Symmetry and anisotropy of the superconducting gap in layered cuprates: Analysis of experiments on photoemission and the influence of defects on the critical temperature

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The anisotropy parameter χ, which appears in the formula for the critical temperature T_c as a function of the concentration of defects, is calculated on the basis of the results of experimental studies of the Fermi surface and superconducting gap Δ in high-T_c superconductors by the method of angle-resolved photoemission spectroscopy. It is shown that the assumption of anisotropic s-pairing makes it possible to correlate the strong angular dependence of Δ in the $a-b$ plane with the relatively weak sensitivity of T_c to atomic disordering. In this case $\chi \approx 0.1$, which is an order of magnitude less than in the case of d-pairing ($\chi = 1$) and strongly anisotropic s-pairing ($\chi \lesssim 1$).

At the present stage of investigations of high-T_c superconductors one of the main problems is to determine the symmetry of the superconducting gap $\Delta(\mathbf{k})$ ($\mathbf{k}$ is the quasi-momentum) in the CuO_2 planes (see, for example, Ref. 1 and the references cited there). The solution of this problem could decrease substantially the number of models of high-T_c superconductivity which are now under discussion. These models can be conventionally divided into two groups: models with s and d symmetry of $\Delta(\mathbf{k})$. The experimental data are ambiguous: there are arguments supporting both s (Ref. 2) and models with d (Ref. 3) symmetry. The only property that has been determined unequivocally[4] is that $\Delta(\mathbf{k})$ is strongly anisotropic in the $a-b$ plane (i.e., in CuO_2 layers). This anisotropy eliminates the possibility of isotropic s pairing in high-T_c superconductors (here and below we are concerned with high-T_c superconductors with hole-type (p-type) doping.

Comparing the experimental data and the results of theoretical calculations of a number of characteristics (penetration depth, nuclear-spin relaxation rate, etc.) in superconductors with different types of pairing can contribute much to the solution of the question of the symmetry of $\Delta(\mathbf{k})$. In the present paper we focus attention on the dependence of the critical temperature T_c on the defect concentration n_{im} or, equivalently, on the momentum relaxation rate of the carriers $1/\tau \sim n_{im}$. It is known that in superconductors with isotropic s pairing T_c does not depend on $1/\tau$ for $1/\tau < E_F$ (Anderson's theorem),[5] where E_F is the Fermi energy (here and below $\hbar = k_B = 1$). In superconductors with d-pairing T_c decreases rapidly with increasing $1/\tau$ and vanishes for $1/\tau_c \approx T_{c0}$, where T_{c0} is the value of T_c in the "pure" sample, which for $T_{c0} \approx 100$ K corresponds to the critical value of the residual resistivity[6] $\rho_0 \approx 50\ \mu\Omega\cdot$cm. It is well known, however, that in high-T_c superconductors T_c is insensitive to sample quality and is virtually identical in films, single crystals, and ceramics with $\rho_0 = 0 - 50\ \mu\Omega \cdot$cm. Moreover, with a controlled change of n_{im} (for example, by radiation action),[7] T_c decreases much more slowly than predicted by the theory for d pairing, although T_c does not remain constant, as in the case of isotropic s pairing.

The alternative is anisotropic s pairing. As shown in Ref. 8, the dependence of T_c on $1/\tau$ is generally determined by the formula

$$\ln\left(\frac{T_{c0}}{T_c}\right) = \chi\left[\psi\left(\frac{1}{2} + \frac{1}{4\pi\tau T_c}\right) - \psi\left(\frac{1}{2}\right)\right], \tag{1}$$

where $\psi(z)$ is the digamma function, and the value of χ is determined by the symmetry and degree of anisotropy of $\Delta(\mathbf{k})$:

$$\chi = 1 - \frac{\langle\Delta(\mathbf{k})\rangle^2}{\langle\Delta^2(\mathbf{k})\rangle}, \quad \langle\ldots\rangle = \frac{\oint(\ldots)\frac{dl}{v(\mathbf{n})}}{\oint\frac{dl}{v(\mathbf{n})}}. \tag{2}$$

The averaging in Eq. (2) is performed over the Fermi contour (we are considering the two-dimensional case); $v(\mathbf{n})$ is the modulus of the Fermi velocity; and, $\mathbf{n} = \mathbf{k}/k$.

