Angular dependence of upper critical field for high-temperature superconductors

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Including Fermi surface anisotropy in addition to the anisotropy of pairing states, we recalculate the angular dependence of the upper critical field $H_{c2}(\theta)$ intending to explain its in-plane anisotropy for the high-temperature superconductors. The results show that two anisotropies arising from different origins compete and the angular dependence of the fourfold symmetry for $H_{c2}(\theta)$ is not unique for all the high-temperature superconductors.

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Recently, Akagawa *et al.*[1] measured the upper critical field H_{c2} of $Ca_{0.5}La_{1.25}Ba_{1.25}Cu_3O_x$ and found its angular dependence with fourfold symmetry for the direction of the magnetic field in the ab plane. It is, however, different by $\pi/4$ from that of $La_{1.86}Sr_{0.14}CuO_4$ (Ref. 2) and $Pb_2Sr_2Ca_{0.38}Cu_3O_8$ (Ref. 3). The angular dependence of the latter materials is qualitatively in agreement with the theoretical results, which are derived from the assumption that the anisotropy arises only from the pairing state with $d_{x^2-y^2}$.[4]

So the theory does not include the anisotropy of the Fermi surface and also does not take the fact into consideration that the transition temperature T_c and the upper critical field for the high-temperature superconductors (HTS's) are much larger than those of conventional superconductors such as Nb and V. Then, in this paper we recalculate $H_{c2}(\theta)$ including the above two effects in addition to the pairing-state anisotropy.

In the following, we adopt one pairing-state approximation for the anisotropic BCS pairing interaction:

$$V_{\boldsymbol{p},\boldsymbol{p}'} = g\,\phi(\hat{\boldsymbol{p}})\,\phi(\hat{\boldsymbol{p}}') \tag{1}$$

where $g(<0)$ is a constant, $\phi(\hat{\boldsymbol{p}})$ expresses the symmetry of the interaction, and $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{p}}'$ are the unit vectors of momentum $\boldsymbol{p}$ and $\boldsymbol{p}'$. For $\phi(\hat{\boldsymbol{p}})$, we consider three cases of the pairing states s, $d_{x^2-y^2}$, and d_{xy}:

$$\phi(\hat{\boldsymbol{p}}) = \begin{cases} 1 & \text{for } s, \\ \sqrt{2}(\hat{p}_X^2 - \hat{p}_Y^2) = \sqrt{2}\cos 2\psi & \text{for } d_{x^2-y^2}, \\ 2\sqrt{2}\hat{p}_X\hat{p}_Y = \sqrt{2}\sin 2\psi & \text{for } d_{xy}, \end{cases} \tag{2}$$

where the coordinate system (X,Y,Z) is defined with respect to the crystalline axes. In this approximation, the order parameter $\Delta_{\boldsymbol{p}}(\boldsymbol{r})$ is expressed by

$$\Delta_{\boldsymbol{p}}(\boldsymbol{r}) = \phi(\hat{\boldsymbol{p}})\tilde{\Delta}(\boldsymbol{r}). \tag{3}$$

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

$$\tilde{\Delta}(\boldsymbol{r}) = K(\boldsymbol{q})\tilde{\Delta}(\boldsymbol{r}), \tag{4}$$

where $\boldsymbol{q} = \hbar\boldsymbol{\nabla}/i - 2e\boldsymbol{A}/c$ and $\boldsymbol{A}$ is the vector potential. The kernel $K(\boldsymbol{q})$ is given by

$$K(\boldsymbol{q}) = |g|T\sum_{n=-\infty}^{\infty}\int\frac{d^3p}{(2\pi\hbar)^3}\phi^2(\hat{\boldsymbol{p}})S(\boldsymbol{p},\boldsymbol{q},\omega_n), \tag{5}$$

where

$$S(\boldsymbol{p},\boldsymbol{q},\omega_n) = G(\boldsymbol{p}+\boldsymbol{q}/2,\omega_n)G(-\boldsymbol{p}+\boldsymbol{q}/2,-\omega_n). \tag{6}$$

The Green's function $G(\boldsymbol{p},\omega_n)$ is defined by

$$G(\boldsymbol{p},\omega_n) = \frac{1}{i\omega_n - \xi(\boldsymbol{p})}, \tag{7}$$

where $\omega_n = (2n+1)\pi T$ is the Matubara frequency and $\xi(\boldsymbol{p}) = \varepsilon(\boldsymbol{p}) - \mu$ with the chemical potential μ.

