High-temperature superconductivity in the Van Hove scenario

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(Received 7 September 1993)

The influence of a logarithmic Van Hove singularity in the electronic density of states is studied in the framework of the BCS theory. We use a simplified model, neglecting effects such as interlayer coupling and pair breaking. Through analytic and numerical analyses it is found that although the model can give rise to high temperatures, there are other properties, such as the isotope effect and specific-heat jump at the transition temperature, which cannot be explained properly with this model, as recent experimental data in the high-T_c oxides show.

I. INTRODUCTION

It is well known that the quasi-two-dimensionality of the CuO planes in high-temperature superconductors gives rise to logarithmic Van Hove singularities (VHS's) in the electronic density of states (DOS). In recent publications[1–4] it has been shown that the incorporation of a VHS to the otherwise standard BCS theory leads to quantitatively different results from those obtained using a constant DOS. Moreover, this VHS model can presumably explain some important features in the high-T_c oxides, such as high critical temperatures, variation of the isotope effect with doping, etc. This proposal has not been widely accepted for several reasons, including the fact that a sharp peak in the DOS can be easily smeared out by three-dimensional (3D) effects such as interlayer hopping, etc., and also the effectiveness of the VHS depends on the fact that it must be placed very close to or at the Fermi level. In such a case, nesting of the Fermi surface is likely to occur, which in turn may give rise to charge- or spin-density waves, which compete with the superconducting state. However, Tsuei *et al.*[5] have given recent thermodynamic data that appear to support the existence of a VHS near ϵ_F in $YBa_2Cu_3O_7$. The dependence of the critical temperature on applied hydrostatic pressure can also be described using the Van Hove scenario,[6] and calculations of the electronic structure and Fermi surface of the new superconductor $HgBa_2CuO_{4+\delta}$ (Ref. 7) provide support for a VHS excitonic pairing mechanism in the new high-T_c oxides.

We believe this is a problem that deserves careful investigation. In this paper we show calculations for the critical temperature, isotope effect exponent, and energy gap, as well as thermodynamic properties for a BCS superconductor with a VHS in the DOS. Recent experimental results on the isotope effect in the high- T_c cuprates will be used to compare with predictions of the Van Hove model. The specific-heat jump is examined in the light of the available data, and the role of a VHS on the behavior of universal BCS ratios such as $2\Delta/k_BT_c$ and $\Delta C(T)/\gamma T_c$ is also discussed. In Sec. II we calculate, analytically and numerically, the critical temperature, zero-temperature energy gap Δ_0, isotope effect exponent β, and ratio $R_1 = 2\Delta/k_BT_c$ for a VHS as a function of its offset from the Fermi energy ϵ_F. We show that, despite the high T_c's that can be obtained, the Van Hove model does not provide an adequate explanation for the small values of β and large ratios R_1 found experimentally. Section III includes calculations of the specific-heat difference between normal and superconducting states, ΔC at $T = T_c$, the normal specific heat $C_N(T)$, and the ratios $R_2 = \Delta C(T_c)/\gamma T_c$ and $R_3 = \gamma T_c^2/H_c^2(0)$. We show that the calculated position of the node in $\Delta C(T)$ and the slope of this curve near T_c are not confirmed by experiments in the high-T_c oxides. Finally, some conclusions are drawn in Sec. IV.

II. CRITICAL TEMPERATURE AND ISOTOPE EFFECT

For the sake of simplicity, but keeping the minimum essential features, we shall use the following 2D-VHS form for the DOS:

$$N(\epsilon) = N_0\left[\ln\left|\frac{\epsilon_F}{\epsilon+\delta}\right| + C\right] , \tag{1}$$

where ϵ is the energy, referred to the Fermi level ϵ_F, N_0 is a normalization factor, and δ is the so-called filling factor, which sets the position of the singularity with respect to the Fermi energy. The constant term N_0C is the background DOS, which must be included, according to tight-binding calculations for a 2D lattice, including nearest- and next-nearest neighbors.[8] Here we shall primarily be concerned with small values of δ since it is presumably close to or at ϵ_F where a VHS is most effective.

