Gap anisotropy in high-T_c superconductors produced as a result of s-wave Cooper pairing of electrons on a multiply connected Fermi surface with spontaneous symmetry breaking

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The "butterfly" anisotropy of the gap observed in the plane of the CuO_2 layers in the high T_c superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ is not a consequence of d-wave Cooper pairing. It is instead due to an anisotropic s-wave pairing of electrons on a multiply connected (multivalley) Fermi surface with flat (congruent) regions and a spontaneous breaking of the symmetry of the electron spectrum as the result of a Peierls structural instability, accompanied by the formation of an insulating gap along one diagonal of the Brillouin zone. The phase shift of Josephson currents along the **a** and **b** axes observed in $YBa_2Cu_3O_{7-\delta}$ single crystals may be due to a difference between the signs of the gap parameters in the CuO_2 layers and the CuO chains. This circumstance might simulate a d-wave pairing. © *1995 American Institute of Physics.*

1. Observation of an anisotropy of the superconducting gap parameter and also of the normal density of states in the plane of the 2D CuO_2 cuprate layers in a $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystal was recently reported[1] on the basis of measurements of the photoelectron energy-loss spectra (the EELS method). According to Ref. 1, the anisotropy of the superconducting gap $\Delta(\mathbf{k})$, which is centered at the Γ point of the Brillouin zone, is at a maximum in the directions of the M points and has minima of different depths in the directions of the X and Y points of the Brillouin zone. As a result, the inequalities $\Delta_{\Gamma-M}>\Delta_{\Gamma-X}\gg\Delta_{\Gamma-Y}>0$ hold.

It follows that the plot of the superconducting gap versus the angle θ in the a–b plane is a "butterfly" with a twofold symmetry axis, not a "rosette" with "petals" of different signs and with zeros of the gap along the diagonals of the Brillouin zone (Fig. 1). The latter prediction follows from the model of a magnon mechanism for superconductivity with a singlet d-wave Cooper pairing of current carriers in the 2D CuO_2 layers, as the result of an exchange of virtual excitations of the spin density (paramagnons) in a nearly antiferromagnetic Fermi liquid.[2–4] The idea of a magnon mechanism for superconductivity in ferro- and antiferromagnets with triplet p-wave Cooper pairing was first expressed in Refs. 5–7. On the other hand, it was recently shown[8] that a predominant d-wave pairing can arise in 2D systems, regardless of the mechanism for the electron–electron interaction with a repulsion at one lattice site and an attraction at neighboring sites.

Measurements of photoelectron spectra by the EELS method at T above the super-

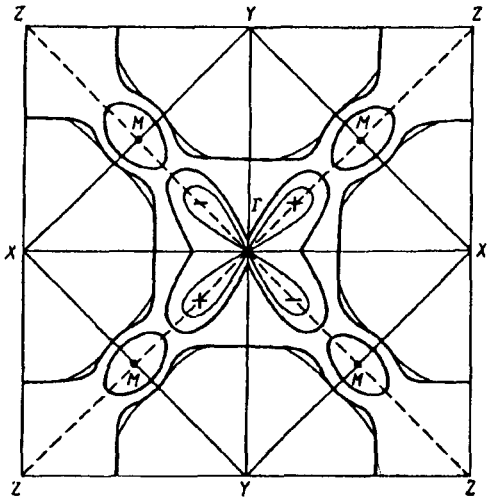

FIG. 1. Cross section of a multiply connected cylindrical Fermi surface of a $Bi_2Sr_2CaCu_3O_{8+\delta}$ single crystal according to Refs. 9 and 10, within an expanded "oxygen" Brillouin zone rotated through an angle of $\pi/4$ with respect to the first Brillouin zone, along with a butterfly angular distribution of the superconducting gap parameter for anisotropic s-wave pairing and a rosette for d-wave pairing[2-4] at the Γ point.

conducting transition temperature T_c have shown[1] that an anisotropy of similar shape (a butterfly) is characteristic of the electron density of states at the Fermi level, $\nu(E_F)$; i.e., those measurements yield $\nu_{\Gamma-M} > \nu_{\Gamma-X} \gg \nu_{\Gamma-Y} > 0$ in the normal state. This circumstance has made it possible to parametrize the anisotropic superconducting gap by means of an exponential formula of the BCS type:[1]

$$\Delta(\theta) = \tilde{\omega} \exp\{-1/\nu(\theta)\tilde{g}\}, \tag{1}$$

where $\tilde{\omega}$ and $\tilde{g}$ are adjustable interaction parameters.

