Delta(0)/T_c$, anomalous isotope effect, pressure coefficient of T_c, temperature variation of specific heat $C_s(T)$ and knight shift etc. Virtually, in all these applications an s-wave interaction has been employed.

However, there are evidences that some of the high-T_c cuprates have singlet d-wave Cooper pairs and the gap parameter has $d_{x^2-y^2}$ symmetry in two dimensions [5]. Recent measurements of the penetration depth $\lambda(T)$ [11, 9, 12] and superconducting specific heat at different temperatures T [11, 9, 12] and related theoretical analyses [13] also support this point of view. According to the isotropic s-wave BCS theory, as $T \to 0$, both observables exhibit exponential dependence on T [3]. The experimental power-law dependencies of these observables on T can be explained by considering anisotropic gap parameter with node(s) on the Fermi surface [4, 13].

We study a weak-coupling renormalized BCS model in two dimensions for s and d waves in the presence of several types of vHs with two objectives in mind. The first objective is to see if these scalings get significantly modified in the presence of a vHs in the DOS. The second objective is to see to what extent the properties of the high-T_c cuprates can be understood by the weak-coupling BCS theory in two dimensions with a vHs in the DOS. The renormalized model yields a high T_c and a small coherence length in the weak coupling region [4] in accord with the recent experimental findings. Moreover it also gives us a linear correlation between T_c and T_F as found in many high T_c materials [14] whereas in the conventional BCS theory we observe a correlation between T_c and T_D. Here T_F is the Fermi temperature and T_D is the Debye temperature. So the the above model seems to be worth studying though it may have some limitations. We work in two dimensions as the cuprates exhibit a conductive structure similar to a two dimensional layer of carriers.

In previous studies of the renormalized weak-coupling BCS model in two and three dimensions we found robust universal scaling among condensation energy ΔU, BCS gap $\Delta(0)$, critical temperature T_c and specific heat per particle $C_s(T_c)$ in non-s waves valid over several decades [4]. There we also calculated the temperature dependencies of different quantities, such as, the BCS gap $\Delta(T)$, spin susceptibility $\chi(T)$, and $C_s(T)$ for $T < T_c$. For isotropic s wave (anisotropic d wave), the BCS theory yields exponential (power-law) dependence on temperature as $T \to 0$ for these observables independent of space dimension [3, 4]. Here we critically reexamine these scalings in the presence of a vHs in the DOS. We find that the scaling relations remain valid in the presence of a vHs with a slightly changed values of the exponents.

We consider a system of N superconducting electrons, each of mass m under the action of a a purely attractive short-range two-electron potential in partial wave l:

$$V_{\mathbf{pq}} = -V_l c_l \cos(l\theta_p)\cos(l\theta_q), \tag{1}$$

where θ_p is the angle of vector $\mathbf{p}$ with any suitable axis and $c_l = 1$ (2) for $l = 0$ ($\neq 0$) as in Ref. [15].

Potential (1) for a arbitrary small V_l and any l leads to Cooper pairing instability at zero temperature in even (odd) angular momentum states for spin-singlet (triplet) state of the two-electron system. The Cooper-pair problem for two electrons over the filled Fermi sea is given by [4]

$$V_l^{-1} = \sum_{\mathbf{q}(q>1)} c_l \cos^2(l\theta)(2\epsilon_q + B_c - 2)^{-1}, \tag{2}$$

with B_c the Cooper binding. Unless the units of the variables are explicitly mentioned, in Eq. (2) and in the following, all energy (momentum) variables are expressed in units of E_F (k_F), such that $T \equiv T/T_F$, $q \equiv q/k_F$, $E_{\mathbf{q}} \equiv E_{\mathbf{q}}/E_F$, $E_F = k_F = 1$, etc.

The summations in Eq. (2) and in the following are evaluated according to

$$\sum_{\mathbf{q}} \to \frac{N}{4\pi}\int_0^\infty n(\epsilon_q)d\epsilon_q \int_0^{2\pi} d\theta, \tag{3}$$

where $\epsilon_q = \hbar^2 q^2/2m$ and $n(\epsilon_q)$ is an integrable vHs in the DOS which tends to a large value on or near the Fermi surface. Here we consider the following three densities of states:

$$n(\epsilon) = \frac{1}{2\ln 2}\ln\left|\frac{\epsilon+1}{\epsilon-1}\right|, \tag{4}$$

$$n(\epsilon) = \frac{2(1-x)}{(\epsilon-1)^x}, \tag{5}$$

$$n(\epsilon) = \frac{\delta}{\arctan(1/\delta)}\frac{1}{(\epsilon-1)^2+\delta^2}, \tag{6}$$

which are a logarithmic vHs, power-law vHs and a Lorentzian DOS, respectively. Here x is a number that decides nature of the power-law vHs and is chosen to be .5 and .75 in this work. We also study the Lorentzian DOS which does not have a singularity at the Fermi surface as it serves the same purpose as a vHs and gives us a wider scope to compare the experimental results. Each of these densities has been normalized such that when all states up to the Fermi surface are filled, the total number of particles is N.

