Anisotropy of Upper Critical Field and Pairing Symmetry

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We calculate the angular dependence of the upper critical field H_{c2}, taking account of the effect of the gap anisotropy and nonlocal correction. If the Fermi surface is nearly isotropic in the a-b plane, the results show that the angular dependence of the upper critical field for $LaSrCuO_4$ in the a-b plane is qualitatively explained by an order parameter Δ with the symmetry of the pairing state $d_{x^2-y^2}$, consistent with a recent experiment by Raman spectroscopy.

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The symmetry of the pairing state of the high temperature oxide superconductors is of great interest. It is extensively investigated by many experimental investigations such as NMR [1], specific heat [2], thermal conductivity [3], penetration depth [4], photoemission spectroscopy [5], Raman spectra [6], and tunneling [7], especially for $YBa_2Cu_3O_7$ and $Bi_2Sr_2CaCu_2O_8$ systems. Besides the above experiments, Hanaguri *et al.* measured the upper critical field H_{c2} of single crystal $La_{1.86}Sr_{0.14}CuO_4$ [8]. They observed a large anisotropy of H_{c2} when the magnetic field is applied in the (1,1,0) plane. The ratio of $H_{c2\perp}$ for $H \perp c$ axis to $H_{c2\parallel}$ for $H \parallel c$ axis is about 10, depending on the temperature. Its angular dependence is well expressed by the effective mass model suitable for anisotropic three-dimensional superconductors. Further they found the anisotropy of H_{c2} about 8% in the a-b plane at the reduced temperature $t = T/T_c \sim 0.9$. Its anisotropy has fourfold symmetry, and H_{c2} takes maxima along the $[\pm 1, 0, 0]$ and $[0, \pm 1, 0]$ directions and minima along the $[\pm 1, \pm 1, 0]$ directions. They considered three possibilities for the fourfold symmetry of the anisotropy of H_{c2} in the a-b plane [8]. The first is due to the twin structure in the orthorhombic phase. If H_{c2} in the orthorhombic phase has twofold symmetry in the c plane, fourfold symmetry of H_{c2} resulting from the superposition of the twofold symmetry is expected from the twin structure. They rejected this possibility because this model leads to minimum H_{c2} for $H \parallel [100]$ and cannot explain the angular dependence of H_{c2}. The second possibility is due to the anisotropy of the critical current density J_c induced by the twin boundary. But since J_c is small near the transition temperature, they could not observe clear anisotropy of J_c. They arrived at the third possibility due to the electronic state in the CuO_2 layer for their sample. The magnitude of the anisotropy in the a-b plane is very large compared to that of conventional superconductors. The anisotropy of the cubic material Nb, for example, is about 10% at $t \sim 0.1$ and decreases with increasing temperature [9]. Its origin has been considered due to the nonlocality and the anisotropy of the Fermi surface. In this Letter, we follow the third possibility of [8] and focus the angular dependence of the upper critical field H_{c2} in the a-b plane for $LaSrCuO_4$. Since the measurements were done near the transition temperature ($t \geq 0.9$), we calculate H_{c2} for pure superconductors near the transition temperature T_c, including the gap anisotropy and the nonlocal correction. The results show that the anisotropy of H_{c2} in the a-b plane is qualitatively explained by the gap anisotropy with the symmetry of the pairing state $d_{x^2-y^2}$ even if the anisotropy of the Fermi surface is small in the a-b plane. For one pairing state approximation, the anisotropic BCS pairing interaction is expressed by

$$V_{\mathbf{k},\mathbf{k}'} = g\phi(\hat{\mathbf{k}})\phi(\hat{\mathbf{k}}'), \tag{1}$$

where g (<0) is a constant, $\phi(\hat{\mathbf{k}})$ expresses the symmetry of the interaction, and $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$ are the unit wave vectors. The order parameter $\Delta_{\mathbf{k}}(\mathbf{r})$ is expressed by

$$\Delta_{\mathbf{k}}(\mathbf{r}) = \phi(\hat{\mathbf{k}})\tilde{\Delta}(\mathbf{r}). \tag{2}$$