For weak disorder ($1/\tau \ll 4\pi T_{c0}$) the dependence of T_c on $1/\tau$ has the form

$$\frac{T_c}{T_{c0}} = 1 - \frac{\pi}{8}\frac{\chi}{\tau T_{c0}}. \tag{3}$$

In the particular cases of isotropic s pairing [$\Delta(\mathbf{k}) =$ const] and d pairing [$\langle\Delta(\mathbf{k})\rangle = 0$] we have from Eq. (2) $\chi = 0$ (i.e., $T_c =$ const) and $\chi = 1$, respectively. In the case of anisotropic s pairing we have $0 < \chi < 1$, and χ increases with increasing anisotropy of $\Delta(\mathbf{k})$. In what follows we shall therefore call χ the anisotropy parameter of the superconducting gap.

While it cannot determine the *sign* of $\Delta(\mathbf{k})$, angle-resolved photoemission[4] indicates that the *modulus* of $\Delta(\mathbf{k})$ is strongly anisotropic in the $a-b$ plane. Therefore, irrespective of whether $\Delta(\mathbf{k})$ does or does not change sign on the Fermi surface [i.e., irrespective of whether or not $\Delta(\mathbf{k})$ possesses d or anisotropic s symmetry], it can be expected that $\chi \approx 1$ ($\chi = 1$ for d-pairing and $\chi \lesssim 1$ for strongly anisotropic s pairing). If, however, $\chi \approx 1$, then, as follows from Eq. (3), the rate of decrease of T_c in the superconductor with anisotropic s pairing is virtually the same as in a superconductor with d pairing [the difference is that for $\chi = 1$ T_c vanishes for $1/\tau_c \approx T_{c0}$, while for $\chi \lesssim 1$ it decreases monotonically with increasing $1/\tau > 4\pi T_c$ (Ref. 8)]. A comparatively low defect concentration [corresponding to $\rho_0 \approx 50\ \mu\Omega \cdot$cm (Ref. 6)] should cause T_c to decrease by several factors, which, as noted above, does not correspond to the experimental situation in high-T_c superconductors. But then it turns out that isotropic s, anisotropic s, and d symmetry all disagree with experiment!

To resolve this discrepancy, we calculated the anisotropy parameter χ not on the basis of simple model considerations, but rather on the results of an experimental study of the Fermi surface[4,9] and $\Delta(\mathbf{k})$[4,10–12] in high-T_c superconductors by the method of angle-

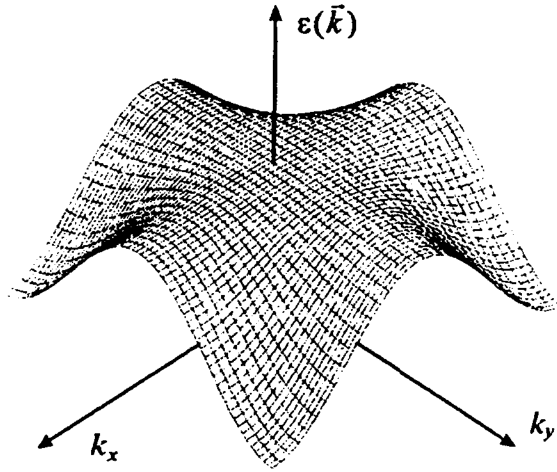

FIG. 1. $\varepsilon(\mathbf{k})$ calculated according to Eq. (4).

resolved photoemission spectroscopy. As will be shown below, $\chi \approx 0.1$, despite the strong angular dependence of $\Delta(\mathbf{k})$; this makes it possible to match the strong angular dependence of Δ in the $a-b$ plane with the relatively weak sensitivity of T_c to atomic disorder.