At a finite T, one has the following BCS equation

$$\Delta_{\mathbf{p}} = -\sum_{\mathbf{q}} V_{\mathbf{pq}}\frac{\Delta_{\mathbf{q}}}{2E_{\mathbf{q}}}\tanh\frac{E_{\mathbf{q}}}{2T} \tag{7}$$

with $E_{\mathbf{q}} = [(\epsilon_q-\mu)^2 + |\Delta_{\mathbf{q}}|^2]^{1/2}$. The order parameter $\Delta_{\mathbf{q}}$ has the following anisotropic form: $\Delta_{\mathbf{q}} \equiv \Delta_0\sqrt{c_l}\cos(l\theta)$, where Δ_0 is dimensionless. The usual BCS gap is defined by $\Delta(T) = \Delta_0$, which is the root-mean-square average of $\Delta_{\mathbf{q}}$ on the Fermi surface. Using Eqs. (1) and (2), Eq. (7) can be written explicitly in terms of the Cooper-pair binding as follows [4]:

$$\int_0^{2\pi} d\theta \cos^2(l\theta)\Big[\int_1^\infty \frac{2n(\epsilon_q)d\epsilon_q}{2\epsilon_q + B_c - 2} - \int_0^\infty \frac{n(\epsilon_q)d\epsilon_q}{E_{\mathbf{q}}}\tanh\frac{E_{\mathbf{q}}}{2T}\Big] = 0. \tag{8}$$

The two terms in equation (8) have ultraviolet divergences and needs a energy cut-off as seen in the conventional BCS case. However, the difference between these terms is finite [4, 16]. Hence we call this a renormalized BCS model . The quantity B_c now plays the role of the coupling of interaction. BCS model (8) has some advantages [4]. Firstly, no arbitrary energy cut-off is explicit in this equation. Secondly, this model leads to an increased T_c in the weak-coupling limit, appropriate for some high-T_c materials [4].

The condensation energy per particle at $T = 0$ is defined by [3]

$$\Delta U = \frac{1}{N}\left[\sum_{\mathbf{q}(q<1)} 2\zeta_q - \sum_{\mathbf{q}}\left(\zeta_q - \frac{\zeta_q^2}{E_{\mathbf{q}}} - \frac{\Delta_{\mathbf{q}}^2}{2E_{\mathbf{q}}}\right)\right], \tag{9}$$

where $\zeta_q = (\epsilon_q - 1)$. The superconducting specific heat per particle is given by

$$C_s(T) = \frac{2}{NT^2}\sum_{\mathbf{q}} f_{\mathbf{q}}(1-f_{\mathbf{q}})\left(E_{\mathbf{q}}^2 - \frac{1}{2}T\frac{d\Delta_{\mathbf{q}}^2}{dT}\right), \tag{10}$$

where $f_{\mathbf{q}} = 1/(1+\exp(E_{\mathbf{q}}/T))$. The normal specific heat C_n is given by Eq. (10) with $\Delta_{\mathbf{q}} = 0$. The jump in specific heat per particle at $T = T_c$ ($\Delta(T_c) = 0$), $\Delta C \equiv [C_s - C_n]_{T_c}$ is given by [3]

$$\Delta C = A^2 B^2 k_B^2 T_c < n(\delta) >_{k_B T_c} \tag{11}$$

where $A^2 = [\Delta(0)/k_B T_c]^2$, $B^2 = -d[\Delta(T)/\Delta(0)]^2/d(T/T_c)$ at $T = T_c$, k_B is the Boltzmann constant and

$$< n(\delta) >_{k_B T} = \int_{-\infty}^{\infty} n(\epsilon)d\epsilon(-\frac{\partial f}{\partial \epsilon}). \tag{12}$$

This gives the jump to T_c ratio in terms of the proper units as found in experiments and not in terms of the dimensionless form which we use for the rest of the calculation. This was mainly done in order to compare the theoretical predictions with the experimental datas. The knight shift can be found from the spin-susceptibility [4] $\chi(T) = (2\mu_N^2/T)\sum_{\mathbf{q}} f_{\mathbf{q}}(1-f_{\mathbf{q}})$, where μ_N is the nuclear magneton.