Now, from the linearized BCS equation[9]

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

for a cutoff frequency ω_D, a constant pairing potential V, and introducing Eq. (1) for $N(\epsilon)$, one finds[4]

$$k_BT_c = 1.36\epsilon_F \exp\left\{C - \sqrt{\frac{2}{N_0V} + \left[\ln\left(\frac{\epsilon_F}{\omega_D}\right) + C\right]^2 + \frac{\delta^2}{2}\left[\frac{1}{(2k_BT_c)^2} + \frac{1}{\omega_D^2}\right] - 1}\right\} , \tag{3}$$

which provides significantly larger values for T_c than the standard BCS formula. Equation (3) shows that T_c is maximum when $\delta=0$, i.e., when the VHS is placed at the Fermi energy. An estimate of T_c using Eq. (3) and the classic BCS formula, $k_BT_c = 1.13\omega_D \exp[-1/N(\epsilon_F)V]$, shows that $T_c^{\rm VHS}$ is at least three orders of magnitude larger than $T_c^{\rm BCS}$.

The zero-temperature BCS gap equation is[9]

$$\frac{2}{V} = \int_{-\omega_D}^{\omega_D} N(\epsilon)\frac{d\epsilon}{\sqrt{\epsilon^2+\Delta_0^2}} , \tag{4}$$

where Δ_0 is the energy gap at $T=0$. Using the VHS model for the DOS, and for small values of Δ_0, one finds the approximate solution

$$\Delta_0 = 2.39\epsilon_F \exp\left\{C - \sqrt{\frac{2}{N_0V} + \left[\ln\left(\frac{\epsilon_F}{\omega_D}\right) + C\right]^2 + \frac{\delta^2}{2}\left[\frac{1}{\omega_D^2} + \frac{1}{\Delta_0^2}\right] - 1}\right\} , \tag{5}$$

which has the same dependence on N_0V, ω_D, ϵ_F, and δ as does the T_c equation [see Eq. (3)], just as occurs in standard BCS theory. Again, Eq. (5) provides larger values for Δ_0 than its BCS counterpart, due to the larger energy scale of the prefactor ϵ_F, and the exponential argument proportional to $1/\sqrt{N_0V}$, rather than $1/N(\epsilon_F)V$.

The ratio R_1 has been calculated numerically from Eqs. (2) and (4), as a function of the parameter δ, and it is compared to its canonical BCS value $R_1=3.53$, in Fig. 1. It is interesting to observe that the introduction of a VHS in the DOS does not change the BCS value of R_1 more than 3% or 4%, unless unphysical values for the parameters are used. The constant background in the DOS, N_0C, changes only the slope of the curves but not their magnitude; also, as the VHS is displaced away from ϵ_F, R_1 goes to the BCS limit. This behavior is qualitatively the same found when using other energy-dependent DOS.[10] In particular, for the choice of parameters $\epsilon_F=500$ meV, $\omega_D=65$ meV, $\delta=0$, and $C=0$ (same used by Tsuei *et al.*[4]), numerical calculation yields $T_c=37.7$ K and $R_1=3.65$. Thus, the VHS model does not explain the large values of R_1 ($\sim$ 5–9) measured in several high-T_c cuprates,[11] unless the coupling constant $N_0V > 1$, which would violate a weak-coupling approximation.

Next we want to consider the isotope effect exponent β, defined as

$$\beta = -\frac{\partial \ln T_c}{\partial \ln M} = -\frac{\omega_D}{2T_c}\frac{\partial T_c}{\partial \omega_D} , \tag{6}$$

where M is the isotopic mass, and the relation $\omega_D \sim M^{-1/2}$ has been used. Thus, differentiating Eq. (2) with respect to ω_D and then performing the integration over energies yields[8]

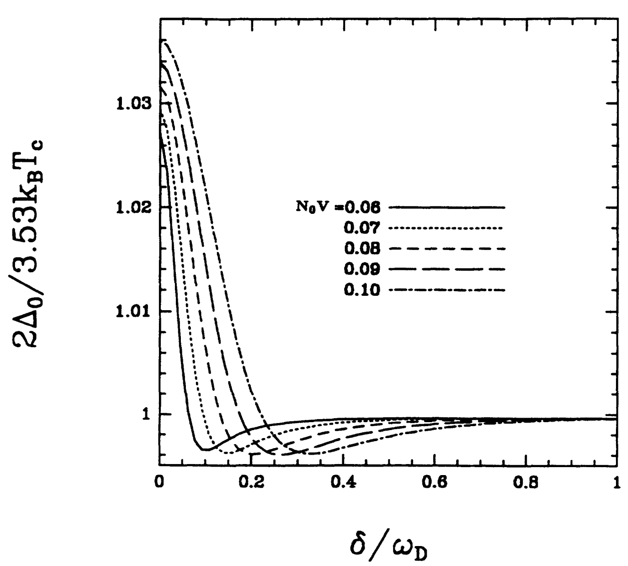

FIG. 1. The ratio $2\Delta_0/k_BT_c$, normalized to the standard BCS value 3.53, for different choices of the coupling constant N_0V, as a function of the filling factor δ, normalized to the cutoff frequency ω_D.

