Specific heat and Knight shift of cuprates within the van Hove scenario

Sujit Sarkar and A. N. Das
Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Calcutta 700 064, India
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The jump in the specific heat at T_c, the specific heat in both the superconducting and normal states, and the Knight shift in the superconducting state are studied within the van Hove singularity scenario considering density of states for a two-dimensional tight-binding system and with an extended saddle-point singularity. The role of the electron-phonon interaction strength, band narrowing, second-nearest-neighbor hopping, and orthorhombic distortion on such properties is investigated. The experimental results on the specific heat and Knight shift of the Y-123 system are compared with the theoretical predictions. [S0163-1829(96)04645-0]

Divergent theories have been proposed so far for the mechanism of superconductivity in high-T_c cuprates. The van Hove singularity (VHS) scenario is one of them. Several papers[1–6] suggested that the high transition temperature, anomalous isotope effect, linear resistivity, and thermoelectric power behavior of high-T_c systems might be understood assuming a presence of a VHS in the density of states (DOS) and its proximity to the Fermi level near optimum doping. Recently angle-resolved photoemission experiments[7,8] have provided direct evidence for the presence of an extended VHS in the DOS of the high-T_c systems.

In this work we investigate the behavior of the specific heat and the Knight shift within the VHS scenario. Previously Tsuei *et al.*[9] studied the specific-heat jump within the VHS scenario and from an analysis of the experimental results of the Y-123 system they concluded that the Fermi level at optimum doping is near a two-dimensional (2D) VHS point. Here we consider a DOS, derived exactly from a tight-binding 2D model where orthorhombic distortion and second-nearest-neighbor hopping have been taken into account.[10] It is well known that a simple 2D band has a saddle point which yields a logarithmic divergence in the DOS. However, recent experiments[7,8] have given direct evidence for a flatband and an extended saddle-point singularity in high-T_c oxide systems. We report in this paper the specific heat and the Knight shift behavior within the VHS scenario for the 2D DOS with simple saddle-point singularities for square and rectangular lattices and also for the DOS corresponding to the extended saddle-point singularity. The role of the band narrowing, electron-phonon (e-ph) interaction strength, second-nearest-neighbor hopping, and orthorhombic distortion on such properties is investigated.

The jump in the specific heat at T_c within the framework of the BCS formalism is given by[9]

$$\Delta C|_{T=T_c}=A^2B^2\int_{-W}^{W}N(\epsilon)f(\xi)[1-f(\xi)]d\epsilon, \qquad (1)$$

where ϵ is the quasiparticle energy, $N(\epsilon)$ is the density of states of the electronic band, W is the half bandwidth, $\xi=\epsilon-E_f$, E_f denotes the Fermi level, and $f(\xi)=[\exp(\beta\xi)+1]^{-1}$ is the Fermi distribution function,

$$A^2=-\frac{T_c}{\Delta_0^2}\frac{d\Delta^2(T)}{dT}, \quad B^2=\left[\frac{\Delta_0}{k_BT_c}\right]^2,$$

$\Delta(T)$ is the superconducting gap at temperature T, and Δ_0 is the gap at $T=0$.

The DOS for a tight-binding model of a rectangular lattice with nearest-neighbor and next-nearest-neighbor hopping is given by[10]

$$N(\epsilon)=\frac{1}{2t\pi^2\sqrt{r_1+r_2\epsilon/2t}}K\left[\frac{\sqrt{(1+r_1)^2-(\epsilon/2t-r_2)^2}}{2\sqrt{r_1+r_2\epsilon/2t}}\right] \qquad (2)$$

for $1+r_1+r_2\geqslant\epsilon/2t\geqslant1-r_1-r_2$ or $-1+r_1-r_2\geqslant\epsilon/2t\geqslant-1-r_1+r_2$, and

$$N(\epsilon)=\frac{1}{t\pi^2\sqrt{(1+r_1)^2-(\epsilon/2t-r_2)^2}}\times K\left[\frac{2\sqrt{r_1+r_2\epsilon/2t}}{\sqrt{(1+r_1)^2-(\epsilon/2t-r_2)^2}}\right] \qquad (3)$$

for $1-r_1-r_2\geqslant\epsilon/2t\geqslant-1+r_1-r_2$, where $K[x]=F(\pi/2,x)$ is the complete elliptic integral of the first kind, r_1 is the ratio of the hopping integrals along the x and y directions, and $r_2=2t_2/t$; t_2 is the second-nearest-neighbor hopping integral. $r_1=1$ corresponds to a square lattice.