At the same time, the shape of the cylindrical, multiply connected (multivalley) Fermi surface of a $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystal was reconstructed in Ref. 9 by angle-resolved photoelectron spectroscopy (ARPES). This surface has a fourfold symmetry axis and is essentially the same in shape as the Fermi surface calculated theoretically in Ref. 10 (Fig. 1). This Fermi surface has flattened regions in the $\Gamma-X$ and $\Gamma-Y$ directions, which are brought into coincidence upon a shift by the "nesting" vector **Q**. It also has regions with an anomalously weak dispersion ("flat zones") near M points. They were interpreted in Refs. 9 and 11 as lines of saddle points in the electron spectrum.

In the present letter we show that the anisotropy of both the superconducting gap parameter and the normal density of state in $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals which was observed in Ref. 1 is the result of (on the one hand) an anisotropic s-wave pairing of electrons on a multiply connected Fermi surface and (on the other) a spontaneous symmetry breaking of the original spectrum as the result of a structural (Peierls) instability accompanied by the onset of an insulating gap and a superlattice along one of the diagonals of the Brillouin zone, because of the flattened regions of the Fermi surface.

In this letter we suggest that the phase shift of π in the Josephson currents along the **a** and **b** axes which has been observed in $YBa_2Cu_3O_{7-\delta}$ single crystals in several experiments[12-14] may be a consequence of different signs of the anisotropic gap param-

eters in the 2D CuO_2 layers and in the ordered 1D CuO chains in the case of an s-wave pairing of current carriers, rather than a consequence of d-wave pairing.

2. It follows from experimental data[9] and numerical calculations[10] that two types of valleys exist within the first Brillouin zone of the layered $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystal: four equivalent valleys at the corners of the Brillouin zone (near the X and Y points) and four valleys near M points (Fig. 1). The relatively wide valleys of the first type (their width is $W>1$ eV) are of "oxygen origin" and stem from a direct overlap of the p-wave orbitals of O^{2-} oxygen ions in the plane of the CuO_2 layers (along the diagonals of the primitive cell). The valleys of the second type result from a hybridization of d-wave orbitals of Cu^{2+} ions with p-wave orbitals of O^{2-} ions (along Cu–O bonds). According to Refs. 9 and 15, they are anomalously narrow (dispersionless) near the M points of the Brillouin zone.

The coexistence of wide and narrow zones (valleys) which overlap in energy but which are hybridized only weakly in momentum space is a necessary and sufficient condition for a plasmon mechanism for superconductivity.[16] That mechanism involves a Cooper pairing of majority carriers through an exchange of low-frequency virtual excitations of the charge density (acoustic plasmons).

According to Refs. 9 and 10, the multivalley Fermi surface of single crystals of the $Bi_2Sr_2CaCu_2O_{8+\delta}$ type has a fourfold symmetry axis in the a–b plane. This assertion contradicts experimental data,[1] according to which the superconducting gap and the normal density of states have twofold symmetry axes. However, it should be kept in mind that the "oxygen" valleys near the X and Y points have flattened regions of the Fermi surface, which are brought into coincidence by a shift by the vector $\mathbf{Q}$. This nesting effect can lead to a structural Peierls instability and to the formation of an insulating gap along one of the diagonals of the Brillouin zone (along the Γ–X or Γ–Y direction), with a spontaneous breaking of the original symmetry of the spectrum.

