Influence of Van Hove singularities on the thermal conductivity of high-T_c superconductors

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We calculate the electronic contribution κ_e to the thermal conductivity of a two-dimensional $d_{x^2-y^2}$-wave superconductor presenting logarithmic Van Hove singularities (VHS) in the density of states. The influence of the position of these VHS from the Fermi level on the thermal conductivity peak observed below T_c is investigated. Experimental results on different $YBa_2Cu_3O_{7-x}$ compounds with various oxygen stoichiometry x can be well described by this model with reasonable values of the physical parameters. [S0163-1829(96)07133-0]

The thermal conductivity $\kappa(T)$ of high-T_c superconductors (HTS's) present a characteristic maximum below the critical temperature T_c.[1] This peak structure has been recently attributed and described as being due to the contribution of normal electrons in the CuO_2 planes.[2–6] On the other hand, high-resolution photoemission data[7–9] on high-T_c compounds have identified the presence of saddle points close to the Fermi energy ε_F in the band structure of these materials, corresponding to two-dimensional logarithmic singularities in the density of states, i.e., Van Hove singularities (VHS).

In this work, we describe the electronic contribution κ_e to the thermal conductivity of a two-dimensional superconductor with saddle points in the band structure. We consider a $d_{x^2-y^2}$-wave gap parameter since recent works suggest that this symmetry is the most probable one in the cuprates.[10–15] It is worth mentioning that Dagotto, Nazarenko, and Moreo[12] have recently proposed a theoretical model which includes both the antiferromagnetic (Hubbard model) and the VHS scenarios for high-T_c superconductivity. This microscopic model predicts a gap parameter of the $d_{x^2-y^x}$-wave type and allows us to explain the main properties of high-T_c compounds.[12] Besides, Newns, Tsuei, and Pattnaik[16] have recently shown that the d-wave version of the Van Hove scenario is ''fully viable.''

The electronic contribution κ_e to the thermal conductivity can be calculated using a variational method described elsewhere.[5,6,17] The thermal conductivity is easily expressed in terms of trial electrical and thermal currents and scattering matrix elements related to the scattering processes which restore the system to equilibrium. We will consider in this work the scattering of electrons by point defects and acoustic phonons only.

We point our that we have neglected so-called coherence factors which appear in the expression of Bardeen, Rickayzen, and Tewordt[18] for the thermal conductivity of BCS-like superconductors. In fact these coherence factors are given as functions of the ratio $\varepsilon(\mathbf{k})/E(\mathbf{k})$ where $\varepsilon(\mathbf{k})$ is the energy spectrum of electrons in the normal state and $E(\mathbf{k})=\sqrt{\varepsilon(\mathbf{k})^2+\Delta(0)^2}$ is the quasiparticle energy spectrum with $\Delta(0)$ the zero-temperature superconducting gap parameter. Since $\Delta(0)$ is larger by a factor of 10–100 in high-T_c compounds compared to conventional low-T_c materials, $E(\mathbf{k})>\varepsilon(\mathbf{k})$ in HTS's and coherence factors can be neglected in a first approximation.

We consider the following electronic energy spectrum:[19,20]

$$\varepsilon(\mathbf{k})-\varepsilon_F(1-\delta)=\frac{\hbar^2}{2m^*_{ab}}k_xk_y, \tag{1}$$

where m^*_{ab} is the effective mass of electrons in the ab (CuO_2) plane. The spectrum described by Eq. (1) gives logarithmic singularities in the density of states at $\varepsilon_{\mathrm{VHS}}=\varepsilon_F(1-\delta)$. The parameter δ thus controls the position of the Van Hove singularity from the Fermi level, see also Ref. 16.

High-T_c superconductors are nonstoichiometric materials containing point defects often corresponding to oxygen atom vacancies or stacking faults. We thus take into account the elastic scattering of electrons by these point defects using the Yukawa potential. In two dimensions and in the Born approximation, the corresponding scattering probability reads[17]

$$C^{(\mathrm{def})}(\mathbf{k},\mathbf{k}')=\frac{2\pi^2}{\hbar S^2}\left(\frac{Ze^2}{\varepsilon_c}\right)^2\frac{N}{|\mathbf{k}-\mathbf{k}'|^2+(\Gamma^{2\mathrm{D}})^2}f^0(E)\times[1-f^0(E')]\delta(E-E'), \tag{2}$$

where S is the surface of a CuO_2 plane, N is the fraction of point defects of effective charge Ze, ε_c is the effective dielectric constant of the material, and $\Gamma^{2\mathrm{D}}$ is the two-dimensional Thomas-Fermi screening factor.

