PHYSICAL REVIEW B VOLUME 48, NUMBER 6 1 AUGUST 1993-II

Strong-coupling effects in d-wave superconductors

J. P. Carbotte and C. Jiang
Physics Department, McMaster University, Hamilton, Ontario, Canada L8S 4M1
(Received 20 April 1993)

At least in some high-T_c oxides there is strong experimental evidence for the existence of a very anisotropic gap and perhaps even for an order parameter of $d_{x^2-y^2}$ symmetry in the CuO plane. To achieve simple BCS fits to data, however, it is often necessary to introduce an arbitrary and substantial increase, over its BCS value, for the ratio of the gap to critical temperature. This is taken as an indication of the importance of strong-coupling corrections. Here we study such effects within a simple Eliashberg separable d-wave model and find only limited support for the above procedure. More elaborate calculations involving other corrections to BCS will be required to achieve a definitive comparison between theory and experiment.

Experimental evidence is accumulating that there exists a very anisotropic gap in some of the high-T_c copper oxide superconductors. Recent angular-resolved photoemission data[1,2] indicate that it is even possible that the gap is of $d_{x^2-y^2}$ symmetry in the two-dimensional (2D) copper oxide plane with zeros on the diagonal of the Brillouin zone. The very recent penetration depth measurements of Hardy *et al.*[3] on high-quality single crystals of Y-Ba-Cu-O give further strong support to this view. The observed linear dependence on temperature (T) for low T is what is expected theoretically for $d_{x^2-y^2}$ symmetry[4] and is in sharp contrast to a nearly constant value found for a BCS superconductor with finite isotropic gap. Many older data have also been interpreted as indicating a d-wave gap and some have been reviewed by Annett and Goldenfeld.[5] There also exists a large theoretical literature on this subject[6–21] which is too extensive to be reviewed in this paper. We will mention explicitly here only one aspect of these works. In the course of considering fits to the NMR as well as Knight shifts with a simple BCS description of the superconducting state, it was found that d-wave models do better than s-wave. However, to obtain a best fit to the available data, it was found necessary to substantially increase, above its BCS value, the ratio of the gap (Δ_0) to critical temperature (T_c).[21] For a separable model of the form $\Delta_0[\cos(k_x a)-\cos(k_y a)]$ with a the in-plane lattice parameter and $\mathbf{k}$ momentum in the copper oxide plane $2\Delta^{\max}/k_B T_c \equiv 4\Delta_0/k_B T_c \cong 4.3$. As $2\Delta^{\max}/k_B T_c$ is arbitrarily scaled upwards within a BCS formalism, the slope of the Knight shift and nuclear-spin-lattice relaxation rate at T_c increase over their BCS values and both curves are lowered in magnitude at all temperatures below T_c. For values of $2\Delta^{\max}/k_B T_c$ of order 6–8, the theoretical curves are close to experiment.[21] This also holds for the penetration depth although, in this case, the low-temperature slope is decreased and the measured normalized inverse of the penetration depth[4] is everywhere above the simple BCS case. This trend in Knight shift, nuclear-magnetic-resonance relaxation rate, and penetration depth can all be understood in the well-studied case for s-wave superconductivity,[22,23] as due to strong-coupling corrections to simple BCS behaviors. To treat strong-coupling effects properly requires numerical solutions of the Eliashberg gap equations.[23] To understand whether or not the simple fitting procedures described above are justified in the case of d-wave superconductors, we have carried out the necessary numerical solutions of a set of two Eliashberg equations written for a simple separable model with an s-wave correction to the normal-state channel[24–27] and have computed, for this model, Knight shift, NMR, and penetration depth. Our results show that the naive expectation that strong-coupling effects can be simulated by a simple rescaling of the ratio $2\Delta^{\max}/k_B T_c$ is not confirmed. While strong-coupling corrections do, in all three cases considered, initially move the curves away from BCS in the direction indicated by experiments, this trend very quickly saturates and then the trend reverses itself. That is, the curves start moving in the opposite direction back towards BCS as the coupling strength is further increased. The saturated value occurs for a value of strong-coupling index around $T_c/\omega_E \cong 0.3$ with ω_E the characteristic energy scale involved in the pairing mechanism which otherwise is left unspecified. In contrast to the s-wave case[22] the ratio $2\Delta^{\max}/k_B T_c$ also saturates around $T_c/\omega_E \cong 0.3$ at a value of approximately 6.5 rather than keep growing and achieving a value of about 13 in the limit $T_c/\omega_E \to \infty$.[22,23]