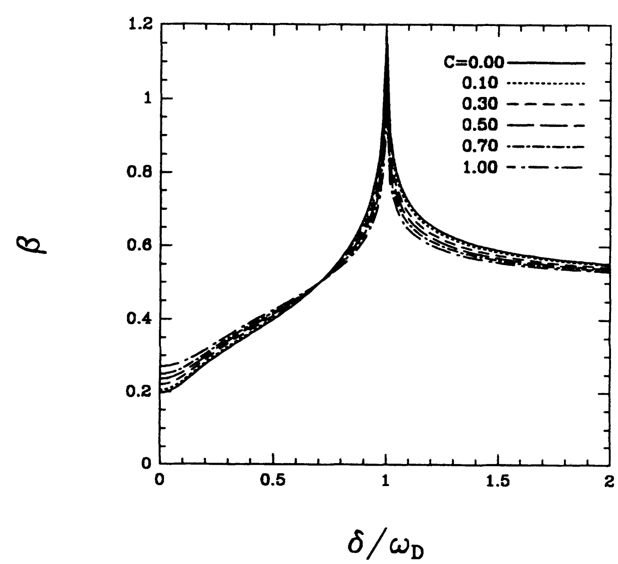

FIG. 2. Isotope effect exponent as a function of δ/ω_D for increasing values of constant C [see Eq. (1)]. Here we have used $\epsilon_F=500$ meV, $\omega_D=65$ meV, and $N_0V=0.084$.

$$\beta = \frac{1}{2}\left[\frac{\ln(\epsilon_F^2/|\omega_D^2-\delta^2|)+2C}{\ln[\epsilon_F^2/|(2k_BT_c)^2-\delta^2|]+(\delta/2k_BT_c)\ln|\frac{\delta-2k_BT_c}{\delta+2k_BT_c}|+2C+2}\right]. \quad (7)$$

A numerical calculation of β based on Eqs. (2) and (6) is shown in Fig. 2 as a function of δ/ω_D, for different values of the constant background in the DOS, N_0C. As shown by both Eq. (7) and Fig. 2, β has a minimum when T_c is maximum, i.e., at δ=0. The peak in this figure corresponds to a singularity occurring when $|\delta|=\omega_D$, as can be easily seen in Eq. (7). Note that the lowest values for β are achieved only when the background N_0C is neglected, whereas for large δ it is found that β goes to the BCS limit, β=0.5. These conclusions are in agreement with Xing *et al.*[8] Originally, Tsuei *et al.* invoked[5] a VHS to explain isotope effect measurements by Crawford *et al.*[12] on the $La_{2-x}Sr_xCuO_{4-y}$ system as a function of doping x. However, recent measurements[13] of the copper and oxygen isotope effect exponents in this system confirm that the minimum values of β ($\sim$ 0.0–0.17) are too small to be accounted for by a simple VHS approach. Experiments in other high-T_c materials seem to support this view.[14,15] The introduction of the constant background N_0C appears to have a strong influence, for it raises the minimum values of β appreciably, and it must be kept, if we want the model to be somewhat realistic. In order to make this point clearer, Fig. 3 shows β as a function of T_c for a VHS with and without the constant background, and the results are compared to recent experiments on the yttrium-based compounds. The lowest values of β remain unattainable with a VHS, and any possible agreement with the data is broken when the background DOS is not zero. Even if a strong-coupling Eliashberg formalism is used, the disagreement remains,[16] and when 3D effects are taken into account β quickly shifts to the BCS limit.[2,8] Under these circumstances, the recent experiments on the isotope effect do not appear to be explained within the context of a model involving DOS alone, even with the inclusion of a VHS.