3. To describe a superconductor with an anisotropic, multiply connected Fermi surface which has nesting along certain directions of the Fermi momentum, we use the Bilbro–McMillan–Nakayama model,[18,19] as in Ref. 17, in an analysis of the magnetic properties of Laves and Chevrel phases. We denote by Σ_1 and Δ_1 the insulating and superconducting gaps on the flattened (congruent) regions of the Fermi surface in the oxygen valleys (near the X and Y points), and we denote by Δ_2 the superconducting gap on the Fermi surface of the "copper–oxygen" valleys (near the M points).[1)] Here is the system of equations for Σ_1, Δ_1, and Δ_2, which incorporates virtual electron transitions between different sheets of the Fermi surface in the BCS approximation:

$$\Sigma_1[1-\tfrac{1}{2}\nu_1(\tilde{V}-3\tilde{U})I(\tilde{\Sigma}_1)]=\tilde{W}, \tag{2}$$

$$\Delta_1=-\tfrac{1}{2}\nu_1(V_1+\tilde{U})\Delta_1\tilde{I}(\tilde{\Sigma}_1)-\nu_2U\Delta_2\tilde{I}(\Delta_2), \tag{3}$$

$$\Delta_2=-\nu_1V_2\Delta_2\tilde{I}(\Delta_2)-\nu_1U\Delta_1\tilde{I}(\tilde{\Sigma}_1). \tag{4}$$

Here V_1 and V_2 are the matrix elements of the intravalley electron–electron interaction, U and $\tilde{U}$ are matrix elements describing two-particle electron transitions between different types of valleys and between coincident flat regions of the Fermi surface of the oxygen valleys, $\tilde{V}$ and $\tilde{W}$ are matrix elements describing the direct (Coulomb interaction)

and one-particle transitions between the flattened regions of the Fermi surface which have become insulating, ν_1 and ν_2 are the average values of the density of states on the congruent and incongruent regions of the Fermi surface, $\tilde{\Sigma}_1 = \sqrt{\Sigma_1^2 + \Delta_1^2}$, and the integral I in (2) is

$$I(\tilde{\Sigma}_1) = \int_0^{\tilde{E}} \frac{d\xi}{\sqrt{\xi^2 + \tilde{\Sigma}_1^2}} \tanh \frac{\sqrt{\xi^2 + \tilde{\Sigma}_1^2}}{2T}, \tag{5}$$

where $\tilde{E}$ is the cutoff energy of the Coulomb interaction (on the order of the Fermi energy E_F). The integral $\tilde{I}$ differs from I in that the upper limit $\tilde{E}$ is replaced by the energy of the effective electron–electron attraction, $\tilde{\omega} \ll \tilde{E}$, due to the exchange of virtual bosons (phonons, plasmons, excitons, etc.).

In contrast with Refs. 17 and 18, we assume that the probabilities for one- and two-particle intervalley transitions are small, and that the states of different valleys are mixed only slightly, in a sufficiently pure single crystal. In the case of a predominant attraction near the Fermi surface in the energy region $\xi \leqslant \tilde{\omega}$, in which we have $V_{1,2} < 0$, $U < 0$, and $\tilde{U} < 0$ (but $\tilde{V} > 0$ and $\tilde{W} > 0$ in the region $\xi \leqslant \tilde{E}$), and under the conditions $|V_{1,2}| \geqslant |U|, |\tilde{U}|$, and $\tilde{V} \geqslant \tilde{W}$, we find a transcendental equation for Σ_1 from (2) in the limit $T \to 0$ (under the condition $\Sigma_1 \geqslant \Delta_1$):

$$1 = \tfrac{1}{2}\nu_1(\tilde{V} + 3|\tilde{U}|)\ln[(\tilde{E} + \sqrt{\tilde{E}^2 + \Sigma_1^2})/\Sigma_1]. \tag{6}$$

Assuming $\Delta_2 \ll \tilde{\omega}$ (but $\Sigma_1 > \tilde{\omega}$), we find from (3)

$$\Delta_1 = \frac{\nu_2|U|\Delta_2 \ln(2\tilde{\omega}/\Delta_2)}{1 - \tfrac{1}{2}\nu_1(|V_1| + |\tilde{U}|)\ln[(\tilde{\omega} + \sqrt{\tilde{\omega}^2 + \Sigma_1^2})/\Sigma_1]}. \tag{7}$$

Comparing (6) and (7), we easily see that the denominator in (7) is positive under the condition $|V_1| < \tilde{V}$ and increases with increasing Σ_1. In other words, the superconducting gap Δ_1 in the regions of the Fermi surface which have become insulating (along the Γ-Y direction) decreases with increasing Σ_1, to a minimum value (under the condition $\Sigma_1 \geqslant \tilde{\omega}$)

$$\Delta_1^{\min} = \nu_2|U|\Delta_2 \ln(2\tilde{\omega}/\Delta_2). \tag{8}$$

Since we have $|\tilde{U}| \ll |V_2|$, we find from Eqs. (4) and (7) that we have $\Delta_1^{\min} \ll \Delta_2$, where the right side is the superconducting gap in the regions of the Fermi surface which have not become insulating (near the M points).