For the energy dispersion for the anisotropic Fermi surface, we assume the simplist form of the tight binding approximation:

$$\varepsilon(\boldsymbol{p}) = \varepsilon_0 + \varepsilon_\parallel\left[2 - \cos\left(\frac{p_X}{p_{0X}}\right) - \cos\left(\frac{p_Y}{p_{0X}}\right)\right] + \varepsilon_\perp\left[1 - \cos\left(\frac{p_Z}{p_{0Z}}\right)\right], \tag{8}$$

where $p_{0X} = \hbar/a$ and $p_{0Z} = \hbar/a'$ with the lattice constants a and a' in the ab plane and between the planes.

Transforming

$$\int\frac{d^3p}{(2\pi\hbar)^3} = \int d\Omega(\boldsymbol{p}_F)N(\boldsymbol{p}_F)\int d\xi(\boldsymbol{p}), \tag{9}$$

where $N(\boldsymbol{p}_F)$ is the density of states of the direction $\boldsymbol{p}_F$ at the Fermi surface and performing the integration over ξ, we have

$$K(\boldsymbol{q}) = |g|N(0)T\sum_{n=-\infty}^{\infty}\left\langle\frac{2\pi i\,\mathrm{sgn}(\omega_n)}{2i\omega_n - \gamma(\boldsymbol{p}_F,\boldsymbol{q})}\right\rangle. \tag{10}$$

Here

$$\langle B\rangle = \frac{1}{N(0)}\int d\Omega(\boldsymbol{p}_F)\phi^2(\hat{\boldsymbol{p}})N(\boldsymbol{p}_F)B(\boldsymbol{p}_F), \tag{11a}$$

$$N(0) = \int d\Omega(\boldsymbol{p}_F)\phi^2(\hat{\boldsymbol{p}})N(\boldsymbol{p}_F), \tag{11b}$$

and

$$\gamma(\boldsymbol{p}_F,\boldsymbol{q})=2p_{0X}V_X\sin\left(\frac{q_X}{2p_{0X}}\right)+2p_{0X}V_Y\sin\left(\frac{q_Y}{2p_{0X}}\right)+2p_{0Z}V_Z\sin\left(\frac{q_Z}{2p_{0Z}}\right), \quad (12)$$

where the velocity $\boldsymbol{V}$ is introduced by

$$\boldsymbol{V}=\left(\frac{\varepsilon_\parallel}{p_{0X}}\sin\left(\frac{p_X}{p_{0X}}\right),\frac{\varepsilon_\parallel}{p_{0X}}\sin\left(\frac{p_Y}{p_{0X}}\right),\frac{\varepsilon_\perp}{p_{0Z}}\sin\left(\frac{p_Z}{p_{0Z}}\right)\right). \quad (13)$$

Expanding Eq. (10) in the power of $\gamma(\boldsymbol{p}_F,\boldsymbol{q})$, we obtain

$$K(\boldsymbol{q})=|g|N(0)\sum_{n=0}^{\infty}A_{2n}\langle\gamma^{2n}(\boldsymbol{p}_F,\boldsymbol{q})\rangle, \quad (14)$$

where

$$A_{2n}=\begin{cases}\ln\dfrac{2\hbar\omega_D\gamma}{\pi k_BT} & \text{for } n=0,\\ \dfrac{2(-1)^n}{(2\pi k_BT)^{2n}}\left(1-\dfrac{1}{2^{2n+1}}\right)\zeta(2n+1) & \text{for } n\geqslant 1.\end{cases} \quad (15)$$

Here, ω_D is the Debye cutoff frequency, $\gamma(=0.577)$ is Euler's constant, and $\zeta(p)$ is Riemann's zeta function. The symmetry properties such as $\langle V_X^2\rangle=\langle V_Y^2\rangle$ in the ab plane give the explicit expression for $\langle\gamma^2(\boldsymbol{p}_F,\boldsymbol{q})\rangle$ as

$$\langle\gamma^2(\boldsymbol{p}_F,\boldsymbol{q})\rangle=(2p_{0X})^2\langle V_X^2\rangle\left[\sin^2\left(\frac{q_X}{2p_{0X}}\right)+\sin^2\left(\frac{q_Y}{2p_{0X}}\right)\right]+(2p_{0Z})^2\langle V_Z^2\rangle\sin^2\left(\frac{q_Z}{2p_{0Z}}\right). \quad (16)$$

In this paper, we restrict ourselves to the temperature region near T_c and keep up to the fourth order terms $\boldsymbol{q}$ in which the fourfold angular dependence of the upper critical field $H_{c2}(\theta)$ first appears. Then, expanding Eq. (16) in the power of $\boldsymbol{q}$, we have

$$\langle\gamma^2(\boldsymbol{p}_F,\boldsymbol{q})\rangle=\Gamma_{2,2}+\Gamma_{2,4}, \quad (17)$$

where

$$\Gamma_{2,2}=\langle V_X^2\rangle(q_X^2+q_Y^2)+\langle V_Z^2\rangle q_Z^2 \quad (18a)$$

and

$$\Gamma_{2,4}=-\frac{\langle V_X^2\rangle(q_X^4+q_Y^4)}{12p_{0x}^2}-\frac{\langle V_Z^2\rangle q_Z^4}{12p_{0z}^2}. \quad (18b)$$

