Dependence of the critical temperature and energy gap of superconductors on a singularity in the density of states

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It is shown how the critical temperature and zero-temperature energy gap decrease by shifting the position of the singularity in the density of states (DOS) with respect to the Fermi energy. The enhancement of the critical temperature due to the singularity (compared with the constant DOS near the Fermi surface) is not as large for strong-coupling superconductors as in the weak-coupling limit. Hence, the singularity in the DOS cannot be the exclusive reason for large values of critical temperatures in high-T_c superconductors.

The most important parameters calculated from the microscopic BCS theory[1] are the energy gap Δ (and its temperature dependence), the critical temperature T_c, and the ratio $R=2\Delta(T=0)/kT_c$. The originally assumed constant density of states (DOS) was already abandoned for some classical superconductors, knowing that the enhanced DOS at or near the Fermi surface can lead to higher values of T_c. For high-T_c superconductors, this effect was even supposed to be responsible for the very large measured values of R (up to about 20, compared with the BCS weak-coupling value 3.53). As shown by Mattis and Molena[2] for the power-law-like singularities and supported by the δ-function singularities,[3] the value of R cannot be greater than 4 in the weak-coupling limit. Therefore, the singularities in DOS cannot explain those experimental results giving higher R values.

In this report, we extend our calculations with δ-function-like singularities to the dependence of the critical temperature and the energy gap on the position of singularity with respect to the Fermi energy. A brief consideration concerning the absolute value of T_c for superconductors with singular DOS is added.

As the highest critical temperatures seem to occur on one side or the other of a van Hove singularity, both symmetric and asymmetric peaks in DOS should be assumed. The use of a δ-function-type singularity in DOS is well justified for many reasons, although it is evidently far from the realistic form. At first, the calculations are extremely simplified (transcendental equations result instead of integral ones). Further, this type of singularity can be considered as the most extreme type of singular DOS. Last but not least, one can construct any form of DOS by the sum of δ functions with different weight factors (in fact, the DOS is defined originally as the sum of δ functions).

As previously,[3] we start with one δ-functional peak in DOS,

$$N(E)=A\delta(E)\ , \tag{1}$$

where $A=$const. The corresponding determining equations for $t=T_c(E)/T_{c0}$ and $d=\Delta_0(E)/\Delta_{00}$ with dependence on the relative position of the singularity $y=E/2kT_{co}=E/\Delta_{00}$ [because $\Delta_{00}/2kT_{c0}=\Delta_0(E=0)/2kT_c(E=0)=1$ corresponds to the result[3] $R_0=\Delta_{00}/2kT_{c0}=4$] are then given by

$$t=y/\tanh^{-1}y\ , \tag{2}$$

$$d=(1-y^2)^{-1/2}\ . \tag{3}$$

The results are given in Fig. 1.

The temperature dependence of the gap in the form

$$\Delta(T)/\Delta_0=\tanh[T_c\Delta(T)/T\Delta_0] \tag{4}$$

derived by Thouless[4] in the strong-coupling limit, is of the same form as the dependence of the off-symmetry on the corresponding critical temperature.

As already mentioned, the singular behavior of the DOS was believed to increase T_c compared with the constant DOS close to the Fermi surface treated in the original BCS theory. Different types of singularities (e.g., the logarithmic one for van Hove singularities[5]) were extensively treated, often with extreme difficulties.[6] Our approach can also be used favorably for treating this problem. Again, the δ-function-type singularity should be considered as the extreme case, giving the limiting values for T_c for a very strong singularity near the Fermi surface.

We compare the situation of constant DOS $N(0)$ from the region $\hbar\omega_0$, in which the attractive interaction of Cooper pairs is assumed (ω_0 is of the order of Debye frequency[1]), to be "compressed" to the Fermi energy. To extend the calculations to the stronger coupling, the most simple procedure is to renormalize the coupling constant $\tau=N(0)V$ in the form $\tau^*=\tau/(1+\tau)$.[7,8] This enables us to include all principle results of strong-coupling without going into details of the phonon spectrum and the Coulomb interaction.