At the same time, it follows from Eqs. (3) and (4) under the conditions $\Sigma_1 = 0$ and $\nu_1|V_1| < \nu_2|V_2|$ that we have $\Delta_2 > \Delta_1$, where the right side is the superconducting gap on the flattened regions of the Fermi surface in the absence of an insulating gap (in the Γ–X direction). Accordingly, for completely realistic relations among the parameters, this anisotropic model of s-wave Cooper pairing leads to the same relations among the values of the superconducting gap in various symmetry directions of the Brillouin zone as in the experiments of Ref. 1:

$$\Delta_2 \equiv \Delta_{\Gamma-M} > \Delta_1 \equiv \Delta_{\Gamma-X} \geqslant \Delta_1^{\min} \equiv \Delta_{\Gamma-Y} > 0. \tag{9}$$

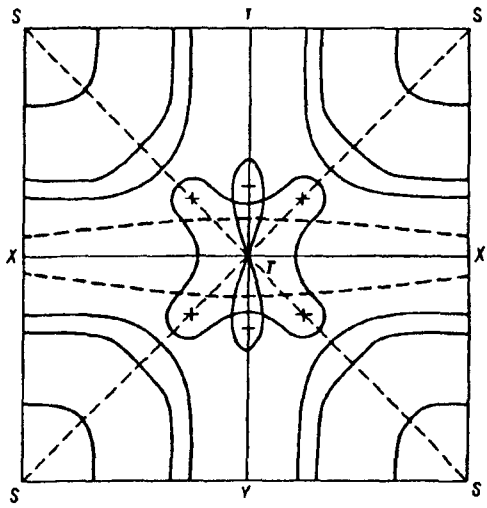

FIG. 2. Cross section of the multiply connected cylindrical Fermi surface of a $YBa_2Cu_3O_7$ single crystal in the system of 2D CuO_2 layers (solid lines) and flattened sheets of the Fermi surface in the system of 1D CuO chains (dashed curves), according to Ref. 22. Shown at the center of the Brillouin zone are suggested angular distributions of the superconducting gap parameters in the 2D CuO_2 layers (a rosette with positive petals) and in the 1D CuO chains (negative petals).

In other words, this model explains the observed (butterfly) angular distribution of the superconducting gap (Fig. 1), incorporating a spontaneous breaking of the symmetry of the electron spectrum due to a Peierls instability. This model also describes the corresponding θ dependence of the normal density of states at $T>T_C$ but $T<T_p$, where the right side is the critical temperature for a structural transition ($T_p \gg T_C$) when the dip in the density of states in the regions of the Fermi surface which have become insulating[2)] is taken into account, and under the condition $\nu_2 > \nu_1$. Empirical formula (1) is thus confirmed. Finally, the dependence of the degree of anisotropy of the superconducting gap on the concentration of doped holes which was observed in Ref. 1 can be linked at a qualitative level in this model with a dependence of the shape and size of the Fermi surface in different valleys on their degree of filling, i.e., on the position of the Fermi level E_F (cf. Ref. 8).

