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# Gap-to-$T_c$ Ratio as a Function of the Fermi Level Shift

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Within the framework of the BCS theory, the gap-to-$T_c$ ratio $R = 2\Delta_0/kT_c$ is evaluated numerically ($\Delta_0$ is the energy gap at $T=0$ and $T_c$ is the critical temperature) for a superconductor with a van Hove singularity (vHs) in the density of states as a function of the shifts ($\delta$) of the Fermi level with respect to the vHs. It is found that $R$ varies asymmetrically with $\delta$ and that the variations are strong near $\delta=0$. Our numerical calculation shows that the largest $R$'s occur at certain values of $\delta \neq 0$.

KEY WORDS: van Hove singularity; gap-ratio; high-$T_c$ superconductor.

The idea that the density of states (DOS) peaks is important for superconductivity was first considered for A15 compounds [1] that show one-dimensional structures. In high-$T_c$ superconductors, the planar structure of the copper oxide layers lead to a vHs of the DOS that can be coincident or very close to the Fermi energy ($E_F$) depending on the doping.

This situation has led many authors [2–8] to consider the possible effect of the logarithmic DOS peak in superconductivity. Tsuei *et al.* [2] showed that there exists a vHs near $E_F$ in $YBa_2Cu_3O_7$. The angle photoemission spectroscopy studies on Y123, Y124, and Bi2122 [3–5] have found that the vHs is almost located at the Fermi level at the composition of optimum $T_c$. It was shown in [6] that a maximum $T_c$ with a minimum isotope shift exponent ($\alpha$) occur when the Fermi level lies at the energy of the vHs and $T_c$ decreases while ($\alpha$) increases as the Fermi level is displaced from the vHs. Sarkar and Das [7] studied the variations of $T_c$, $\alpha$, and the pressure coefficient of $T_c$ with the shift ($\delta$) of the Fermi level from the vHs. They also examined the gap-to-$T_c$ ratio ($R$) for the case $\delta=0$, and found that $R$ lies within the range from 3.53 to 4.00. The question arises if there is a possibility to enhance the gap ratio taking into account a nonzero shift of the Fermi level from the vHs.

The purpose of this paper is to extend the study of [7] by evaluating the exact $R$ (numerical) as a function of $\delta$ for different sets of parameters. In particular, we would like to examine the change in $R$ as the shift $\delta$ is varied.

We compute the zero-temperature gap $\Delta_0$ in the framework of the standard BCS mean field formalism

$$\frac{2}{V} = \int_{-\omega_D}^{\omega_D} d\varepsilon \, \frac{N(\varepsilon)}{\sqrt{\varepsilon^2 + \Delta_0^2}} \tag{1}$$

where $N(\varepsilon)$ is the density of states, $\omega_D$ is a cutoff frequency, and $V$ is a constant pairing potential, nonzero only within a range $2\omega_D$ centered about the Fermi level.

The linearized $T_c$ equation can be written as

$$\frac{2}{V} = \int_{-\omega_D}^{\omega_D} d\varepsilon \, \frac{N(\varepsilon)}{\varepsilon} \tanh\left(\frac{\varepsilon}{2T_c}\right) \tag{2}$$

We use the $2D$ vHs form for the DOS [7],

$$N(\varepsilon) = N_0 \ln\left|\frac{E_F - \delta}{\varepsilon - (E_F - \delta)}\right| \tag{3}$$

where $N_0$ is a normalization factor, and $\delta = E_F - E_{vHs}$ indicates the displacement of the Fermi level with respect to the vHs ($E_{vHs}$). This form of DOS is relevant in high-$T_c$ cuprates because the Fermi level shifts with doping, and $\delta$ changes correspondingly.

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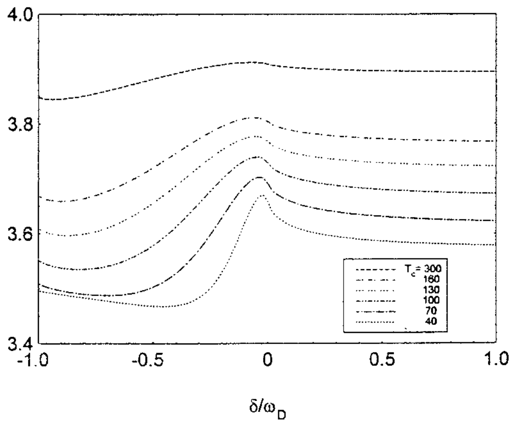


**Fig. 1.** The ratio $R$ for different choices of the parameter $T_c$, as a function of $\delta/\omega_D$. $E_F = 4000$ K, $\omega_D = 500$ K.