The upper critical field H_{c2} is the maximum field for which the linearized Ginzburg-Landau equation of the order parameter $\Delta_{\mathbf{k}}(\mathbf{r})$ has a nontrivial solution

$$\tilde{\Delta}(\mathbf{r}) = K(\mathbf{q})\tilde{\Delta}(\mathbf{r}), \tag{3}$$

where $\mathbf{q} = \hbar\nabla/i - 2e\mathbf{A}/c$ and $\mathbf{A}$ is the vector potential. For the pure superconductors near the transition temperature T_c, the kernel $K(\mathbf{q})$ is given by [10,11]

$$K(\mathbf{q}) = |g|N(0)\sum_{n=0}^{\infty} A_{2n}\langle\phi^2(\hat{\mathbf{k}})(\mathbf{v}\cdot\mathbf{q})^{2n}\rangle, \tag{4}$$

where $N(0)$ and $\mathbf{v}$ are the average density of states and the velocity at the Fermi surface, respectively. Further,

$$A_{2n} = \begin{cases} \ln\frac{2\hbar\omega_D\gamma}{\pi k_B T} & \text{for } n = 0, \\ \frac{2(-1)^n}{(2\pi k_B T)^{2n}}\left(1 - \frac{1}{2^{2n+1}}\right)\zeta(2n+1) & \text{for } n \geq 1, \end{cases} \tag{5}$$

where ω_D is the Debye cutoff frequency, γ ($= 0.577$) Euler's constant, and $\zeta(z)$ Riemann's zeta function. The angular brackets in Eq. (4) denote the average at the Fermi surface, namely,

$$\langle A\rangle = \frac{\int d\Omega\, N(\Omega)A}{\int d\Omega\, N(0)}.$$

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The upper critical field of Eq. (3) with the kernel $K(\mathbf{q})$ up to $n = 1$ corresponds to that of the effective mass model for uniaxial materials. The terms $n \geq 2$ in Eq. (4) are the nonlocal correction to the effective mass model. The factor $\phi(\hat{\mathbf{k}})$ which expresses the gap anisotropy appears on the average at the Fermi surface in product form with the Fermi velocity [12]. First we consider the eigenvalue equation for the $n = 1$ part of Eq. (4),

$$\langle \phi^2(\hat{\mathbf{k}})\,(\mathbf{v}\cdot\mathbf{q})^2\rangle \tilde{\Delta}_0(\mathbf{r}) = \lambda \tilde{\Delta}_0(\mathbf{r})\,. \tag{6}$$

The lowest eigenvalue λ and the eigenfunction $\tilde{\Delta}_0(\mathbf{r})$ are given by

$$\lambda = \frac{4e\hbar H\langle \phi^2(\hat{\mathbf{k}}) v_x^2\rangle}{c\eta} \quad \text{and} \quad \tilde{\Delta}_0(\mathbf{r}) = e^{-(eH/c\hbar\eta)x^2}, \tag{7}$$

where

$$\eta = \sqrt{\frac{\langle \phi^2(\hat{\mathbf{k}}) v_x^2\rangle}{\langle \phi^2(\hat{\mathbf{k}}) v_y^2\rangle}}\,. \tag{8}$$

We have chosen the coordinate system (x, y, z) in which the z axis is parallel to the external magnetic field, the x axis is in the a-b plane, and the y axis is directed along the c axis. The vector potential is taken as $\mathbf{A} = (0, Hx, 0)$. The parameter η of Eq. (8) gives the anisotropy in the effective mass model. Next we include the nonlocal correction due to the terms $n \geq 2$ in Eq. (4). With respect to the eigenfunction $\tilde{\Delta}_0(\mathbf{r})$, the kernel $K(\mathbf{q})$ is separated into the diagonal part $K_d(\mathbf{q})$ and the off-diagonal part $K_{od}(\mathbf{q})$:

$$K(\mathbf{q}) = K_d(\mathbf{q}) + K_{od}(\mathbf{q})\,. \tag{9}$$

Let us introduce quantities $\tilde{\mathbf{r}}$, $\tilde{\mathbf{v}}$, $\tilde{\mathbf{q}}$, and $\tilde{H}$, which are defined by

$$\tilde{\mathbf{r}} = (x, \eta y), \quad \tilde{\mathbf{v}} = (v_x, \eta v_y), \quad \tilde{\mathbf{q}} = \left(q_x, \frac{q_y}{\eta}\right), \quad \text{and} \quad \tilde{H} = \frac{H}{\eta}\,. \tag{10}$$