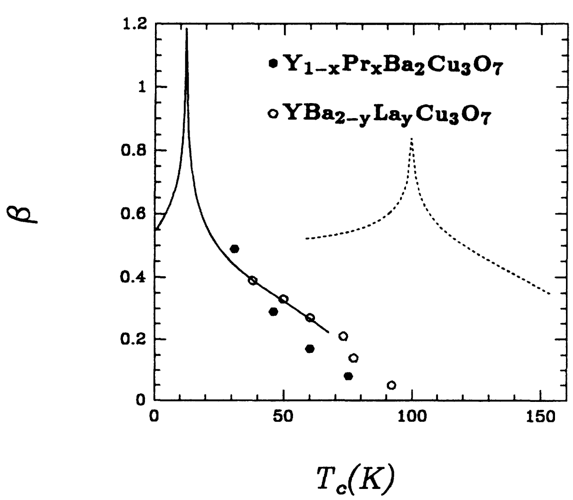

FIG. 3. Isotope effect exponent as a function of T_c. The solid line corresponds to C=0, while the dotted line is for C=2. The parameters are kept the same as in Fig. 2, except N_0V=0.11 for both curves. Experimental data are taken from Franck *et al.* (Ref. 14) (open circles) and Bornemann and Morris (Ref. 15) (solid hexagons).

III. THERMODYNAMIC PROPERTIES OF A VHS

Solving numerically the temperature-dependent BCS gap equation has revealed that the logarithmic structure in the DOS has no appreciable influence in the temperature dependence of the energy gap $\Delta(T)$; i.e., the gap behaves as a function of temperature just as if the DOS was a constant. This has been confirmed by Getino *et al.*[23] who show that the deviation of $\Delta(T)/\Delta(0)$ for a VHS in the DOS from that using a constant DOS is *at most about* 0.5%. Therefore, for the purposes of calculation of thermodynamic properties of a VHS, and to a very good approximation, we shall use here $[\Delta(T)/\Delta(0)]_{\rm VHS}=[\Delta(T)/\Delta(0)]_{\rm BCS}$. Hence, for temperatures close to T_c it is possible to show[17] that

$$\Delta^2(T)\sim(1.736)^2\left(1-\frac{T}{T_c}\right)\Delta_0^2 \quad (8)$$

and therefore

$$\left.\frac{\partial\Delta^2(T)}{\partial T}\right|_{T_c} = -k_B^2(1.736)^2(1.765)^2T_c\ , \quad (9)$$

where we have used R_1=3.53, considering that departures from this value for a VHS are negligible, as was discussed above. This result will prove useful in the calculation of the specific-heat difference at T_c, which in BCS theory is given by[9]

$$\Delta C(T_c) = -(k_BT_c)^3\int N(\epsilon)\epsilon\frac{e^{\epsilon/k_BT_c}}{(1+e^{\epsilon/k_BT_c})}\left.\frac{\partial\Delta^2(T)}{\partial T}\right|_{T_c}; \quad (10)$$

introducing Eqs. (1) and (9) in the expression above, and for δ=0, the specific-heat jump is approximately given by

$$\Delta C(T_c) = 9.38N_0k_BT_c\left\{\ln\left(\frac{\epsilon_F}{k_BT_cM}\right)+C\right\}, \quad (11)$$

with $M\equiv 0.8813$. The normal specific heat for a VHS at the Fermi energy is

$$C_N(T) = 2N_0k_B^2T\frac{\pi^2}{3}\left[\ln\left(\frac{\epsilon_F}{k_BT}\right)+C-1\right], \quad (12)$$

which shows that the normal specific-heat coefficient, commonly denoted by γ, is proportional to $\ln(1/T)$, confirming a prediction by Hirsch and Scalapino.[18] From Eqs. (11) and (12) one finds that the ratio $R_2\equiv\Delta C(T_c)/\gamma T_c$ deviates very little from its BCS universal value 1.43, for δ=0. However, when the VHS is displaced far away from ϵ_F one gets the approximate expression

$$R_2 = 1.43 \left[\frac{\ln|\epsilon_F/\delta| + \frac{\pi^2}{6}(k_B T_c/\delta)^2 + C}{\ln|\epsilon_F/\delta| - \frac{7\pi^2}{10}(k_B T_c/\delta)^2 + C} \right] \tag{13}$$

for $k_B T_c/\delta \ll 1$. In Fig. 4 this ratio is calculated numerically for five choices of the constant background in the DOS. The departures from the BCS value are reduced as the background DOS is increased, and of course, as the singularity moves off the Fermi energy. Phillips *et al.*[19] have estimated the specific-heat to T_c ratio for $YBa_2Cu_3O_{7-y}$, and report a value of 4.8. Junod *et al.*[20] find a similar estimate. These values cannot be explained with the Van Hove scenario, at least in the simple version we are presenting here, and they deserve further analysis.