We solve Eq. (8) numerically and calculate the BCS gap $\Delta(0)$, T_c, $C_s(T_c)$, ΔU at $T = 0$ as well as $\Delta(T)$, $C_s(T)$, and $\chi_s(T)$ in s and d waves in the weak-coupling region. In the absence of a vHs in two dimensions we established $\Delta(0) = 2\sqrt{\Delta U}$, $T_c = 2\sqrt{\Delta U}/A$, and $C_s(T_c) \sim \sqrt{\Delta U}$ where $A \equiv \Delta_0/T_c$ is the universal BCS ratio. In the presence of a vHs or Lorentzian DOS, we establish in the present study scalings $\Delta(0) \sim \sqrt{\Delta U}$ and $T_c \sim \sqrt{\Delta U}$. The exponent of these scalings are unchanged in the presence of the vHs in the DOS although the prefactor gets changed. In the presence of a vHs in the DOS the scaling $C_s(T_c) \sim \sqrt{\Delta U}$ and the ratio A increases slowly from its BCS universal value 1.764 for $l = 0$ (1.513 for $l = 2$) [4] with the increase of ΔU or coupling. However, as noted before the ratio A is always limited by 2.

One of the most interesting aspects of introducing a vHs in the DOS is that it increases the jump in specific heat $\Delta C(T_c)/C_n(T_c)$ above its BCS value of 1.43 for $l = 0$ and 1.0 for $l = 2$ for all T_c [4]. Many of the high-T_c cuprates yield a significantly higher value for this ratio experimentally [6, 7]. In Fig. 1 we plot the jump $\Delta C/T_c$ for different T_c in case of s and d waves for the power law vHs $x = .5$ and .75 respectively and $\Delta C/T_c$ is in J/K^2/mole and T_c is in kelvin. $< n(\delta) >_{k_B T_c}$ is chosen to be 2.5 ev^{-1} spin^{-1} and 1.5 ev^{-1} spin^{-1} for both s and d waves. The above values of $< n(\delta) >_{k_B T_c}$ are in reasonable agreement with the values estimated from other experiments [17]. As the s-wave problem has been studied before [6, 7] here we pay our attention mostly to d-wave. From Fig. 1 we find that $\Delta C/T_c$ increases with T_c. In both s and d waves $\Delta C/T_c$ exhibits a very slow increase with temperature initially but above $T_c = 80$K the jump increases steeply with temperature. For a fixed T_c and the same DOS, the s-wave jump is always greater than the d-wave jump.

The calculated results are compared with experimental results [18]. In terms of the overall T_c dependence the agreement between the theory and experimental is quite reasonable.

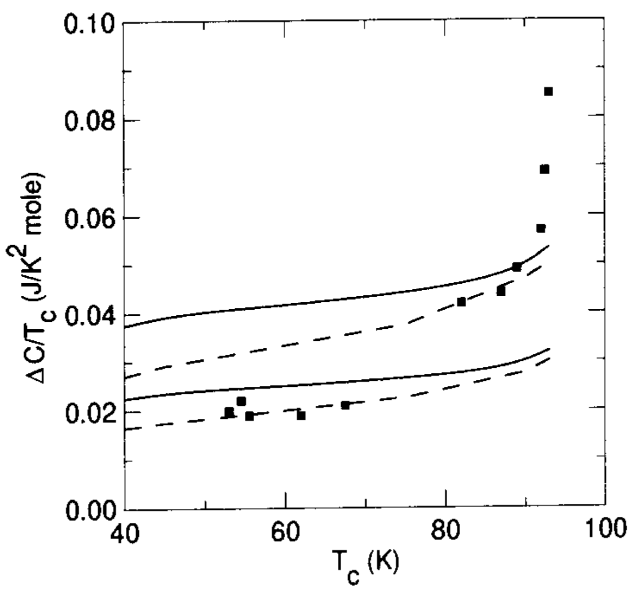

Figure 1. Specific heat jump $\Delta C/T_c$ versus T_c in s (solid line) and d (dashed line) waves for PL – vHs (5)for s(d) wave with $x = 0.5(0.75)$. The lower(upper) set of lines are for $< n(\delta) >_{k_B T_c}$ =1.5 (2.5) ev^{-1} spin^{-1}. Experimental results of the Y-123 system (Daumling) are shown.