We begin with Eliashberg equations for a separable d-wave model.[24–26] Our aim in this paper is quite limited in that we would like to consider the simplest possible model which contains strong-coupling effects. With this in mind, it is sufficient here to consider an electron dispersion relation of the form

$$\epsilon_{\mathbf{k}} = -2t[\cos(k_x a)+\cos(k_y a)]-\mu \tag{1}$$

with t the nearest-neighbor transfer matrix element in the CuO plane and μ the chemical potential. To simplify the calculations, we follow Pines and coworkers[16,17] and Nicol, Jiang, and Carbotte[15] and use the transformation

 ©1993 The American Physical Society

$$\cos(k_x a)=-\epsilon-[1-|\epsilon|]\cos\theta\ , \tag{2a}$$

$$\cos(k_y a)=-\epsilon+[1-|\epsilon|]\cos\theta \tag{2b}$$

$-1\le\epsilon\le 1$, $0\le\theta\le\pi$. In addition, the van Hove singularity in the 2D electronic density of states is neglected and the energy integral performed after pinning all slowly varying functions to the Fermi surface. This maps the gap in the CuO plane[15]

$$\Delta_k=(\Delta_0/2)[\cos(k_x a)-\cos(k_y a)] \tag{3}$$

into

$$\Delta_\theta=\alpha\Delta_0\cos\theta\ , \tag{4}$$

where $\alpha=1-\bar{\mu}$ with $\bar{\mu}=\mu/4t$. The two gap equations are[24–26]

$$\tilde{\Delta}(i\omega_n;\theta)=\pi Tg\sum_m\cos\theta\lambda(m-n)\left\langle\frac{\cos(\theta')\tilde{\Delta}(i\omega_m;\theta')}{\sqrt{\tilde{\omega}(i\omega_m;\theta')^2+\tilde{\Delta}(i\omega_m;\theta')^2}}\right\rangle' \tag{5a}$$

and

$$\tilde{\omega}(i\omega_n;\theta)=\omega_n+\pi T\sum_m\lambda(m-n)\left\langle\frac{\tilde{\omega}(i\omega_m;\theta')}{\sqrt{\tilde{\omega}(i\omega_m;\theta')^2+\tilde{\Delta}(i\omega_m;\theta')^2}}\right\rangle' . \tag{5b}$$

In (5a) and (5b), the brackets $\langle\ \rangle'$ indicate an average over the angles, $\omega_n=\pi T(2n-1)$, $n=0\pm1,\pm2,\ldots,g$ is a parameter specifying the d- and s-wave admixture[27] in our model. For definiteness, g can be taken to be 1 and also $\bar{\mu}$ was set to zero. In Eqs. (5a) and (5b), the kernel $\lambda(m-n)$ is related to an electron-boson spectral density which sets the energy scale for the interaction (ω_E, also called $\omega_{\log}$)[28] and its magnitude determines the desired size for T_c. We note from (5b) that $\tilde{\omega}(i\omega_n;\theta)$ is independent of θ in this work. The shape of the spectral density is of little consequence in our numerical work. For Knight shift and nuclear-magnetic-resonance rate, we will use a Pb (Ref. 23) spectrum while a δ function is used for the penetration depth calculations.