The initial critical temperature for constant DOS is then

$$kT_{c,\mathrm{BCS}}=1.14\hbar\omega_0\exp(-1/\tau)\ , \tag{5}$$

$$kT_{c,McM}=1.14\hbar\omega_0\exp[-(1+\tau)/\tau]\ . \tag{6}$$

Assuming the same value for the constant interaction po-

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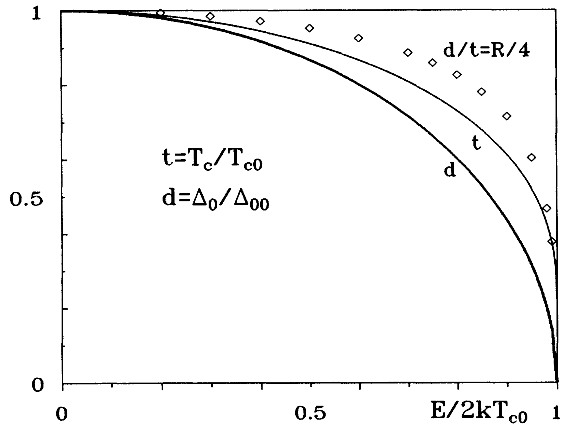

FIG. 1. The reduced critical temperature $t=T_c/T_{c0}$ (1), the reduced zero-temperature energy gap $d=\Delta_0/\Delta_{00}$ (2), and their ratio $R/4$ (3) with dependence on the off-symmetric position of the singularity in DOS, $E/2kT_{c0}$.

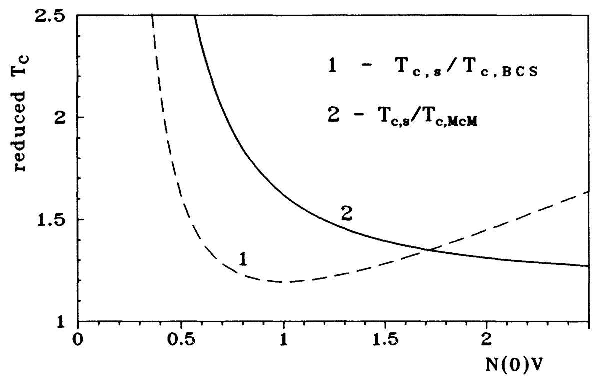

FIG. 2. The reduced critical temperature for singular DOS compared with T_c obtained from constant DOS in the BCS weak-coupling limit (dashed line) and in the modified case for the strong-coupling electron-phonon interaction (full line) with dependence on the coupling strength $N(0)V$.

tential V, we obtain for the singular DOS the equation

$$1=V\int_0^\infty \frac{d\sigma}{\sigma}N_0\delta(\sigma)\tanh\frac{\sigma}{2kT_c}=\frac{VN_0}{2kT_c}\ , \tag{7}$$

with $N_0=N(0)\hbar\omega_0$. This leads to (label s means singular)

$$T_{c,s}/T_{c,BCS}=(\tau/2.28)\exp(t/\tau)\ , \tag{8}$$

$$T_{c,s}/T_{c,McM}=(\tau^*/2.28)\exp(1/\tau^*)\ . \tag{9}$$

Both functions are given in Fig. 2 with dependence on the coupling strength τ.

The strong increase of T_c for singular DOS in the weak-coupling limit was realized earlier (see, e.g., Ref. 9). The calculated results for the van Hove singularity in the region $\tau=0.081\div0.12$ (Ref. 10) are in very good agreement with our weak-coupling results (dashed line in Fig. 2).

We would like to emphasize, however, that this increase is much smaller for stronger coupling (Fig. 2, full line). The explanation of this effect is as follows. As can be seen from Fig. 1, the singularity in DOS contributes to T_c nearly equally for $E\lesssim0.8kT_c\approx0.4\tau\hbar\omega_0/(1+\tau)$. This region is very narrow in the weak-coupling limit ($\tau\ll1$), whereas it is comparable with $\hbar\omega_0$ in the strong-coupling case. The immediate consequence is that T_c does not change very much by pressing the states closer to the Fermi energy.

Therefore, for high-T_c superconductors with supposed values of $\tau\approx1$, the enhanced DOS cannot be the exclusive reason for much higher critical temperatures compared with classical superconducting materials.

Another effect enhancing T_c could be the higher *total* DOS determining the pairing interaction. Then, the real bandwidth would not be determined by the characteristic phonon frequency ω_0, but by other parameters such as the Fermi energy (e.g., for the excitonic or plasmonic pairing mechanisms).

In conclusion, we have calculated the dependence of the critical temperature and the zero-temperature energy gap on the position of the singularity in DOS (with respect to the Fermi energy) in the weak-coupling limit. Enhanced attention should be paid to the elaboration of the procedure to include the singularities in the strong-coupling case more precisely. However, we believe that the full curve of Fig. 2 is qualitatively correct, at least for the phonon-mediated mechanism of superconductivity. Nevertheless, it is not excluded that the increase of T_c due to the singular behavior of the DOS for other pairing mechanisms can be as strong as in the case of weak-coupling electron-phonon mechanism.

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