The temperature dependence of the specific-heat difference, $\Delta C(T)$, is shown in Fig. 5 for a VHS at the Fermi level, one at δ=100 meV, and for a constant DOS (standard BCS case). It is found that the VHS shifts the zero in ΔC toward lower reduced temperatures, as compared with the BCS node, especially when δ=0. From Fig. 5, the change of sign in $\Delta C(T)/\Delta C(T_c)$ occurs for a VHS with δ=0 (T_c=92 K) at T/T_c=0.5, the BCS prediction is 0.55, and experiments[20] in the oxides give a value of 0.86. Indeed, Junod *et al.*[20] have measured $\Delta C(T)$ for $YBa_2(Cu_{1-x}Fe_x)_3O_{7-y}$ and have found that the peak at the critical temperature is very sharp, the node in ΔC occurs at considerably higher temperatures than for the BCS curve, and its minimum is surprisingly lower. These findings, along with other thermodynamic data,[21] are clearly inconsistent with the predictions of the Van Hove scenario. Moreover, a more detailed strong-coupling calculation for a somewhat more realistic VHS corroborates this conclusion.[22] We have also found that increasing the value of the constant background DOS does not change the position of the node in $\Delta C(T)$.

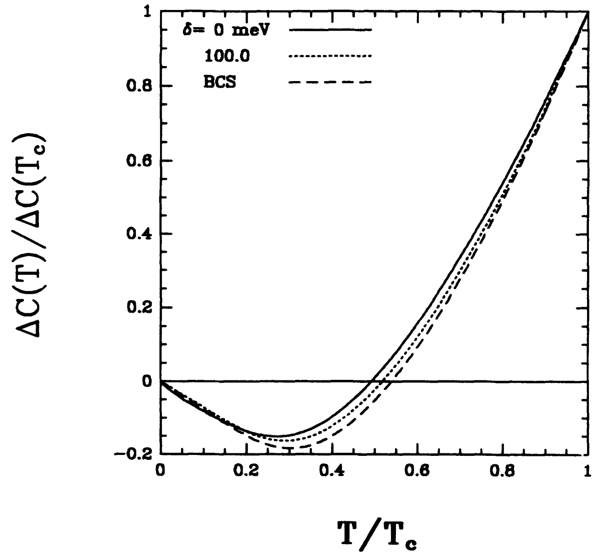

FIG. 5. Specific-heat difference $\Delta C(T)$, normalized to its value at T_c, as a function of the reduced temperature. The following values have been used: ϵ_F=500 meV, ω_D=65 meV, C=0, and N_0V=0.2.

Another universal ratio of interest in BCS theory is $R_3 \equiv \gamma T_c^2/H_c^2(0)$, where γT_c is the normal state specific heat at the critical temperature, and $H_c(0)$ is the thermodynamic critical magnetic field at zero temperature. R_3 is equal to 0.168 for a constant DOS. Starting from the zero-temperature condensation energy with a VHS, we calculate $H_c(0)$ and evaluate R_3 as a function of the filling factor δ (Fig. 6). For $k_B T_c \ll 1$, R_3 is approximately given by

$$R_3 = 0.168 \left[1 - \frac{7\pi^2}{10} \frac{(k_B T_c/\delta)^2}{\ln|\epsilon_F/\delta| + C} \right] , \tag{14}$$