From solutions of Eqs. (5a) and (5b), one can compute, quite directly, the temperature-dependent penetration depth[24,25]

$$\left[\frac{1}{\lambda_{xx}(T)}\right]^2\propto\left\langle\sum_{n=1}\frac{\tilde{\Delta}(i\omega_n;\theta)(1-\cos^2\theta)}{\sqrt{\tilde{\omega}(i\omega_n;\theta)^2+\tilde{\Delta}(i\omega_n;\theta)^2}}\right\rangle , \tag{6}$$

while, for the Knight shift and nuclear-spin-lattice relaxation rate, it is necessary to perform an analytic continuation to the real axis as described by Marsiglio, Schossmann, and Carbotte.[29] This yields real frequency quantities $\tilde{\Delta}(\omega+i\delta;\theta)$ and $\tilde{\omega}(\omega+i\delta;\theta)$ with δ infinitesimal. The Yosida function $Y(T)$, which determined the Knight shift, is given by[30]

$$Y(T)=\frac{K_s}{K_n}=2\int_0^\infty d\omega\left[-\frac{\partial f(\omega)}{\partial\omega}\right]N(\omega) \tag{7}$$

and the nuclear-spin-lattice relaxation rate

$$\frac{R_s}{R_n}=2\int_0^\infty d\omega\left[-\frac{\partial f(\omega)}{\partial\omega}\right][N^2(\omega)+M^2(\omega)] \tag{8}$$

with

$$N(\omega)=\left\langle\mathrm{Re}\left\{\frac{\tilde{\omega}(\omega+i\delta;\theta)}{\sqrt{\tilde{\omega}(\omega+i\delta;\theta)^2+\tilde{\Delta}(\omega+i\delta;\theta)^2}}\right\}\right\rangle \tag{9a}$$

and

$$M(\omega)=\left\langle\mathrm{Re}\left\{\frac{\tilde{\Delta}(\omega+i\delta;\theta)}{\sqrt{\tilde{\omega}(\omega+i\delta;\theta)^2+\tilde{\Delta}(\omega+i\delta;\theta)^2}}\right\}\right\rangle . \tag{9b}$$

Our numerical results are presented in Figs. 1–3 for Yosida function, nuclear-spin-lattice relaxation rate, and penetration depth, respectively. The solid curve in Fig. 1 is $Y(T)$ for the case $T_c/\omega_{\log}=0.1$, which is intermediate coupling. We note clearly the linear, rather than exponential dependence, at low T. This linear dependence is characteristic of the d wave. It is to be noticed that as the coupling is increased, the curves initially do not change much in shape or in magnitude. Comparing the solid curve with that for $T_c/\omega_{\log}=0.2$ (dotted), we see that $Y(T)$ is everywhere reduced but by only a very small amount, while for $T_c/\omega_{\log}=0.3$ this trend has already saturated and even reversed, i.e., started to move back towards the BCS case ($T_c/\omega_{\log}\to 0$). For $T_c/\omega_{\log}=0.6$, the largest value of the coupling strength shown, the dash-dotted curve, has already moved above the solid curve except at low temperature. This series of curves is quite different from those shown in Fig. 9 of Bulut and Scalapino[21] where the curves show much more variation with increasing value of $2\Delta^{\max}/k_BT_c$. As this ratio ranges from 3.52 to 8.0, their curves drop to ~ 0.2 for a reduced temperature of $T/T_c\cong 0.6$, while our lowest value is only slightly under 0.4, which occurs for $T_c/\omega_{\log}$ in the range 0.2–0.3. In fact, in our calculations $2\Delta^{\max}/k_BT_c=4.3$, 4.8, 6.4, 4.7, and 1.6 for $T_c/\omega_{\log}=0.01$, 0.1, 0.3, 1.0, and 4.0, respectively. It is clear that $2\Delta^{\max}/k_BT_c$ peaks at a value of about 6.5 for $T_c/\omega_{\log}\cong 0.3$ and after that it decreases. This ratio can never have a value as large as 8 for the d wave, nor is the value of $Y(T)$ at any reduced temperature ever reduced as much in realistic calculations as is indicated by scaled BCS calculations.[21] Such a procedure is clearly not justified. This means that strong-coupling effects alone cannot be invoked to explain the discrepancy that exists between present data and simple BCS results. Some other effects must also be