Since the order parameter for the upper critical field does not contain the z coordinate, we have dropped the z component of $\tilde{\mathbf{r}}$, $\tilde{\mathbf{v}}$, and $\tilde{\mathbf{q}}$. By use of the quantities defined by Eqs. (5) and (10), $K_d(\mathbf{q})$ and $K_{od}(\mathbf{q})$ are written as

$$K_d(\mathbf{q}) = |g|N(0)\{A_0 + (2p+1)A_2\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^2\rangle\epsilon + 3(2p^2+2p+1)A_4\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^4\rangle\epsilon^2\}, \tag{11}$$

$$K_{od}(\mathbf{q}) = |g|N(0)A_4[\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^2\tilde{v}_-^2\rangle\overline{q_+^3 q_-} + \langle \phi^2(\hat{\mathbf{k}})\tilde{v}_-^4\rangle q_+^4], \tag{12}$$

where

$$\tilde{q}_\pm = \tilde{q}_x \mp i\tilde{q}_y, \quad p = \frac{\tilde{q}_+\tilde{q}_-}{\epsilon}, \quad \tilde{v}_\pm = \frac{\tilde{v}_x \pm i\tilde{v}_y}{2},$$

$$\tilde{v}_\perp^2 = \tilde{v}_+\tilde{v}_-, \quad \text{and} \quad \epsilon = \frac{4e\hbar\tilde{H}}{c}\,.$$

The bar over the product $q_+^3 q_-$ in Eq. (12) means that we take the sum of all the permutations of q_+ and q_-. To retain the lowest order of the anisotropy H_{c2}, it is sufficient to keep only the diagonal part $K_d(\mathbf{q})$, because the off-diagonal part $K_{od}(\mathbf{q})$ is the first order of the anisotropy [$\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^2\tilde{v}_-^2\rangle$ and $\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_-^4\rangle$] and its contribution to the eigenvalue is the second order. After some calculations, we obtain the upper critical field H_{c2} in a form

$$\frac{4e\hbar H_{c2}}{c\eta} = \frac{\delta}{A_2\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^2\rangle} - \frac{3A_4\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^4\rangle\delta^2}{[A_2\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^2\rangle]^3}\,, \tag{13}$$

where $\delta = \ln(T/T_c)$. For the magnetic field applied in the direction $(H\cos\theta,\ H\sin\theta,\ 0)$ with respect to the crystallographic axes, the velocity $\mathbf{v}$ is expressed by $\mathbf{v} = (-V_X\sin\theta + V_Y\cos\theta, V_Z, V_X\cos\theta + V_Y\sin\theta)$, where $\mathbf{V}$ is the velocity with respect to the crystallographic axes. Using the relations

$$\langle \phi^2(\hat{\mathbf{k}})V_X^{2n}\rangle = \langle \phi^2(\hat{\mathbf{k}})V_Y^{2n}\rangle \neq \langle \phi^2(\hat{\mathbf{k}})V_Z^{2n}\rangle,$$
$$\langle \phi^2(\hat{\mathbf{k}})V_X V_Y\rangle = 0\,,$$

and other similar symmetry relations, we have

$$\eta = \sqrt{\frac{\langle \phi^2(\hat{\mathbf{k}})V_X^2\rangle}{\langle \phi^2(\hat{\mathbf{k}})V_Z^2\rangle}}\,, \tag{14a}$$

$$\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^2\rangle = \tfrac{1}{2}\langle \phi^2(\hat{\mathbf{k}})V_X^2\rangle, \tag{14b}$$

and

$$\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^4\rangle = A + B\cos 4\theta\,, \tag{14c}$$

where

$$A = \frac{1}{16}\left\langle \phi^2(\hat{\mathbf{k}})\left\{(V_X^2 + \eta^2 V_Z^2)^2 - \frac{V_X^4 - 3V_X^2V_Y^2}{4}\right\}\right\rangle, \tag{15}$$

$$B = \frac{1}{64}\langle \phi^2(\hat{\mathbf{k}})\,(V_X^4 - 3V_X^2V_Y^2)\rangle\,. \tag{16}$$