For high-T_c oxide systems where the motion of charge carriers is important in planes an orthorhombic structure generally corresponds to $r_1\neq1$. However, in the low-temperature tetragonal phase of La-214 the Cu-O bond distances in a particular CuO_2 plane are different along the x and y directions,[11] and $r_1\neq1$ may still be relevant.

The DOS described by Eqs. (2) and (3) has a logarithmic van Hove singularity for $r_1=1$ and $r_2=0$. For $r_1\neq1$ the VHS peak splits into two which appear at $\epsilon=\pm2t(1-r_1)$ whereas for $r_1=1$ and $r_2\neq0$ the VHS peak shifts by $-4t_2$ and the DOS becomes asymmetric.[10,12]

The DOS corresponding to an extended saddle point has a power law (square root) singularity and is approximately given by[8,13]

$$N(\epsilon)=\frac{1}{2}\frac{1}{\sqrt{W-\epsilon_0}}\frac{1}{\sqrt{\epsilon-\epsilon_0}}\quad(\epsilon>\epsilon_0)$$
$$=0\quad(\text{otherwise}),\tag{4}$$

where W is the half bandwidth and ϵ_0 is the singularity point in the DOS.

Tsuei *et al.*[9] found that $A=1.74$ and $B=1.84$ for a DOS with a VHS when the chemical potential lies close to the singularity point of the DOS (2) and (3). We also obtained similar values of A and B, which are almost independent of r_1 and r_2 for for $1\leqslant r_1\leqslant 0.9$ and $r_2\leqslant 0.4$ and near optimum doping concentration.[12] using $A=1.74$ and $B=1.84$ one obtains a simplified expression for

$$\Delta C|_{T=T_c}=10.25k_B\int_{-W}^{W}N(\epsilon)f(\xi)[1-f(\xi)]d\epsilon.\tag{5}$$

This expression is simple and describes reasonably the jump in the specific heat within the VHS scenario.

We have also studied the specific heat in the normal and superconducting states using the standard formulas

$$C_n=\frac{1}{k_BT^2}\int_{-W}^{W}N(\epsilon)f(\xi)[1-f(\xi)]\epsilon^2d\epsilon,\tag{6}$$

$$C_s=\frac{1}{k_BT^2}\int_{-W}^{W}N(\epsilon)f(E)[1-f(E)]\times\left(E^2-\frac{1}{2}T\frac{d\Delta^2(T)}{dT}\right)d\epsilon\tag{7}$$

where $E=\sqrt{(\epsilon-E_f)^2+\Delta^2(T)}$. The gap parameter $\Delta(T)$ is obtained from the standard gap equation

$$\frac{2}{v}=\int_{E_f-\omega_D}^{E_f+\omega_D}N(\epsilon)\frac{1}{\sqrt{(\epsilon-E_f)^2+\Delta^2(T)}}\times\tanh\left(\frac{\sqrt{(\epsilon-E_f)^2+\Delta^2(T)}}{2T}\right)d\epsilon,\tag{8}$$

where v represents the electron-phonon interaction strength. The temperature gradient of $\Delta^2(T)$ is given by the expression

$$\frac{d\Delta^2(T)}{dT}=\frac{1}{I_1-I_2}\frac{1}{2k_BT^2}\int_{E_f-\omega_D}^{E_f+\omega_D}N(\epsilon)\text{sech}^2(E/2k_BT_c)d\epsilon,\tag{9}$$

$$I_1=\frac{1}{4k_BT_c}\int_{E_f-\omega_D}^{E_f+\omega_D}\frac{N(\epsilon)}{E^2}\text{sech}^2(E/2k_BT_c)d\epsilon,\tag{10}$$

$$I_2=\frac{1}{2}\int_{E_f-\omega_D}^{E_f+\omega_D}N(\epsilon)\frac{1}{E^3}\tanh(E/2k_BT_c)d\epsilon.\tag{11}$$

The jump in the specific heat and the specific heat in the normal state as well as in the superconducting state are evaluated numerically using Eqs. (5)–(9) using the DOS (2) and (3) and the DOS (4). It may be mentioned that for the DOS (4) the lower limit of integration is determined by the singularity point of the electronic DOS instead of the Debye frequency.