We introduce Eq. (3) into Eqs. (1) and (2), and obtain the following equation:

$$\int_0^{\omega_D} \frac{dx}{x} \tanh(x) \ln\left|\frac{E_F - \delta}{2T_c x + \delta}\right| = \int_0^{2\omega_D/RT_c} \frac{dx}{\sqrt{1+x^2}} \ln\left|\frac{E_F - \delta}{RT_c x/2 + \delta}\right| \tag{4}$$

From this integral equation the numerical values of $R$ have been evaluated exactly as a function of the parameter $\delta/\omega_D$ for various values of $T_c$. We have performed the calculation for the same parameters as that of Sarkar and Das [7], namely $E_F = 4000$ K and $\omega_D = 500$ K.

We can see from the graph $R$ vs. $\delta/\omega_D$ (Fig. 1) that there is a large departure of $R$ from the canonical BCS value of 3.53 as $\delta$ varies. The shift $\delta$, therefore, has a strong influence on $R$. The plot shows that the variation of $R$ is not symmetric about $\delta = 0$; $(d/d\delta)R$ is positive for underdoped samples and changes signs for the overdoped cases. The general trend is that $R$ decreases for $\delta > 0$ more rapidly than for $\delta < 0$. We note also that as $E_F$ is displaced away from vHs, i.e., $|\delta|$ increases, $R$ decreases, and the value of $R$ always increases as $\omega_D/T_c$ decreases. Moreover, as $\omega_D/T_c$ increases, $R$ is suppressed and goes to the BCS limit of 3.53.

Our numerical calculation shows also that there is a maximum value of $R$ occurring at a certain nonzero value of $\delta/\omega_D$. To find the value of $\delta/\omega_D$ where $R_{\max}$ occurs, we differentiate Eq. (4) with respect to $\delta/\omega_D$ and set $dR/d(\delta/\omega_D)$ equal to zero, and we arrive at the following equation:

$$\int_0^{\omega_D/2T_c} \frac{dx}{x} \tanh x \frac{(2T_c x + E_F)}{(2T_c x + \delta)} = \int_0^{2\omega_D/RT_c} \frac{dx}{\sqrt{1+x^2}} + \left(\frac{E_F}{\omega_D} - \frac{\delta}{\omega_D}\right) \times \int_0^{2\omega_D/RT_c} \frac{dx}{\sqrt{1+x^2}\,(RT_c x/2\omega_D + \delta/\omega_D)} \tag{5}$$

We evaluate $R_{\max}$ and $\delta/\omega_D$ numerically using the two integral equations (4) and (5). To do that we have to choose three parameters: $T_c$ and the Fermi and cutoff energies. The numerical results are presented in Table I.

We note that the peak position in $R$ shifts to the underdoped region with increasing $T_c$.

In summary, based on the BCS theory, we have studied the effects of the Fermi level shift with respect to the vHs on the gap-to-$T_c$ ratio. The general behavior of $R$ is that it is largest at some optimum doping, $\delta \neq 0$. We show that there is an asymmetric gap ratio in doped superconductors.

Recently Giraldo and Baquero [9] evaluated the van Hove singularity shift from the Fermi level as a function of composition and found an approximately linear behavior as a function of doping. It is therefore of interest to investigate experimentally the gap-to-$T_c$ ratio as a function of the doping concentration as a quantitative check of our theory.

**Table I.** Value of $R$ Estimates for a DOS with a vHs for Different $T_c$ Values, and $\delta/\omega_D$ Where $R_{\max}$ Occurs ($E_F = 4000$ K and $\omega_D = 500$ K)

| $T_c$ (K) | $R_{\max}$ | $\delta/\omega_D$ |
|---|---|---|
| 300 | 3.912 | −0.073 |
| 160 | 3.811 | −0.059 |
| 130 | 3.777 | −0.055 |
| 100 | 3.740 | −0.043 |
| 70 | 3.703 | −0.035 |
| 40 | 3.671 | −0.021 |

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