4. In $YBa_2Cu_3O_{7-\delta}$ single crystals with $\delta \ll 1$, a spontaneous symmetry breaking in the spectrum occurs because of an ordering of the 1D CuO chains along one of the Cu–O bonds (the **b** axis). Here one observes a significant anisotropy of the conductivity in the a–b plane (the conductivity is higher along the **b** axis than along the **a** axis). This situation is evidence that an insulating gap does not form on the flattened parts of the Fermi surface in the system of 1D chains (possibly because of a fairly pronounced corrugation of the Fermi surface). At the same time, numerical calculations on the band spectrum[22] of $YBa_2Cu_3O_7$ and experiments on photoelectron spectroscopy[23] and the de Haas–van Alphen effect[24] show that the cylindrical parts of the Fermi surface corresponding to a quasi-2D spectrum of electrons (holes) in the CuO_2 cuprate layers (Fig. 2) do not have a pronounced nesting. In this case we can use system of equations (3), (4) with $\Sigma_1 = 0$ and $\tilde{U} = \tilde{W} = 0$, under the assumption that quantities with a subscript 1 refer to the 1D CuO chains, while quantities with a subscript 2 refer to the 2D CuO_2 layers. The anisotropy of the superconducting gap, $\Delta_1(\theta)$, is at a maximum along the Γ–Y direction (i.e., along the normals to the flat sheets of the Fermi surface). It is zero in the perpendicular direction, Γ-X. The superconducting gap $\Delta_2(\theta)$ is at a maximum toward

the corners of the Brillouin zone, at which there are four valleys with a high density of states near s points. It is at a minimum in the $\Gamma-X$ and $\Gamma-Y$ directions, in which the Fermi surface is open (Fig. 2).

Let us assume that the strongest electron–electron attraction is in pairs of CuO_2 cuprate layers because of an interaction with dipole-active optical vibrations of O^{2-} ions and with collective low-frequency excitations of the charge density of nearly localized heavy charge carriers in anomalously narrow 2D zones,[16] positioned near s points,[25] while a Coulomb repulsion is predominant in the CuO chains, so that we have $V_2<0$ but $V_1>0$ and[3] $U>0$. We then find the following results from (3) and (4) (under the conditions $|V_2|\gg U$ and $T\to 0$):

$$\Delta_1=-\frac{\nu_2\Delta_2\ \ln(2\tilde{\omega}/\Delta_2)}{1+\nu_1 V_1\ \ln(2\tilde{\omega}/|\Delta_1|)},\quad \Delta_2=2\tilde{\omega}\ \exp\left\{-\frac{1}{\nu_2|V_2|}\right\}. \tag{10}$$

It follows that the signs of the parameters Δ_1 and Δ_2 are opposite (e.g., $\Delta_1<0$ with $\Delta_2>0$). If the maximum absolute value of the superconducting gap Δ_1 induced by intervalley transitions in the $\Gamma-Y$ direction is larger than the minimum value of the anisotropic superconducting gap Δ_2 in this direction (Fig. 2), then the overall sign of the order parameter along the **b** axis will be the same as the sign of Δ_1 ($\Delta_1+\Delta_2^{\min}<0$). However, since the induced gap in the 1D chains along the $\Gamma-X$ direction is $\Delta_1=0$, the sign of the superconducting order parameter along the **a** axis is the same as the sign of the gap Δ_2 in the 2D layers ($\Delta_2^{\min}>0$). Such a change in the sign of the superconducting gap parameter upon rotation through an angle of $\pi/2$ (from the **a** axis to the **b** axis) could simulate a d-wave pairing[2–4,8] in tunneling experiments[12–14] on $YBa_2Cu_3O_{7-\delta}$ single crystals, giving rise to a phase shift of π in the Josephson currents.

The results of recent numerical calculations[26] of the superconducting order parameter in $YBa_2Cu_3O_{7-\delta}$ on an anisotropic, multiply connected Fermi surface support the model of an anisotropic structure of gaps in 2D layers and 1D chains proposed in the present letter. An anisotropy of the absolute value of the superconducting gap in BiSrCaCuO (and also TlBaCaCuO and HgBaCaCuO) could simulate a d-wave pairing in experiments in which the phase of the order parameter is unimportant (e.g., in Raman scattering). On the other hand, "first-principles" numerical calculations[27] of d-wave pairing due to an exchange of antiferromagnetic magnons lead to extremely low values $T_c\sim 1$ K, because of a predominant repulsion over the entire volume of the Brillouin zone.

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[1)]We mean the average values of the gap parameters $\Delta(\theta)$ and $\Sigma(\theta)$ on the corresponding regions of the Fermi surface.

[2)]A finite density of states within the insulating gap, $\Sigma_1(\theta)$, may be due to defects (in particular, domain walls) in the incommensurate superlattice.[20,21]

[3)]In this case, U determines the probability for one-electron transitions between 1D chains and 2D layers.

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