It is convenient to use the coordinate system (x,y,z), where the x and y axes rotate by the angle θ along the Z axis relative to the X and Y axes. Further, we assume the direction of the applied magnetic field parallel to the y axis and we choose the gauge $(0,0,-Hx)$. Since there is no spatial variation of the order parameter along the magnetic field, we have $q_y=0$ and the above expressions reduce to

$$\Gamma_{2,2}=\langle V_X^2\rangle q_x^2+\langle V_Z^2\rangle q_z^2, \quad (19a)$$

$$\Gamma_{2,4}=-\frac{3+\cos 4\theta}{4}\frac{\langle V_X^2\rangle q_x^4}{12p_{0x}^2}-\frac{\langle V_Z^2\rangle q_z^4}{12p_{0z}^2}. \quad (19b)$$

The fourth-order term of $\gamma^4(\boldsymbol{p}_F,\boldsymbol{q})$ in Eq. (14) is approximated as

$$\langle\gamma^4(\boldsymbol{p}_F,\boldsymbol{q})\rangle=\langle(V_xq_x+V_zq_z)^4\rangle, \quad (20)$$

where

$$V_x=V_X\cos\theta+V_Y\sin\theta,\quad V_z=V_Z. \quad (21)$$

Collecting the terms, we obtain the kernel $K(\boldsymbol{q})$ of Eq. (4):

$$K(\boldsymbol{q})=|g|N(0)[\tilde{K}_0(\boldsymbol{q})+\tilde{K}_4(\boldsymbol{q})], \quad (22)$$

where

$$\tilde{K}_0(\boldsymbol{q})=A_0+A_2\Gamma_{2,2}, \quad (23a)$$

$$\tilde{K}_4(\boldsymbol{q})=A_2\Gamma_{2,4}+A_4\langle(V_xq_x+V_zq_z)^4\rangle. \quad (23b)$$

In the term $\tilde{K}_4(\boldsymbol{q})$ with q_i^4, the first term has been usually neglected because the ratio of the first term to the second is $[k_BT/(p_FV_F)]^2$.

Substituting Eqs. (23) into Eq. (4), we have the equation to determine the upper critical field. To solve it, we use the perturbation method and we treat the term $\tilde{K}_0(\boldsymbol{q})$ as the unperturbed part and the term $\tilde{K}_4(\boldsymbol{q})$ as a perturbation. The eigenfunction of $\tilde{K}_0(\boldsymbol{q})$ is

$$\Delta_0(\boldsymbol{r})=e^{-(eH/c\hbar\eta)x^2}, \quad (24)$$

where

$$\eta=\sqrt{\frac{\langle V_X^2\rangle}{\langle V_Z^2\rangle}}. \quad (25)$$

Including $\tilde{K}_4(\boldsymbol{q})$, we have the upper critical field

$$H_{c2}(T)=\frac{C_1\delta}{A_2}\left(1+\frac{C_2\delta}{A_2}\right), \quad (26)$$

where $\delta=\ln(T/T_c)$,

$$C_1=\frac{c}{2e\hbar\sqrt{\langle V_X^2\rangle\langle V_Z^2\rangle}}, \quad (27)$$

and

$$C_2=\frac{1}{16}\left(\frac{3+\cos 4\theta}{4p_{0X}^2\langle V_X^2\rangle}+\frac{1}{p_{0Z}^2\langle V_Z^2\rangle}\right)-\frac{3A_4}{4A_2}\left\langle\left(\frac{V_x^2}{\langle V_X^2\rangle}+\frac{V_Z^2}{\langle V_Z^2\rangle}\right)^2\right\rangle. \quad (28)$$

The anisotropic part is contained in the term with C_2

$$C_2=B_0+B_4\cos 4\theta, \quad (29)$$

where

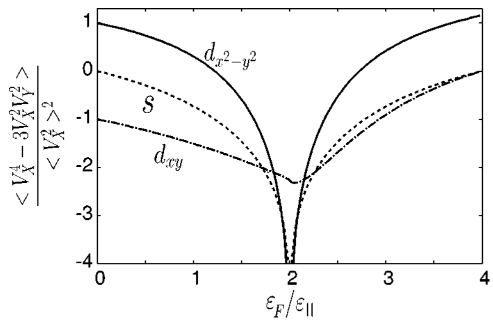

FIG. 1. The dependence of $\langle V_X^4 - 3V_X^2V_Y^2\rangle/\langle V_X^2\rangle^2$ on ε_F for the pairing states s (dotted line), $d_{x^2-y^2}$ (solid line), and d_{xy} (dot-dashed line).