Next we studied the temperature dependence of $\Delta(T)$, $C_s(T)$, and knight shift for $T < T_c$. The gap function $\Delta(T)$ has essentially the same universal behavior as in s wave [3]. For $T \approx T_c$, we find $\Delta(T)/\Delta(0) = B\,(1 - T/T_c)^{1/2}$, with $B = 1.74$ (1.70) for $l = 0$ $(= 2)$. The value of the constant B is essentially independent of the presence of a vHs.

In our attempt to study the specific heat jump with vHs in the DOS we consider the compounds $YBa_2Cu_3O_{7-x}$ (s-wave cuprate in two dimensions) and $Bi_2Sr_2CaCu_2O_8$ (d-wave cuprate in two dimensions) [8]. For $YBa_2Cu_3O_{7-x}$, $T_c = 93$ K, $T_F = 8800$ K, $T_c/T_F \approx 0.01$ and $\Delta C/C_n(T_c) \approx 5$. For $Bi_2Sr_2CaCu_2O_8$, $T_c = 100$ K, $T_F = 4200$ K, $T_c/T_F \approx 0.024$ and $\Delta C/C_n(T_c) \approx 2$ [8]. In order to simulate these two cuprates we considered DOS (4), (5) and (6) with $T_c = 0.01$ (s wave) and $T_c = 0.025$ (d wave).

In Fig. 2 we plot the s-wave superconducting and normal specific heats $C(T)/C_n(T_c)$ versus T/T_c for DOS (5) with $x = 0.75$, and (6) with $\delta = 0.01$. The jump $\Delta C/C_n(T_c)$ in these two cases is approximately equal to the experimental value (5) quoted above for the s-wave cuprate. The jump in specific heat for (4) is small and is not considered here.

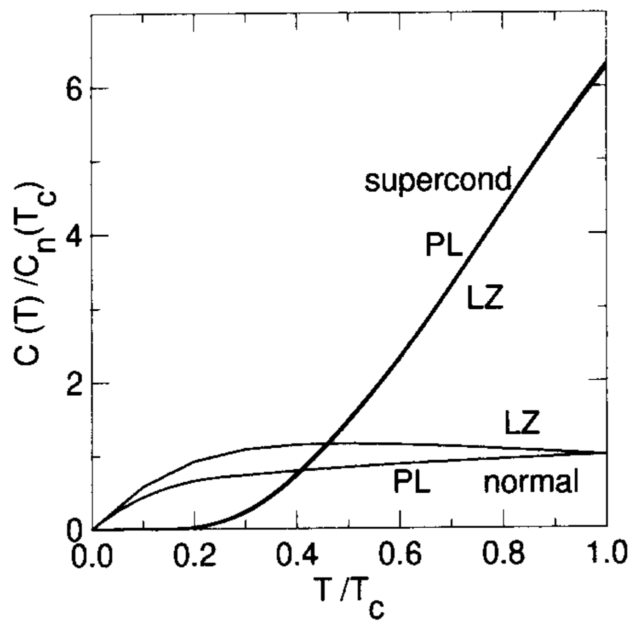

Figure 2. Normal and superconducting specific heats $C(T)/C_n(T_c)$ versus T/T_c for s wave: PL – vHs (5) with $x = 0.75$, LZ – DOS (6) with $\delta = 0.01$.

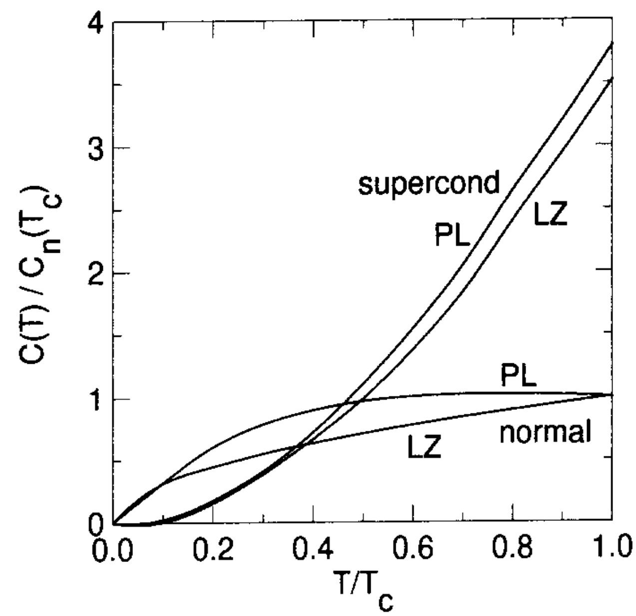

Figure 3. Normal and superconducting specific heats $C(T)/C_n(T_c)$ versus T/T_c for d wave: PL – vHs (5) with $x = 0.5$ (dashed curve), LZ – DOS (6) with $\delta = 0.04$ (solid curve).