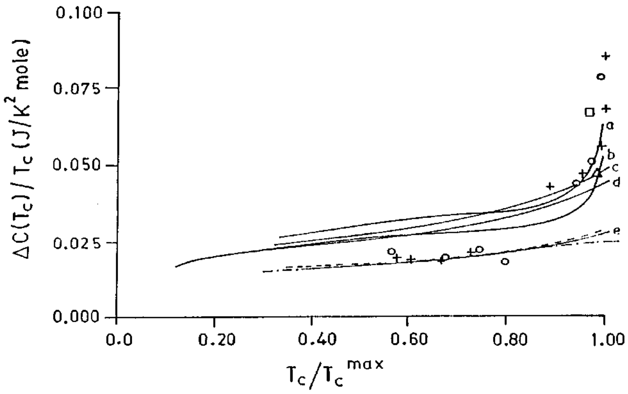

FIG. 1. $\Delta C(T_c)/T_c$ as a function of $T_c/T_c^{\max}$. Solid curves (a) and (b) are for the DOS (4) (a) $t=600$ K, $v=1000$ K, and $\epsilon_0=500$ K, (b) $t=1000$ K, $v=1000$ K, and $\epsilon_0=1000$ K. Solid curves (c), (d), and (e) are for the DOS (2) and (3) and for $r_1=1$ and $r_2=0$. (c) $t=400$ K, $v=1000$ K; (d) $t=400$ K, $v=1200$ K; (e) $t=800$ K, $v=1600$ K. Dashed and dashed-dot curves, adjacent to curve (e), are for $r_1=1$, $r_2=0.4$ and $r_1=0.9$, $r_2=0$, respectively, and for $t=800$ K and $v=1600$ K. Experimental results of the Y-123 system are shown: circles (Wuhl *et al.*), triangles (Inderhees *et al.*), squares (Junod *et al.*), + (Daumling).

Figure 1 shows the variation of $\Delta C(T_c)/T_c$ with T_c for different values of t and v. The effects of r_1 and r_2 for the DOS (2) and (3) on the specific-heat jump are shown in the same figure. The value of $\Delta C(T_c)/T_c$ is high at optimum doping where $T_c=T_c^{\max}$ ($T_c^{\max}$ is the maximum transition temperature) and it decreases sharply with decreasing T_c as the Fermi level shifts from the VHS point. Similar results were reported by Tsuei *et al.*[9] It is found that $\Delta C(T_c)/T_c$ decreases with increasing bandwidth (W) and increasing v. Orthorhombic distortion and second-nearest-neighbor hopping have little effect on the specific heat jump. The value of $\Delta C(T_c)/T_c$ increases slightly with the introduction of r_2, while it decreases near optimum doping as the orthorhombic distortion is introduced.

The DOS (4) corresponding to the extended saddle point has a much stronger singularity than the DOS (2) and (3). This gives rise to a much sharper fall of $\Delta C(T_c)$ with T_c as T_c decreases (Fig. 1). The experimental data on $YBa_2Cu_3O_{7-\delta}$ systems[14–16] are shown in the same figure. The fall of $\Delta C(T_c)/T_c$ with decreasing T_c, as observed experimentally, agrees qualitatively with the predictions of the VHS theory, as emphasized by Tsuei *et al.*[9] The results for the extended saddle-point singularity are closer to the experimental situation. It may be mentioned that in the Y-123 system ΔC is large and continues to rise in the overdoped regime[17] because of a chain contribution, which has not been considered in our work.

We have also studied $\Delta C(T)/C_n(T)$ as a function of T/T_c for optimum doping. $\Delta C(T)[=C_s(T)-C_n(T)]$ and $C_n(T)$ are calculated using the exact expressions (6) and (7). It is found that value of the ratio $\Delta C(T)/C_n(T)$ at T_c is 2.13 for the DOS (2) and (3), which is considerably higher than the BCS value of 1.43, and $\Delta C(T)$ changes sign at $T/T_c\sim 0.5$, similar to the result obtained by Goicochea.[18] For