On the other hand, the scattering of electrons by acoustic phonons can be modeled as in the deformation potential approximation,[17] which is supposed to be valid in the case of long-wavelength acoustic phonons, assumed to be the dominant scattering centers of heat carriers in high-T_c materials.[1] In the Born approximation, the corresponding scattering probability is given by[21]

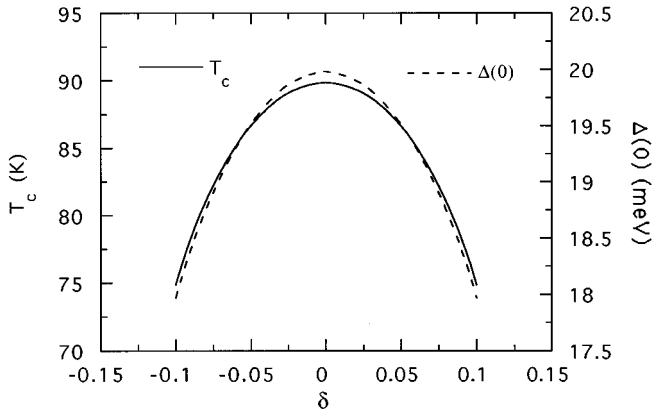

FIG. 1. Critical temperature T_c and zero-temperature energy gap $\Delta(0)$ vs the shift δ of the Fermi level from the energy of the Van Hove singularities.

$$C^{(\mathrm{ph})}(\mathbf{k},\mathbf{k}') = \frac{(\lambda_{\mathrm{tr}}\varepsilon_F q)^2}{8\pi^2 M\omega_q} f^0(E)[1-f^0(E')]N_q \times \delta(E-E'+\hbar\omega_q), \quad (3)$$

where $q=|\mathbf{k}'-\mathbf{k}|$ is the phonon wave vector, λ_{tr} is the in-plane electron-phonon transport coupling constant, ω_q is the phonon frequency (we have assumed a linear two-dimensional acoustic-phonon spectrum $\hbar\omega_q=\hbar s\sqrt{q_x^2+q_y^2}$, with s the sound velocity in the crystal), M is the mass of the crystal, and N_q is the Bose-Einstein distribution function.

In Eqs. (2) and (3), $E(\mathbf{k})=\sqrt{(\varepsilon(\mathbf{k})-\varepsilon_F)^2+\Delta(\mathbf{k})^2}$ is the quasiparticle energy spectrum with $\Delta(\mathbf{k})$ the k dependent gap parameter. The wave vector and temperature dependence of the $d_{x^2-y^2}$-wave gap parameter is approximated by[10]

$$\Delta_{d_{x^2-y^2}}(\mathbf{k},T)=\Delta(0)[\cos(\hat{k}_x) - \cos(\hat{k}_y)]\tanh(\alpha\sqrt{(T_c-T)/T}), \quad (4)$$

where $\hat{k}_x=k_x a$ and $\hat{k}_y=k_y b$ with a and b the crystallographic parameters along the a and b axis, respectively and $\alpha\approx 2$.[10]

We point out that we can also take into account the dependence of the critical temperature T_c and zero-temperature energy gap $\Delta(0)$ on the parameter δ. In the Van Hove scenario of high-T_c superconductivity, T_c and $\Delta(0)$ are maximum for $\delta=0$, i.e., when the Fermi level lies at the Van Hove singularities.[16] T_c and $\Delta(0)$ then decrease when δ is increased, and this behavior is symmetric with respect to δ,[16,22] see Fig. 1.

The theoretical temperature dependence of the normalized electronic contribution $\kappa_e/\kappa_e(T_c)$ to the thermal conductivity is shown in Fig. 2 as a function of the δ parameter. These curves have been obtained by fixing the following realistic values of the physical parameters:[23,24] T_c $(\delta=0)=90$ K, $\Delta(0)(\delta=0)=20$ meV, $m_{ab}^*=4m_0$, $\varepsilon_F=0.1$ eV, $Z=2$, $\Gamma^{2D}=15$ (Å)$^{-1}$, and $\varepsilon_c=12\varepsilon_0$ where ε_0 is the dielectric constant in vacuum. The transport electron-phonon coupling constant λ_{tr} and the fraction of point defects N are arbitrarily fixed to 0.3 (Refs. 25 and 26) and 0.05, respectively, for display in Fig. 2. One can see that κ_e increases below T_c due to the inelastic scattering of electrons by acoustic phonons, presents a peak near $0.6T_c$ for $\delta=0$ and then decreases at lower temperature due to the scattering of low-energy quasiparticles by point defects. The height of the maximum in κ is lowered in magnitude and shifted towards higher temperatures as δ is increased, i.e., when the Fermi level is shifted away from the energy of the Van Hove singularities $\varepsilon_{\mathrm{VHS}}$. This behavior arises from the decrease of the quasiparticle density of states at the Fermi level when δ is increased, resulting in a weaker enhancement of the electronic thermal conductivity below T_c.