Now we turn to the interesting case of the d-wave specific heat. In Fig. 3 we plot the d-wave superconducting and normal specific heats $C(T)/C_n(T_c)$ versus T/T_c for DOS (5) with $x = 0.5$ and (6) with $\delta = 0.04$. We studied the scaling properties in this case and found

$C_s(T) \sim (T/T_c)^{\beta_C}$, with $\beta_C = 1.8$ for both square-root vHs in the DOS and Lorentzian DOS. In order to extract this exponent β_C we had to plot Fig. 3 in log-log scale (not shown). In the absence of the vHs in the DOS in two dimensions $\beta_C = 2$ [4]. The exponent $\beta_C = 2$ has been observed in the experimental work of Phillips et al [19].

Finally, we study the knight shift. We plot $K(T)/K(T_c)$ versus T/T_c in Fig. 4 for DOS (6) with $\delta = 0.01$ (s wave) and $\delta = 0.04$ (d wave), and DOS (4). The s wave results essentially lead to a single curve. The two d-wave possibilities considered also lead to very similar results. In this case we establish the following power-law dependencies on T/T_c for $l = 2$: $K(T)/K(T_c) \sim (T/T_c)^{\beta_k}$ with $\beta_k = 1.0$ for almost the entire temperature range. In two dimensions in the absence of a vHs we found the exponent to be 1.2 [4]. We also plot the experimental points [20] and it is seen that the theoretical predictions from our model fit reasonably the data.

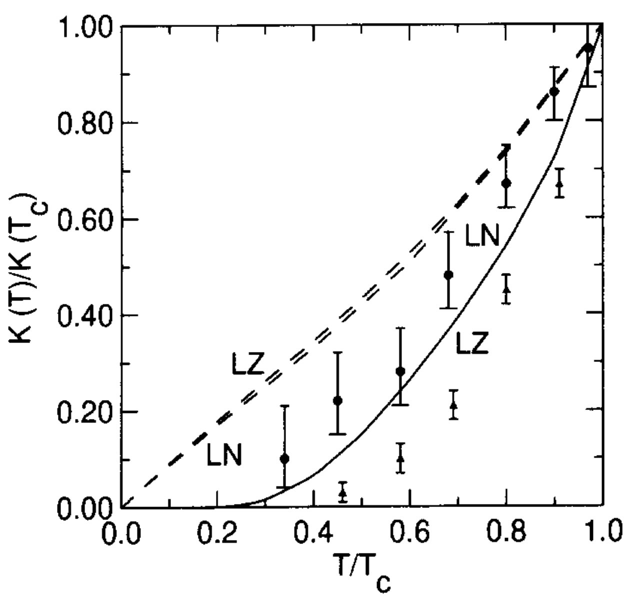

Figure 4. $K(T)/K(T_c)$ versus T/T_c for s (solid line) and d (dashed line) waves. LZ – DOS (6) with $\delta = 0.01$ for s wave, LZ – DOS (6) with $\delta = 0.04$ for d wave and LN – DOS (4). Experimental data points on Y-123 system : circle(perpendicular) triangle (parallel) (ref. 15).

To summarize, we studied a renormalized weak-coupling BCS model in s and d waves in the presence of a van Hove and Lorentzian DOS. Scalings are established among $\Delta(0)$ and T_c as function of ΔU: $\Delta(0) \sim \sqrt{\Delta U}$ and $T_c \sim \sqrt{\Delta U}$. Identical scalings have been established recently in the absence of a vHs [4]. The temperature dependencies of $C_s(T)$ and $\chi_s(T)$ below T_c in d wave are found to exhibit power-law scalings distinct to some high-T_c materials at low energies [11, 9, 12]. No power-law T dependence is found in s wave for these observables. For $l = 2$ we obtained $C_s(T)/C_n(T_c) \sim (T/T_c)^{1.8}$ and $K(T)/K(T_c) \sim (T/T_c)^{1.0}$ for almost the entire temperature range in the presence of a vHs. Similar scalings, with a slightly different exponent were found to exist in the absence of a vHs [4]. In the presence of a vHs, the jump in specific heat $\Delta C/C_n(T_c)$ could have values much larger than the standard BCS value 1.43 (1.0) for $l = 0$ (2) [4]. Such large values were observed experimentally for some high-T_c cuprates [6, 8]. The ratios $\Delta C/T_c$ and $A = \Delta(0)/T_c$ were both found to increase with coupling (T_c). Although there are controversies about a microscopic formulation of high-T_c cuprates, it seems that the present renormalized BCS model with a vHs can be used to explain some of their universal properties.

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