According to Refs. 4 and 9, a two-dimensional model with the dispersion relation

$$\epsilon(\mathbf{k}) = -2t[\cos(k_x a) + \cos(k_y a)] + 4t' \cos(k_x a)\cos(k_y a), \tag{4}$$

where the matrix elements t and t' of a hop between the nearest and next-to-nearest sites are chosen in such a way that the computed Fermi surface coincides with the experimental surface (in what follows we shall require only the ratio $t'/t = 0.45$ (Ref. 9)], can be used to describe the antibonding $dp\sigma$ band (which crosses the Fermi level in hole-doped high-T_c superconductors). The function $\varepsilon(\mathbf{k})$ is shown in Fig. 1. We underscore the fact that it agrees qualitatively with the dispersion law relation obtained on the basis of a more complicated model of singlet-correlated motion of oxygen holes in the CuO_2 planes.[13]

We use the following expression for Δ as a function of $\mathbf{k}$:

$$\Delta(\varphi) = \gamma_1 \cos(2\varphi) + i\gamma_2 \cos(\varphi + \varphi_0), \tag{5}$$

which was proposed in Ref. 10 on the basis of measurements of $|\Delta(\varphi)|$ at symmetric points of the Brillouin zone of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals. Here φ is the angle between $\mathbf{k}$ and the $\Gamma - M$ direction (the Cu–O bond in real space). As shown in Ref. 10, for most samples

$$\gamma_1 = 13.1 \text{ meV}, \quad \gamma_2 = 6.09 \text{ meV}, \quad \varphi_0 = 118.0°. \tag{6}$$

We emphasize that Eq. (5) is a fit for the *modulus* $|\Delta(\varphi)|$, so that the presence in it of terms with $d_{x^2-y^2}$ symmetry (first term) and $d_{xz} + d_{yz}$ symmetry (second term) cannot be regarded as evidence of d symmetry of $\Delta(\mathbf{k})$. The superconducting gap in the form (5) can be equally regarded as a manifestation of anisotropic s pairing, if it is assumed that $\Delta(\mathbf{k})$ is equal to the modulus of expression (5), which is consistent with experiment. We

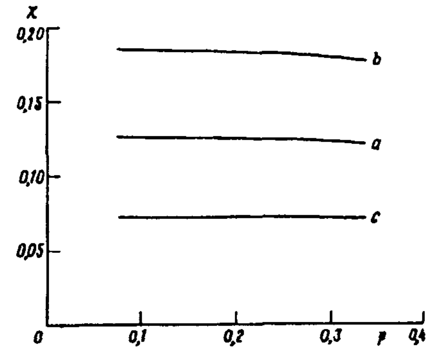

FIG. 2. Anisotropy parameter χ as a function of the number p of excess holes (per copper atom) for anisotropic s pairing and different values of γ_1, γ_2, and φ_0 [a—see Eq. (6), b—(7), c—(8)] in the approximation formula $\Delta(\mathbf{k})=|\gamma_1\cos(2\varphi)+i\gamma_2\cos(\varphi+\varphi_0)|$.

calculated the value of χ, using expression (5) and setting $\Delta(\mathbf{k})=|\Delta(\varphi)|$ in Eq. (2). In this case $v(\mathbf{n})=[(\partial\epsilon(\mathbf{k})/\partial k_x)^2+(\partial\epsilon(\mathbf{k})/\partial k_y)^2]^{1/2}$, where $\epsilon(\mathbf{k})$ is determined by Eq. (4), and the two-dimensional Fermi surface is given by the expression $\epsilon(\mathbf{k})=E_F$, where E_F is found from the constraint on the total number of holes n_h (per copper atom).

Figure 2 shows χ as a function of the concentration of excess holes $p=n_h-1$ ($p=0$ in the undoped dielectric state; $p=0.1-0.3$ corresponds to the "superconducting section" of the $p-T$ phase diagram).[1] The same figure shows the curves $\chi(p)$ for two sets of values, different from the values (6), of γ_1, γ_2, and φ_0 in expression (5):

$$\gamma_1=19.8\ \text{meV},\quad \gamma_2=2.82\ \text{meV},\quad \varphi_0=0.0°, \tag{7}$$

$$\gamma_1=12.6\ \text{meV},\quad \gamma_2=16.1\ \text{meV},\quad \varphi_0=15.3°. \tag{8}$$

The set (7) was proposed in Ref. 10 for describing the data of Ref. 12 and the set (8) was found in Ref. 10 for a small number of samples [we note that the existence of two different dependences $\Delta(\mathbf{k})$ in $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals was also noted in Ref. 11].