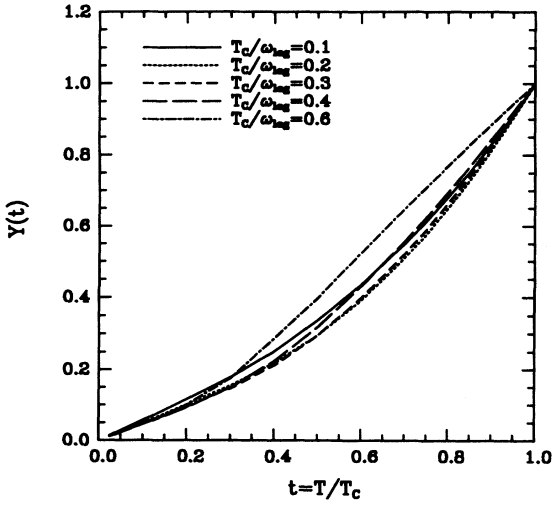

FIG. 1. The Yosida function vs the reduced temperature $t=T/T_c$ for various values of coupling strength $T_c/\omega_{\log}$: 0.1 (solid), 0.2 (dotted), 0.3 (short dashed), 0.4 (long dashed), and 0.6 (short dashed dotted).

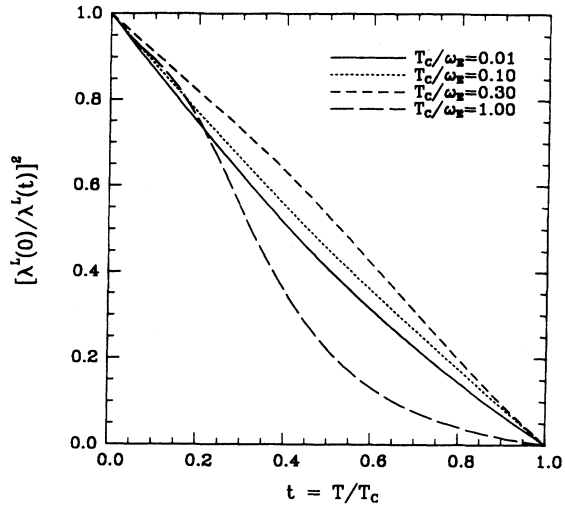

FIG. 3. The inverse of the square of the penetration depth in the London limit normalized to its zero-temperature value as a function of reduced temperature $t=t/T_c$ for different values of coupling strength T_c/ω_E: 0.01 (solid), 0.1 (dotted), 0.3 (short dashed), and 1.0 (long dashed).

involved. Similar conclusions are reached when the nuclear-spin-lattice relaxation rate and penetration depth are considered. Results are shown in Figs. 2 and 3, respectively. Strong-coupling effects initially reduce the ratio R_s/R_n over its BCS value at all reduced temperatures, and the results show saturation with reversal of behavior occurring for $T_c/\omega_{\log}\cong 0.3$, in which case our results are considerably below the BCS curve given in Fig. 13 [frame (a)] of Ref. 21 and so are closer to experiment. This fact has clear implications for the d-wave fits obtained in Bulut and Scalapino,[21] but full calculations including the proper form factors would be needed to make a convincing comparison. In Fig. 3, we show results for the square of the normalized inverse of the London penetration depth. In this case, the maximum upward deviation from the solid line which holds for $T_c/\omega_E=0.1$ (intermediate coupling) is attained for $T_c/\omega_E=0.3$ (short-dashed curve). This curve is still far below a $1-(T/T_c)^2$ law. The data of Hardy *et al.*[3] start below this reference curve at low temperature but ends up considerably above at higher temperatures. Such a behavior is obtained in a scaled BCS calculation if the ratio $2\Delta^{\max}/k_BT_c$ is taken to fall between 6 and 8 (see Fig. 2 in Scalapino).[31] It is clear from our work here that such a fit is meaningless and is not justified as due to strong-coupling corrections. Further, a value of $2\Delta^{\max}/k_BT_c=8$ cannot occur in a separable strong-coupling d-wave model of the kind studied here. It is important in closing to point out that Arberg, Mansor, and Carbotte[4] have studied strong-coupling effects on $\lambda^L(T)$ for a more complicated model than the one considered here. In their work, no Fermi-surface approximations have been introduced and the van Hove singularity is properly included. Their work essentially confirms the results found here in that the simplifications introduced in the present paper do not importantly affect strong-coupling corrections, which we can safely conclude are usually fairly small. On the other hand, Lenck and Carbotte[32] have carried out detailed studies of the penetration depth using the nonseparable phenomenological model of Millis, Monien, and Pines[20] for the spin susceptibility. A BCS formalism is used but the gap is solved for, without making the simplifying ansatz that it vary as $\Delta_0[\cos(k_xa)-\cos(k_ya)]$. While d-wave symmetry comes out of these calculations automatically, the variation of Δ_k over the Brillouin zone can be quite different from (3). These differences are found to importantly affect the temperature variation of $\lambda^L(T)$ as does the underlying band structure used and the value of chemical potential.[33] For some cases, curves closer to the data of Hardy *et al.*[3] can be obtained.

