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Reduced-Gap Ratio of High-T_c Cuprates Within the *d*-Wave Two-Dimensional Van Hove Scenario

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The gap-to-T_c ratio (R) of high-temperature superconductors is calculated in the context of d symmetry of the superconducting order parameter and a two-dimensional Van Hove singularity in the density of states, using the BCS theory for weak coupling. Exact numerical calculation and an analytic formula for R are given. The ratios are found to be substantially larger than the BCS weak coupling limit of 3.53. The overall dependence of R on ω_D/T_c, where ω_D is the cutoff frequency, is given.

KEY WORDS: BCS; gap-to-T_c ratio; *d*-wave superconductors; Van Hove singularity.

The gap-to-T_c ratio is an important parameter that can be used to investigate the nature of phase transition, and the symmetry of the pairing state [1]. In BCS theory the ratio $R=2\Delta(0)/T_c$ is a constant quantity and equal to 3.53, where $\Delta(0)$ is the value of the order parameter at zero temperature. But in high-temperature cuprate superconductors, this ratio has been found to be greater than the BCS value [2]. Recently the explanation of this discrepancy has been attributed to the *d*-wave symmetry of the order parameter [3], and calculations based on the BCS approach with a constant density of states showed that the ratio R for the d wave is 4.28, which is larger than 3.53 for the s wave.

There is now much direct evidence, from high-resolution angle-resolved photoemission (ARPES) measurements [4] and band structure calculations [5], that most of the high-T_c cuprates have *d*-wave pairing symmetry [6], and that these cuprates have a quasi-2D electronic dispersion structure with a logarithmic Van Hove singularity in the normal-state density of states. It is therefore natural to consider whether the combination of *d*-wave symmetry of the gap parameter and Van Hove singularity can explain the large increase in R over its BCS value.

The main purpose of this paper is to perform a numerical computation for R as a function of ω_D/T_c, where ω_D is the cutoff energy in the BCS theory. In this investigation we assume that the pairing is of d symmetry, and the effect of the Van Hove singularity in the density of states is also taken into consideration. An analytic expression for R within the BCS approach will also be derived.

We begin with the linearized BCS gap equation

$$\Delta_{\vec{k}}(T)=\sum_{\vec{k}'}\frac{V_{\vec{k}\vec{k}'}\Delta_{\vec{k}'}}{2\sqrt{(\varepsilon_{\vec{k}'}-E_F)^2+\Delta_{\vec{k}'}^2}}\times\tanh\frac{\sqrt{(\varepsilon_{\vec{k}'}-E_F)^2+\Delta_{\vec{k}'}^2}}{2T} \qquad (1)$$

where $\Delta_{\vec{k}}$ is the BCS gap parameter, T is the temperature, $V_{k\vec{k}'}=V_d\cos 2\phi\cos 2\phi'$ for $|\varepsilon_k-E_F|\le\hbar\omega_D$, and $V_{\vec{k}\vec{k}'}=0$ otherwise; here V_d is a constant pairing potential within the energy range around the Fermi energy E_F. The angle ϕ is defined in our two-dimensional model as $\phi=\tan^{-1}(k_y/k_x)$.

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For this particular form of the scattering matrix, the d-wave order parameter takes the form

$$\Delta_{\vec{k}}(T)=\Delta_d(T)\cos 2\phi \tag{2}$$

and for the high-T_c cuprates, it is justified to use the 2D tight binding dispersion to model the Cu–O square lattice where the pairing interaction is located [4–6]. The presence of saddle points in the Brillouin zone gives rise to a logarithmic singularity near the Fermi level of the form

$$N(\varepsilon_{\vec{k}})=N_0 \ln\left|\frac{E_F}{\varepsilon_{\vec{k}}-E_F}\right| \tag{3}$$

Here N_0 is a constant. Upon substituting Eqs. (2) and (3) in Eq. (1), one obtains the following equation:

$$\frac{1}{N_0V_d}=\int_{-\omega_D}^{\omega_D} d\varepsilon \int_0^{2\pi}\frac{d\phi}{2\pi}\frac{\cos^2 2\phi \ln|E_F/\varepsilon|}{2\sqrt{\varepsilon^2+\Delta_d^2(T)\cos^2 2\phi}} \times \tanh\left(\frac{\sqrt{\varepsilon^2+\Delta_d^2(T)\cos^2 2\phi}}{2T}\right) \tag{4}$$