As one can see from Fig. 2, for all values of γ_1, γ_2, and φ_0 considered χ is found to be an order of magnitude smaller (≈ 0.1). This was expected on the basis of the strong angular dependence of Δ (we obtained the same result for other values $t'/t=0-0.4$ also). It is interesting that χ is virtually independent of the degree of doping in the entire range $p=0.1-0.3$, decreasing slightly as p increases. The small value of χ makes it possible to understand the relative insensitivity of T_c of high-T_c superconductors to defects. Indeed, considering the interrelation between $1/\tau$ and ρ_0 (see Ref. 6 for a more detailed discussion), for $\chi\approx 0.1$ we obtain $dT_c/d\rho_0\approx -0.1$ K/$\mu\Omega\cdot$cm. Therefore, for typical values $\rho_0\leq 50$ $\mu\Omega\cdot$cm we have $T_{c0}-T_c\leq 5$ K, which agrees well with the experimentally observed sample-to-sample variation of T_c (caused by very small changes in the composition and/or the presence of a small number of defects). We note that $dT_c/d\rho_0\approx -0.3$ K/$\mu\Omega\cdot$cm was obtained by controlling the defect concentration in

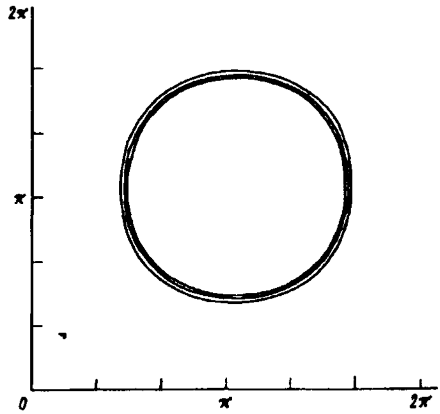

FIG. 3. Two-dimensional Fermi surfaces for excess hole concentrations $p=0.1$ (inner curve), 0.2 (middle curve), and 0.3 (outer curve). The surfaces were obtained by sectioning the surface $\epsilon(\mathbf{k})$ (see Fig. 1) by the planes $\epsilon=E_F$ (E_F depends on p).

$YBa_2Cu_3O_{7-\delta}$ single crystals by electron irradiation.[14] In terms of the anisotropy parameter, this corresponds to $\chi\approx0.3$, which is close to (though somewhat greater than) the value of χ which we computed for $Bi_2Sr_2CaCu_2O_{8+\delta}$.

In conclusion, we briefly discuss the physical reason for the low value of χ, which at first glance appears to contradict the strongly angular dependence of $\Delta(\mathbf{k})$ (5) in the CuO_2 plane. The point is that the degree of anisotropy of $\Delta(\mathbf{k})$ is determined not only by the character of the dependence of Δ on $\mathbf{k}$, but also by the specific shape of the Fermi surface. For example, for the dispersion relation $\epsilon(\mathbf{k})=-2t[\cos(k_xa)+\cos(k_ya)]$ an anisotropic (in $\mathbf{k}$ space) s wave $\Delta(\mathbf{k})=\Delta_0[\cos(k_xa)+\cos(k_ya)]$ is equivalent to an isotropic s wave, since $\Delta(\mathbf{k})=\Delta_0=$ const on the Fermi surface (and we have $\chi=0$ with all the consequences that follows). Therefore, the low value of χ which we found is a consequence of the small change in $\Delta(\mathbf{k})$, described by the dispersion relation (4), on the Fermi surface. As far as the weak p-dependence of χ is concerned, it is associated with the weak effect of doping on the shape and area of the Fermi surface with $p=0.1-0.3$ (see Fig. 3).

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