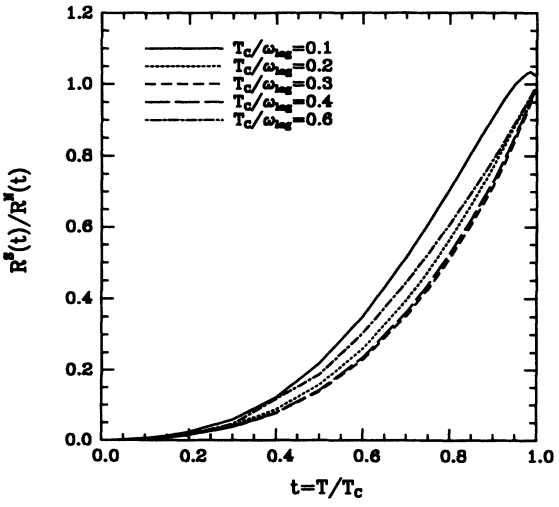

FIG. 2. The nuclear-spin-lattice relaxation rate $R^S(t)/R^N(t)$ vs reduced temperature $t=T/T_c$ for various coupling strengths $T_c/\omega_{\log}$: 0.1 (solid), 0.2 (dotted), 0.3 (short dashed), 0.4 (long dashed), and 0.6 (short-dashed dotted).

We have carried out numerical solutions of Eliashberg equations in a separable d-wave model. We use the solutions to study the modifications which strong-coupling effects introduce to the Knight shift, nuclear-spin-lattice relaxation rate, and penetration depth. While such effects reduce the Knight shift and spin-lattice relaxation rate, they increase the penetration depth at all reduced temperatures when compared to pure BCS results. As the coupling increases, these effects soon saturate for $T_c/\omega_{\log} \cong 0.3$ and then begin to move back in the opposite direction, i.e., towards their original BCS values. This also holds when the gap to T_c ratio is considered. For the d-wave, $2\Delta_0/k_B T_c$ saturates at a value of about 6.5, which occurs when $T_c/\omega_E \cong 0.3$. Then, it starts to drop and can fall below the BCS value of ~ 4.2 for sufficiently strong coupling. This behavior is completely different from that of an s-wave phonon-mediated superconductor for which $2\Delta_0/k_B T_c$ keeps rising with increasing $T_c/\omega_{\log}$ and saturates to a value of ~ 13 (Refs. 22 and 23) only in the infinite limit $T_c/\omega_{\log} \to \infty$. On the whole, we find here only very limited justification for the procedure of simulating strong-coupling effects, approximately, within a BCS model by simply scaling the dimensionless ratio $2\Delta_0/k_B T_c$ upwards. This scaling has been used to obtain satisfactory agreement between theory and experiment for various physical properties of the CuO's. Our work should not be interpreted, however, as a strong argument against a d-wave model. Rather, it points to the fact that strong coupling cannot be invoked simply to achieve a good fit with experiment. More complicated calculations will be required and further corrections to BCS will need to be found elsewhere. It has already been stressed by Pines and co-workers[16–19] that in theories of superconductivity stabilized by antiferromagnetic spin fluctuations, it may be necessary to take careful account of the detailed form of the susceptibility in order to obtain quantitatively correct results. Calculations[32,33] have already shown that band-structure effects can importantly change the nuclear-spin relaxation[33] rate and penetration depth[32] and by implication, possibly other quantities. Deviation from a strict $[\cos(k_x a) - \cos(k_y a)]$ model for the order-parameter variation over the Brillouin zone[32] can also be important. All of these effects, and possibly others, will need to be carefully included in any final comparison of theory with experiment.