Thus, η and $\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^2\rangle$ are isotropic and the anisotropy with the fourfold symmetry appears in the term $\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^4\rangle$. For $\phi(\hat{\mathbf{k}})$, we consider two cases of the pairing states $d_{x^2-y^2}$ and d_{xy}:

$$\phi(\hat{\mathbf{k}}) = \begin{cases} \sqrt{2}\,(\hat{k}_X^2 - \hat{k}_Y^2) = \sqrt{2}\cos 2\psi & \text{for} \quad d_{x^2-y^2}\,, \\ 2\sqrt{2}\,\hat{k}_X\hat{k}_Y = \sqrt{2}\sin 2\psi & \text{for} \quad d_{xy}\,, \end{cases} \tag{17}$$

where $\hat{\mathbf{k}}$ is the unit wave vector in the a-b plane and $\phi(\hat{\mathbf{k}})$ is normalized as

$$\int_0^{2\pi} \frac{d\psi}{2\pi}\,\phi^2(\hat{\mathbf{k}}) = 1\,.$$

If we assume that the Fermi surface is isotropic in the a-b plane, it it easy to show that

$$\langle \phi^2(\hat{\mathbf{k}})\tilde{v}_\perp^2\rangle = \tfrac{1}{4}\langle V_\perp^2\rangle_Z \tag{18}$$

and

$$B = \begin{cases} \langle V_\perp^4\rangle_Z/4^4 & \text{for} \quad d_{x^2-y^2}\,, \\ -\langle V_\perp^4\rangle_Z/4^4 & \text{for} \quad d_{xy}\,, \end{cases} \tag{19}$$

where $V_\perp$ is the magnitude of the velocity in the a-b plane and $\langle\cdots\rangle_Z$ means the average with respect to the Z direction at the Fermi surface. Since $A_2 < 0$ and $A_4 > 0$ from Eq. (5), the expression (13) for the upper critical field along the $[\pm 1, 0, 0]$ and $[0, \pm 1, 0]$ directions takes the maxima for the symmetry of the pairing state $d_{x^2-y^2}$ and the minima for the symmetry of d_{xy}. From experiments [8], we conclude the pairing state as $d_{x^2-y^2}$ for $LaSrCuO_4$. In the recent Raman spectroscopy experiment for $LaSrCuO_4$ [13], the symmetry of the gap is favored for $d_{x^2-y^2}$. Thus, we have the consistent symmetry of the pairing state $d_{x^2-y^2}$ in both experiments. We estimate roughly the magnitude of the anisotropy of H_{c2} near the transition temperature for $\langle V_\perp^2\rangle_Z^2 \sim \langle V_\perp^4\rangle_Z$ in the following. Using Eqs. (13), (16), and (19), it is given by

$$\frac{\Delta H_{c2}}{H_{c2}} \sim \frac{6A_4 B|\delta|}{(A_2\langle\phi^2\tilde{v}_\perp^2\rangle)^2} \sim 0.2(1-t). \qquad (20)$$

This value is smaller than the experimental one by about a factor of 4. The origin of the quantitative discrepancy may be caused by our assumption of the isotropic Fermi surface.

In conclusion, we have calculated the upper critical field H_{c2}, taking account of the gap anisotropy and the nonlocal correction. The results show that the symmetry of the pairing state $d_{x^2-y^2}$ is consistent with both the anisotropy of H_{c2} and Raman spectroscopy. We desire to measure the upper critical field H_{c2} in the a-b plane of other high temperature oxide superconductors to clarify its origin of the anisotropy.

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