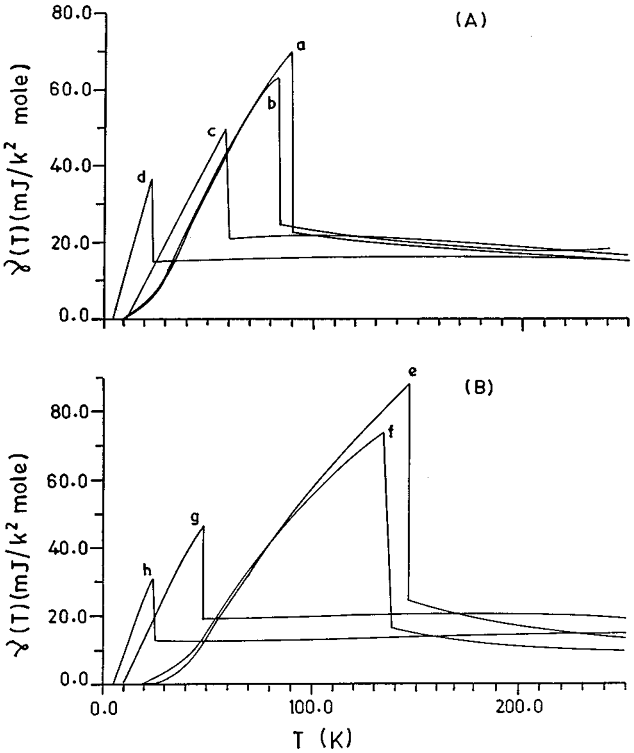

FIG. 2. Plot of $\gamma(T)$ vs T, (A) for the DOS (2) and (3) and (B) for the DOS (4). Upper curves (A) $t=400$ K, $v=1000$ K, (a) $E_f=-40$ K, (b) $E_f=-160$ K, (c) $E_f=-400$ K, (d) $E_f=-800$ K. Lower curves (B) $t=600$ K, $v=1000$ K, and $\epsilon_0=500$ K for curves (e) and (g), the values of $E_f=800$ K, and 1600 K, respectively. $t=1000$ K, $v=1000$ K, and $\epsilon_0=1000$ K for the curves (f) and (h), the values of $E_f=1200$ K and 2500 K, respectively.

the DOS (4) the ratio $\Delta C(T)/C_n(T)$ at T_c is much larger (3.38 for $t=v=1000$ K, $\epsilon_0=1000$ K) and is closer to the experimental value [4.8 (Ref. 19) compared to the case with a simple VHS. The value of T/T_c where $\Delta C(T)$ changes sign is slightly higher than 0.5 for the DOS (4). However, the experimental results of high-T_c system give a much higher value of T/T_c (~ 0.86) where $\Delta C(T)$ changes sign.

In Fig. 2 we plot the variation of $\gamma(T)(=C_e/T)$ with temperature T. In the superconducting state $\gamma(T)$ exhibits an exponential behavior at very low temperatures and then increases almost linearly and has a sharp fall at T_c. For the optimally doped samples this jump in the specific heat is large and in the normal state $\gamma(T)$ decreases with increasing T. As the Fermi level shifts from the VHS point T_c decreases and the jump in the specific heat also decreases. For sufficiently underdoped samples [curves (c) and (d), and (g)] $\gamma(T)$ for $T>T_c$ slightly increases with T and then decreases. The general trend of the results for $\gamma(T)$ is the same for both the cases of the DOS (2) and (3) and the DOS (4); only the value of $\gamma(T)$ and the jump in $\gamma(T)$ at T_c are larger for the DOS (4) compared to the DOS (2) and (3) as evident in Fig. 1.

Loram *et al.*[20] made a systematic study of the specific heat of the $YBa_2Cu_3O_{6+x}$ system as a function of temperature and oxygen content. They found that for samples close to optimum doping $\gamma(T)$ in the normal state decreases with increasing T, while for underdoped samples it exhibits a broad peak which moves to higher temperature with decreasing carrier concentration (oxygen content). Comparing our results of Fig. 2 with that of Fig. 4 of Ref. 20 we find that their experimental results are reasonably consistent with the theoretical predictions for both the simple and extended VHS models.

It may be mentioned that the broad peak in the specific heat observed for underdoped samples at a temperature higher than T_c may be a signature of formation of a spin gap in the spin excitation spectrum. Inelastic neutron scattering experiments[21,22] suggest that a spin gap develops in high-T_c oxides well above T_c. The resistivity (ρ) and susceptibility (χ) behavior of high-T_c oxide systems also indicates the formation of the spin gap.[23] The development of the spin gap suppresses the spin fluctuations and the spin fermions form singlet pair. This should be manifested in the specific heat as a peak. Within the VHS scenario similar feature in the specific heat is obtained for underdoped samples without considering any gap in the spectrum.

We have studied the effect of second-nearest-neighbor hopping and orthorhombic distortion on $\gamma(T)$ for the DOS (2) and (3) and found that $\gamma(T)$ has similar variation with temperature for all the cases.