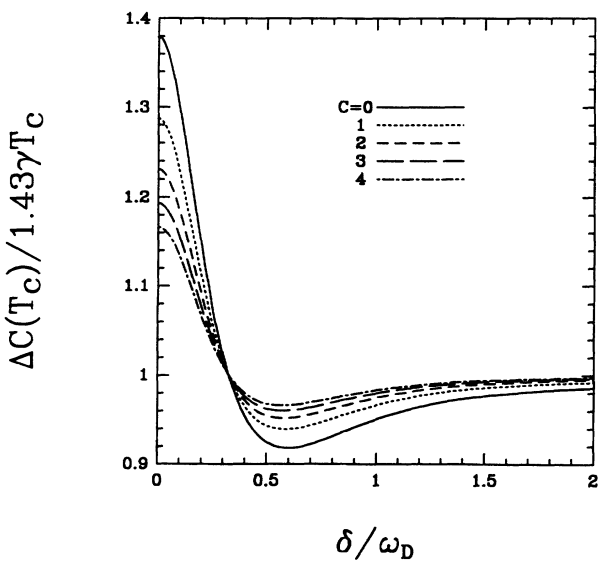

FIG. 4. Specific-heat jump to T_c ratio normalized to the BCS value 1.43, as a function of the filling factor δ. For the calculations, the following parameters were chosen: ϵ_F=500 meV, ω_D=65 meV, and T_c=92.0 K.

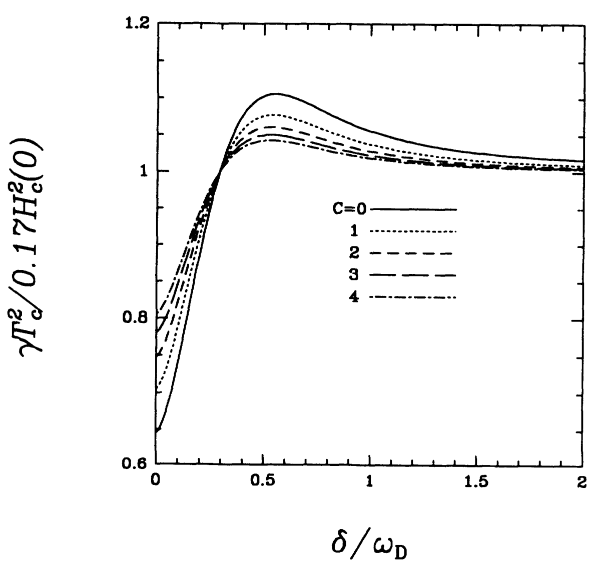

FIG. 6. Ratio R_3 (see text) normalized to 0.17 (BCS limit) for different choices of the constant background in the DOS. Same parameters as in Fig. 4.

while for $\delta=0$ it is basically equal to the BCS limit. In Fig. 6 we compare R_3 for several values of N_0C, for a superconductor with T_c=92 K, ω_D=65 meV, and ϵ_F=500 meV. Here, the background DOS makes R_3 go to the BCS limit faster than when C is not included. Comparison with experiment here is very difficult because, to the best of our knowledge, there are no precise, reliable measurements of the specific-heat coefficient γ or of the zero-temperature critical field for most high-T_c superconductors. As observed in the other universal ratios that we considered here, the maximum departures from the BCS value occur when the VHS is located at the Fermi energy. For a superconductor with T_c=92.0 K, ϵ_F=500 meV, and ω_D=65 meV, Fig. 6 shows that R_3 can deviate from the BCS value up to 35%, when no background DOS is included.

IV. CONCLUSIONS

The consequences of the introduction of a logarithmic energy-dependent DOS in BCS theory have been studied with the purpose of exploring how useful this approach is to describe the recently discovered high-temperature superconductors. After analytic and numerical work we have found that the Van Hove model does predict critical temperatures in the 100 K range, even with modest values of the coupling constant. It may also explain the observed doping dependence of the transition temperature. By contrast, there are other characteristics of the superconducting state that do not agree with some available data in the oxides. In particular, we have found that the lowest values of the isotope effect exponent are too low to be described properly by a VHS, especially when a background in the DOS is included. Also, the prediction of the position of the node in the specific-heat difference between the normal and superconducting states is much smaller than found experimentally. In addition, the Van Hove model does not appear to support extreme variations in the values of universal BCS ratios, in contradiction with a number of experiments. However, one must bear in mind that our model neglects some features that may be essential for a detailed comparison with experiments. Examples of such aspects are inelastic scattering, interlayer coupling, disorder, etc. In particular inelastic scattering acts as a pair breaking mechanism and it may be strong near a VHS.[24] It is also known to grow with temperature. Therefore Eq. (3) will overestimate the critical temperature, for pair breaking was not included in its derivation. But inelastic scattering vanishes as the temperature is lowered, so that $\Delta(0)$ will be correctly given by Eq. (5). This leads to large values of ratio R_1, in agreement with experiment.[25]

ACKNOWLEDGMENT

The author wishes to thank J. P. Carbotte for useful discussions.

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