When $T=T_c$, $\Delta_d(T_c)=0$, Eq. (4) is reduced to

$$\frac{1}{N_0V_d}=\int_0^{\omega_D}\frac{d\varepsilon}{\varepsilon}\int_0^{\pi}\frac{d\theta}{\pi}\cos^2\theta \ln\left(\frac{E_F}{\varepsilon}\right)\tanh\left(\frac{\varepsilon}{2T_c}\right) =\frac{1}{2}\int_0^{\omega_D/2T_c}\frac{dx}{x}\ln\left(\frac{E_F}{2T_c x}\right)\tanh x \tag{5}$$

Now, when $T=0$, $\Delta_d(T)$ becomes $\Delta_d(0)$, and we have

$$\frac{1}{N_0V_d}=\int_0^{\omega_D} d\varepsilon \frac{\ln|E_F/\varepsilon|}{\sqrt{\varepsilon^2+\Delta_d^2(0)\cos^2\theta}} \times \int_0^{\pi} d\theta \frac{\cos^2\theta}{\pi} \tag{6}$$

Replacing $\Delta_d(0)$ by $RT_c/2$ in Eq. (6), one finds

$$\frac{1}{N_0V_d}=\int_0^{\pi}\frac{d\theta}{\pi}\cos^2\theta \times\left\{K\ln\left(\frac{4E_F}{RT_c|\cos\theta|}\right)-\frac{1}{2}Li_2(e^{-2K})-\frac{K^2}{2}+\frac{\pi^2}{12}\right\} \tag{7}$$

where $K=\sinh^{-1}(2\omega_D/T_c/R|\cos\theta|)$ and $Li_2(x)=\sum_{k=1}^{\infty} x^k/k^2$ is Euler's dilogarithmic function [7].

Combining Eqs. (5) and (7), we obtain the exact integral equation for R within the BCS scheme as

$$\int_0^{\omega_D/2T_c} dx\frac{\tanh x}{x}\ln\left(\frac{E_F}{2T_c x}\right) =\frac{2}{\pi}\int_0^{\pi} d\theta\cos^2\theta \times\left\{\sinh^{-1}\left(\frac{2\omega_D/T_c}{R|\cos\theta|}\right)\ln\left(\frac{4E_F}{RT_c|\cos\theta|}\right) -\frac{1}{2}Li_2\left(\exp\left[-2\sinh^{-1}\left(\frac{2\omega_D/T_c}{R|\cos\theta|}\right)\right]\right) -\frac{1}{2}\left(\sinh^{-1}\left(\frac{2\omega_D/T_c}{R|\cos\theta|}\right)\right)^2+\frac{\pi^2}{12}\right\} \tag{8}$$

We compute R numerically and plot it as a function of ω_D/T_c for value of $E_F/\omega_D=20$. On the same graph, we also plot R for the s wave, using the same set of parameters [8]. From Fig. 1 we can see that for given ω_D/T_c the d-wave case yields R values larger than the s-wave results of [8].

Since one can typically expect the ratio $\omega_D/T_c>1$, the expansion

$$\sinh^{-1}x=\ln|2x| + \sum_{k=1}^{\infty}\frac{(-1)^{k+1}(2k)!}{2^{2k}(k!)^2 2k x^{2k}} \quad (x\geq 1) \tag{9}$$

may be employed in the integral term on the right-hand side of Eq. (8); for the same reason that

Fig. 1. Variation of reduced gap-to-T_c ratio $R=2\Delta_d(0)/T_c$ with ω_D/T_c for d-wave pairing. Curves 1 and 2 correspond to exact R and approximate R as calculated from Eqs. (8) and (12), respectively. We also show, for comparison, curve 3 which corresponds to the s-wave case. Here we have used $E_F/\omega_D=20$.

$\omega_D/T_c > 1$, we neglect the Li_2 term in the integral because $\lim_{x\to 0} Li_2(x) = 0$. Using the expansion

$$\frac{1}{y}\tanh y = 2\sum_{n=0}^{\infty}\frac{1}{y^2+[\pi(n+\frac{1}{2})]^2} \tag{10}$$

and straightforward integration, we obtain, after lengthy algebra, the following result:

$$\begin{aligned}
&\frac{1}{2}\left[\frac{\pi^2}{4}-\frac{3}{4}-\ln^2\left(\frac{E_F}{\omega_D}\right)+\ln^2\left(\frac{8E_F}{\sqrt{e}RT_c}\right)\right] \\
&+\frac{1}{2}\ln\left(\frac{E_F}{\omega_D}\right)\sum_{k=1}^{\infty}\frac{(-1)^{k+1}(2k+2)!\,(2k)!}{(2k)[k!\,(k+1)!]^2}\left(\frac{RT_c}{8\omega_D}\right)^{2k} \\
&-\frac{1}{4}\sum_{k=1}^{\infty}\frac{(2k+2)!}{[k(k+1)!]^2}\left[\frac{RT_c}{8\omega_D}\right]^{2k} \\
&-\frac{1}{4}\sum_{k=1}^{\infty}\sum_{p=1}^{\infty}\frac{(-1)^{p+k}(2k)!\,(2p)!}{(2k)(2p)} \\
&\times\frac{(2p+2k+2)!}{[k!\,p!\,(p+k+1)!]^2}\left(\frac{RT_c}{8\omega_D}\right)^{2(p+k)} \\
&=\sum_{n=0}^{\infty}\frac{4}{\pi(n+1)}\left\{\ln\left(\frac{E_F}{\omega_D}\right)\tan^{-1}\left(\frac{\omega_D}{(2n+1)\pi T_c}\right)\right. \\
&+\frac{\pi}{2}\ln\left(\frac{\omega_D}{(2n+1)\pi T_c}\right) \\
&\left.+\sum_{k=0}^{\infty}\frac{(-1)^k}{(2k+1)^2}\left(\frac{(2n+1)\pi T_c}{\omega_D}\right)^{2k+1}\right\}
\end{aligned} \tag{11}$$

To obtain an explicit expression for R, we neglected all terms of order $(RT_c/\omega_D)^n$ for any n, except the logarithmic term in Eq. (11), and solving for R by exponentiation gives the approximate expression

$$R \cong \frac{8E_F}{\sqrt{e}T_c}\exp\left\{-\sqrt{\frac{11-\pi^2}{4}-\ln^2\left(\frac{4e^\gamma}{\pi}\right)+\ln^2\left(\frac{2e^\gamma E_F}{\pi T_c}\right)}\right\}$$

Here e^γ is Euler's constant. In the limit $E_F/T_c \to \infty$, we find that Eq. (12) gives $R = 8E_F/\sqrt{e}T_c \times \pi T_c/2e^\gamma E_F = 4.28$, as obtained in [3], where the condition $\omega_D/T_c \gg 1$ was considered. We note that our approximate formula for R for the d-wave superconductor depends only on the ratio E_F/T_c.

In order to test the validity of our expression for R, we compute R from Eq. (12) and compare the values obtained with those obtained by direct computation of Eq. (8). We can see from the graph that the agreement between the exact result and the value computed by using Eq. (12) tends to improve as the ratio ω_D/T_c increase, and when $\omega_D/T_c > 20$, our approximate analytic formula gives R values almost identical to those obtained by direct computation.

It is readily seen from Fig. 1 that, in spite of not making any weak coupling approximation $N_0 V_d \ll 1$, the energy gap in terms of $2\Delta_d(0)/T_c$ is still significantly enhanced from its BCS value, 3.53. The maximal value of R is ~ 5 when $\omega_D/T_c \to 0$, and the minimal value is predicted to be 4.3 in the limit $\omega_D/T_c \to \infty$. Hence our theory yields R values within the range of the conventional strong coupling value of 4–5. The explanation for the "large" values of R is that, in this model, the expression for R [Eq. (12)] has the prefactor for $\Delta_d(0)$ which is an electronic energy rather than the usual Debye frequency.

As is obvious from the graph where three curves are given for comparison, we can see that for both s- and d-pairing symmetries, R always decreases with the increase of ω_D/T_c, and that for $\omega_D/T_c > 20$, R does not change appreciably. We observe that the exact R as determined from Eq. (11) is slightly larger than the approximate R as given by Eq. (12) for the same parameter space. The difference is, however, only about 0.2% when $\omega_D/T_c > 10$. Here we have used the parameter $E_F/\omega_D = 20$, for this value is consistent with our previous study [18] where we calculated R for the s-wave Van Hove superconductors.

Recently Wei *et al.* [9] showed that for optimally doped Hg-1201, Hg-1212, and Hg-1223, the corresponding maximum reduced gap ratios are 7.9, 9.5, and 13, respectively. A comparison of these figures with our graphical solution in Fig. 1 indicates that there are still large discrepancies between our predictions and the experiments. Hence the BCS formalism of the d-wave two-dimensional Van Hove scenario does not explain the observed data. Larger values for this ratio may be produced by the unconventional strong coupling theory of Eliashberg.

To summarize the present work, we have studied the effect of Van Hove singularity in the density of states on the gap-to-T_c ratio for d-wave pairing symmetry within the BCS scheme. We have derived an integral equation and found a general expression for the ratio. From our study it is revealed that the variation of R with ω_D/T_c is moderated considerably by the d-wave pairing as compared to the s-wave symmetry [8], for the same material parameters. Yet the maximum value of R is much lower than some experimental results [9].

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