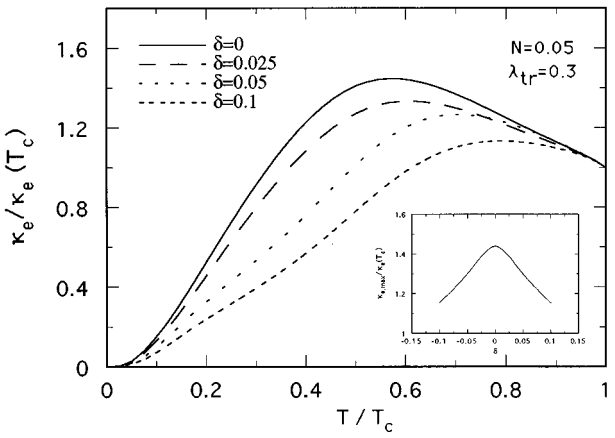

FIG. 2. Normalized electronic thermal conductivity $\kappa_e/\kappa_e(T_c)$ vs reduced temperature T/T_c as a function of the position of the Fermi energy δ relative to the energy of the Van Hove singularities. The fraction of point defects N and the electron-photon transport coupling constant λ_{tr} are fixed, respectively, to 0.05 and 0.3. Inset: Normalized maximum value $\kappa_{e,\max}/\kappa_e(T_c)$ of the electronic thermal conductivity vs δ at $N=0.05$ and $\lambda_{\mathrm{tr}}=0.3$.

The maximum value of the electronic thermal conductivity $\kappa_{e,\max}$ is shown in the inset of Fig. 2 as a function of the δ parameter at such fixed values of N and λ_{tr}. One observes that $\kappa_{e,\max}$ is lowered when δ is increased and that this be-

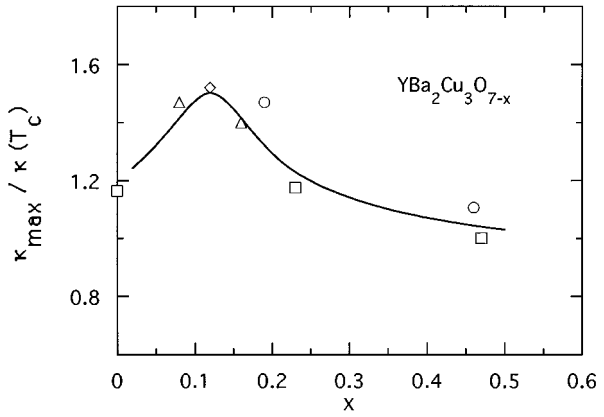

FIG. 3. Normalized maximum value $\kappa_{\max}/\kappa(T_c)$ of the thermal conductivity of $YBa_2Cu_3O_{7-x}$ compounds as a function of the oxygen content x. Squares indicate the experimental results of Zavaritskii, Samoilov, and Yurgens;[27] circles indicate the experimental results of Jezowksi *et al.* (Ref. 28); diamonds and triangles indicate the experimental data of Cohn *et al.* (Ref. 29).

havior is symmetric with respect to δ, as in the case of the electronic specific-heat jump at T_c indeed.[16]

Recently some search was made for empirical relations between characteristic features. One is the relationship between $\kappa_{\max}$ and T_c. In Fig. 3, we show the thermal conductivity maximum $\kappa_{\max}$ of various $YBa_2Cu_3O_{7-x}$ samples[27–29] as a function of the oxygen stoichiometry x. We observe that the highest value of $\kappa_{\max} \approx 1.5$ is obtained for $x \approx 0.1$, i.e., near optimal doping ($T_c \approx 92$ K). On the other hand, the value of $\kappa_{\max}$ is decreased as the oxygen content x is shifted from this value.

The solid line in Fig. 3 is the fit from our theoretical model, assuming that the highest value of $\kappa_{\max}$ observed in $YBa_2Cu_2O_{6.9}$ corresponds to the optimally doped case, i.e., that the Van Hove singularity coincides then with the Fermi level ($\delta = 0$). The fit is in very good agreement with the experimental results for reasonable values of the free parameters $\lambda_{tr} = 0.32$ and $N = 0.048$.

To summarize, the behavior of the thermal conductivity of $YBa_2Cu_3O_{7-x}$ at different oxygen doping level can be explained as follows. At optimal doping $x \approx 0.1$, one may assume that the Fermi level coincides with the energy of the Van Hove singularities ($\delta = 0$). As the oxygen concentration is modified by annealing the sample, the Fermi energy is changed and does not coincide any more with the Van Hove singularities, resulting in a decrease of the quasiparticle density of states at the Fermi level. As a result, the electronic thermal conductivity maximum below T_c is lowered, in agreement with experimental data.