This work was supported in part by the Canadian Institute for Advanced Research (CIAR), the Ontario Centre for Materials Research (OCMR), and the Natural Sciences and Engineering Research Council of Canada (NSERC).

[1]Z. K. Shen *et al.*, Phys. Rev. Lett. **70**, 1553 (1993).
[2]B. O. Wells *et al.*, Phys. Rev. B **46**, 11 830 (1992).
[3]W. Hardy *et al.*, Phys. Rev. Lett. **70**, 3999 (1993).
[4]P. Arberg, M. Mansor, and J. P. Carbotte, Solid State Commun. **86**, 671 (1993).
[5]J. F. Annett and N. Goldenfeld, J. Low Temp. Phys. **89**, 197 (1992).
[6]M. R. Norman, Phys. Rev. B **37**, 4987 (1988); **41**, 170 (1990).
[7]N. E. Bickers, R. T. Scalettar, and D. J. Scalapino, Int. J. Mod. Phys. B **1**, 687 (1987).
[8]D. J. Scalapino, E. Loh, and J. E. Hirsch, Phys. Rev. B **34**, 8190 (1986).
[9]R. J. Radtke, S. Ullah, K. Levin, and M. R. Norman, Phys. Rev. B **46**, 11 975 (1992).
[10]A. J. Millis, S. Sachdev, and C. M. Varma, Phys. Rev. B **37**, 4975 (1988).
[11]P. Monthoux, A. V. Balatsky, and D. Pines, Phys. Rev. Lett. **67**, 3448 (1991).
[12]A. J. Millis, Phys. Rev. B **45**, 13 047 (1992).
[13]S. Wermbter and L. Tewordt, Phys. Rev. B **43**, 10 530 (1991).
[14]St. Lenck and J. P. Carbotte, Phys. Rev. B **46**, 14 850 (1992).
[15]E. J. Nicol, C. Jiang, and J. P. Carbotte, Phys. Rev. B **47**, 8131 (1993).
[16]H. Monien, P. Monthoux, and D. Pines, Phys. Rev. B **43**, 275 (1991).
[17]P. Monthoux and D. Pines, Phys. Rev. Lett. **69**, 961 (1992).
[18]D. Pines, Physica C **185-189**, 120 (1991).
[19]P. Monthoux and D. Dines, Phys. Rev. B **47**, 6069 (1993).
[20]A.J. Millis, H. Monien, and D. Pines, Phys. Rev. B **42**, 167 (1990).
[21]N. Bulut and D. J. Scalapino, Phys. Rev. B **45**, 2371 (1992).
[22]J. P. Carbotte, F. Marsiglio, and B. Mitrovic, Phys. Rev. B **33**, 6135 (1986).
[23]J. P. Carbotte, Rev. Mod. Phys. **62**, 1027 (1990).
[24]M. Prohammer and J. P. Carbotte, Phys. Rev. B **43**, 5370 (1991).
[25]C. Jiang and J. P. Carbotte, Phys. Rev. B **45**, 10 670 (1992).
[26]A. Perez-Gonzalez and J. P. Carbotte, Phys. Rev. B **45**, 9894 (1992).
[27]P. J. Williams and J. P. Carbotte, Phys. Rev. B **39**, 2180 (1989).
[28]P. B. Allen and R. C. Dynes, Phys. Rev. B **12**, 905 (1975).
[29]F. Marsiglio, M. Schossmann, and J. P. Carbotte, Phys. Rev. B **37**, 4965 (1988).
[30]C. Jiang and J. P. Carbotte, J. Low Temp. Phys. **87**, 95 (1992).
[31]D. J. Scalapino, J. Phys. Chem. Solids (to be published).
[32]St. Lenck and J. P. Carbotte, J. Phys. Chem. Solids (to be published).
[33]Q. Si, Y. Zha, K. Levin, and J. P. Lu, Phys. Rev. B **47**, 9055 (1993).