$$B_4 = \frac{1}{64p_{0X}^2\langle V_X^2\rangle} - \frac{3A_4\langle V_X^4 - 3V_X^2V_Y^2\rangle}{16A_2\langle V_X^2\rangle^2}. \tag{30}$$

Thus, the anisotropy of the upper critcal field is roughly estimated by

$$\frac{\Delta H_{c2}}{\overline{H}_{c2}} \sim \frac{B_4\delta}{A_2}, \tag{31}$$

where $\overline{H}_{c2}$ is the term independent of the angle θ. In the previous paper,[4] the first term of Eq. (30) for B_4, which is always positive, has been neglected and the average of $\langle\cdots\rangle$ has been evaluated using the isotropic energy dispersion in the ab plane. The upper critical fields for HTS's are much higher and the average velocities are smaller than those for conventional superconductors such as Nb and V. Then, the first term of Eq. (30) is important for HTS's.

Using the ratio of the upper critical fields, $H_{c2\perp}/H_{c2\|}$, we can estimate the ratio of $\varepsilon_\perp/\varepsilon_\|$ as $\varepsilon_\perp/\varepsilon_\| \sim aH_{c2\perp}/(a'H_{c2\|}) \ll 1$. Then, in evaluation of $\langle\cdots\rangle$ at the Fermi surface, the p_Z dependence can be safely neglected.

In Fig. 1, we show the dependence of $\langle V_X^4 - 3V_X^2V_Y^2\rangle$ on ε_F normalized by $\langle V_X^2\rangle^2$ for the pairing states s, $d_{x^2-y^2}$, and d_{xy}. The divergence at $\varepsilon_F/\varepsilon_\| = 2$ for the s and $d_{x^2-y^2}$ states is due to the contributions from the points $\boldsymbol{p} = (\pm\pi p_{0X}, 0)$ and $\boldsymbol{p} = (0, \pm\pi p_{0X})$ to the density of states $N(0)$ for Eq. (11b). For the d_{xy} state, this divergence is canceled by the pairing function $\phi_{xy}(\boldsymbol{p})$. For the dispersion (8), the limiting case $p/p_{0X} \ll 1$ corresponds to the isotropic Fermi surface considered in the previous work.[4] From the figure, we see the fact that only the quantity $\langle V_X^4 - 3V_X^2V_Y^2\rangle$ for the $d_{x^2-y^2}$ pairing state becomes positive at low $\varepsilon_F/\varepsilon_\|$. As increasing anisotropy, two anisotropic effects for the $d_{x^2-y^2}$ pairing state compete and it becomes negative.

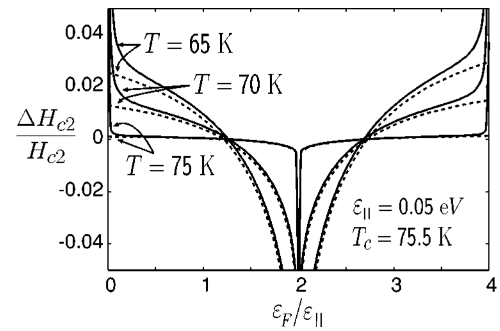

FIG. 2. The relative magnitude of anisotropy $\Delta H_{c2}/H_{c2}$ as a function of ε_F for the $d_{x^2-y^2}$ pairing state for T=65, 70, and 75 K with T_c=75.5 K with the full expression (solid line) and without the first term (dotted line) for B_4 term of Eq. (30) . Here $\varepsilon_\|$ is taken as 0.05 eV.

In Fig. 2, the ratio of the anisotropy $\Delta H_{c2}/H_{c2}$ is shown as a function of ε_F for the $d_{x^2-y^2}$ pairing state for the temperatures T=65, 70, and 75 K with T_c=75.5 K and $\varepsilon_\| = 0.05$ eV. To find the relative value of the first term of Eq. (30), the full expression of $\Delta H_{c2}/H_{c2}$ and that without the first term of Eq. (30) are shown by the solid lines and the dotted lines. Thus, we see that the term is important at smaller ε_F and lower temperatures.

In conclusion, we have shown that the anisotropy of the upper critical field arises from two effects: one is the symmetry of the pairing state and the other is the anisotropy of the Fermi surface. Although we assumed the simple dispersion for the latter anisotropy, they compete in general and different angular dependences are expected as observed by experiments, depending on the Fermi energy. The term $\Gamma_{2,4}$ which has usually been neglected is important for HTS's in which the critical temperature is much higher and the upper critical field is much greater than those of conventional superconductors. In the present approximation, the results are valid only near the transition temperature. If we extend the study to the lower-temperature region and make similar calculations as before,[5] we will find the competition effect on the flux line lattice about its structure and its correlation between the crystal lattice.[6]

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