We have thus shown that the behavior of the thermal conductivity maximum in various $YBa_2Cu_3O_{7-x}$ samples as a function of oxygen doping x can be well explained within the Van Hove scenario of high-T_c superconductivity and is of electronic origin indeed.

Notice that a d-wave gap parameter has been considered in this work. However, a Van Hove model with an s-wave gap parameter should reproduce the thermal conductivity peak as well. In view of Ref. 5 this calculation does not seem necessary. Nevertheless, we stress that the main difference between the two gap parameter symmetries should be observable at very low temperatures[15] due to the presence of lines of nodes in the d-wave gap. It should be thus of interest to measure the very low-temperature behavior of the thermal conductivity of high-T_c materials with various oxygen content.

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[1] For a review, see, C. Uher, J. Supercond. **3**, 337 (1990).
[2] R. C. Yu, M. B. Salamon, J. P. Lu, and W. C. Lee, Phys. Rev. Lett. **69**, 1431 (1992); **71**, 1658 (1993).
[3] P. B. Allen, X. Du. L. Mihaly, and L. Forro, Phys. Rev. B **49**, 9073 (1994).
[4] M. Houssa and M. Ausloos, Phys. Rev. B **51**, 9372 (1995).
[5] M. Houssa, M. Ausloos, and S. Sergeenkov, J. Phys. Condens. Matter **8**, 2043 (1996).
[6] M. Houssa and M. Ausloos, Physica C **257**, 321 (1996).
[7] D. S. Dessau, Z, X. Shen, D. M. King, D. S. Marshall, L. W. Lombardo, P. H. Dickinson, A. G. Loeser, J. DiCarlo, C. H. Park, A. Kapitulnik, and W. E. Spicer, Phys. Rev. Lett. **71**, 2781 (1993).
[8] K. Gofron, J. C. Campuzano, A. A. Abrikosov, M. Lindroos, A. Bansil, H. Ding, D. Koelling, and B. Dabrowski, Phys. Rev. Lett. **73**, 3302 (1994).
[9] J. Ma, C. Quitmann, R. J. Kelley, P. Alméras, H. Berger, G. Margaritondo, and M. Onellion, Phys. Rev. B **51**, 3832 (1995).
[10] J. H. Xu, J. L. Shen, J. H. Miller, and C. S. Ting, Phys. Rev. Lett. **73**, 2492 (1994).
[11] D. J. Scalapino, Phys. Rep. **250**, 329 (1995).
[12] E. Dagotto, A. Nazarenko, and A. Moreo, Phys. Rev. Lett. **74**, 310 (1995).
[13] A. Sudbø and S. P. Strong, Phys. Rev. B **51**, 1338 (1995).
[14] F. Onufrieva, Physica C **251**, 348 (1995).
[15] M. Houssa and M. Ausloos, Europhys. Lett. **33**, 695 (1996).
[16] D. M. Newns, C. C. Tsuei, and P. C. Pattnaik, Phys. Rev. B **52**, 13 611 (1996).
[17] J. M. Ziman, *Electrons and Phonons* (Clarendon, Oxford, 1963).
[18] J. Bardeen, G. Rickayzen, and L. Tewordt, Phys. Rev. **113**, 982 (1959).
[19] P. C. Pattnaik, C. L. Kane, D. M. Newns, and C. C. Tsuei, Phys. Rev. Lett. **45**, 5714 (1992).
[20] D. M. Newns, C. C. Tsuei, R. P. Huebener, P. J. M. van Bentum, P. C. Pattnaik, and C. C. Chi, Phys. Rev. Lett. **73**, 1695 (1994).
[21] K. Durczewski and M. Ausloos, J. Magn. Magn. Mater. **53**, 243 (1985).
[22] A. Gama Goicochea, Phys. Rev. B **49**, 6864 (1994).
[23] D. R. Harshman and A. P. Mills, Phys. Rev. B **45**, 10 684 (1992).
[24] M. Di Stasio, K. A. Müller, and L. Pietronero, Phys. Rev. Lett. **64**, 2827 (1990).
[25] M. Gurvitch and A. T. Fiory, Phys. Rev. Lett. **59**, 1337 (1987).
[26] D. B. Tanner and T. Timusk, in *Physical Properties of High Temperature Superconductors*, edited by D. M. Ginsberg (World Scientific, Singapore, 1992), Vol. 3, p. 416.
[27] N. V. Zavaritskii, A. V. Samoilov, and A. A. Yurgens, JETP Lett. **48**, 242 (1988).
[28] A. Jezowksi, J. Klamut, R. Horyn, and K. Rogacki, Supercond. Sci. Technol. **1**, 296 (1989).
[29] J. L. Cohn, S. A. Wolf, T. A. Vanderah, V. Selvamanickam, and K. Salama, Physica C **192**, 435 (1992).