The Knight shift may be found from the static spin susceptibility

$$\chi(q\rightarrow 0,\omega=0)=\chi_0(0,0)/[1-U\chi_0(0,0)], \tag{12}$$

where

$$\chi_0(0,0)=-\sum_k \frac{\partial f(E_k)}{\partial E_k}=\frac{1}{k_B T_c}\int_{-W}^{W} f(E)[1-f(E)]N(\epsilon)d\epsilon. \tag{13}$$

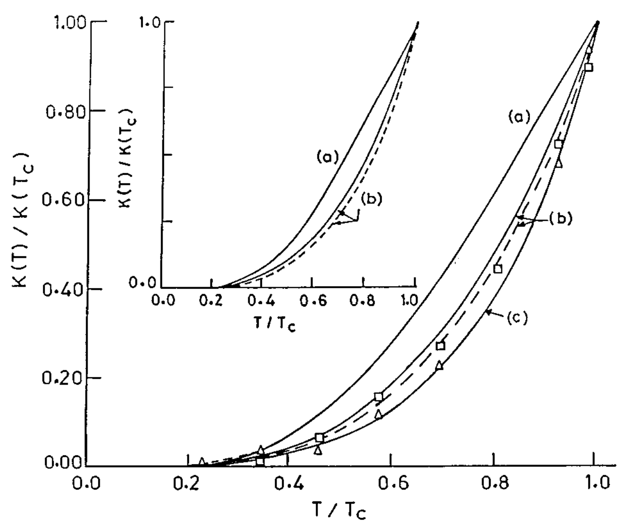

FIG. 3. Variation of $K(T)/K(T_c)$ with T/T_c. Curves (a) and (b) are for the DOS (2) and (3) ($r_1=1$ and $r_2=0$) and the curve (c) corresponds to the DOS (4). For curves (a) and (b) $t=400$ K, $v=1000$ K (solid line); $t=400$ K, $v=800$ K (dashed line); (a) $U=0$, (b) $U=2t$. Curve (c) $t=600$ K, $v=1000$ K, $\epsilon_0=500$ K, $U=1.4t$. Experimental data points on the Y-123 system: square (perpendicular), triangle (parallel) (Refs. 24 and 25). Inset curves are for the DOS (2) and (3): solid line ($t=400$ K, $v=1000$ K), dashed ($t=800$ K, $v=1600$ K). (a) $U=0$, (b) $U=2t$.

Near the transition temperature the number of thermally excited quasiparticles is large and the picture of noninteracting quasiparticles is not valid. This requires consideration of Fermi liquid correction in the superconducting state.[24] The denominator of Eq. (12) takes account of such corrections within the simple random phase approximation (RPA) scheme; U denotes the strength of the Fermi liquid correction.

Figure 3 shows the variation of $K(T)/K(T_c)$ with T/T_c for different values of v, W, and for $U=0$ and $U=2t$ for the DOS (2) and (3) and for $U=1.4t$ for the DOS (4). For the DOS (2) and (3) the Stoner enhancement factor for $U=2t$ at T_c is 1.95 for $t=400$ K and $v=800$ K, 1.80 for $t=400$ K and $v=1000$ K, and 2.1 for $t=800$ K and $v=1600$ K (for the first and third sets of parameters we obtain $T_c \sim 90$ K). For the DOS (4) the Stoner enhancement factor is 1.97 for $U=1.4t$ (for $t=600$ K, $v=1000$ K, and $\epsilon_0=500$ K). This enhancement factors are reasonable.[24] With increasing value of v the ratio $K(T)/K(T_c)$ is supressed at very low temperature. Similar observation was made by Sudbo *et al.*[24] Positive curvature in the Knight shift (Fig. 3) is enhanced considerably as the Fermi liquid correction is considered. In the intermediate-temperature range the ratio $K(T)/K(T_c)$ increases with increasing e-ph interaction strength. This result is consistent with that obtained in a previous study.[24] In the inset of Fig. 3 the effect of the change in the band width on $K(T)/K(T_c)$ for the DOS (2) and (3) is shown. The ratio remains almost unchanged for $U=0$; however, for $U=2t$, it decreases with increasing bandwidth for the intermediate temperature range. For the DOS (4) the positive curvature in the Knight shift enhances rapidly with U as the Fermi liquid correction is considered. The experimental results of the Y-123 system[25] are also shown in Fig. 3. It is seen that the theoretical predictions for the DOS (2) and (3) with $U=2t$ and for the DOS (4) with $U=1.4t$ fit reasonably with the experimental data points.

In summary we have studied the specific heat and the Knight shift within the VHS scenario and found that an extended VHS can reasonably account for some of the observed results.

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