Splitting of the superconducting transition in high-temperature superconductors due to a slight orthorhombic nature

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The splitting of a superconducting transition which has been observed in $YBa_2Cu_3O_7$ [S. E. Inderhees *et al.*, Phys. Rev. Lett. **60**, 1178 (1988); M. Ishikawa *et al.*, Technical Reports of ISSP (Japan), A No. 1907, University of Tokyo, Institute of Solid State Physics, February 1988] is similar to the splitting of the superfluid transition in ^{3}He-A which is caused by a magnetic field. In the superconducting case, the role of the magnetic field is played by an orthorhombic distortion of the tetragonal crystal symmetry. This similarity suggests the possibility of d pairing in this high-temperature superconductor.

Experiments by Inderhees *et al.*[1] and Ishikawa *et al.*[2] on the heat capacity of $YBa_2Cu_3O_7$ have revealed a fine structure in the superconducting transition: The transition splits in two, and the new transitions are separated from each other by a short interval, on the order of 3–4 K. The jumps in the heat capacity are comparable in magnitude. If we put aside the possibility that there are two different crystal modifications, with approximately equal superconducting transition temperatures, we are struck by the analogy with the splitting of the superfluid transition in ^{3}He-A caused by an arbitrarily weak magnetic field: The temperature interval between the transitions is small, being proportional to the strength of the magnetic field, while the jumps in the heat capacity are comparable and independent of the field.

The splitting of the transition in ^{3}He-A is of a purely symmetry origin. A magnetic field, distorting the structure of ^{3}He-A, lowers the symmetry of this phase to the extent that the liquid cannot undergo a transition to ^{3}He-A directly from the normal state ^{3}He-N. The transition thus occurs in two steps, with successive lowerings of the symmetry: $^3\text{He-N}\rightarrow{}^3\text{He-}A_1\rightarrow{}^3\text{He-}A$. Both of these transitions are second-order. The possibility of a splitting of this sort, due to the symmetry, of a superconducting transition in high-temperature superconductors was pointed out in Ref. 4. Since a splitting has been seen experimentally, we would like to analyze this possibility in more detail.

An orthorhombic perturbation of a tetragonal crystal lattice may play the role of a weak perturbation which lowers the symmetry and initiates a splitting of the transition in high-temperature superconductors. Since the superconductivity plays out primarily in CuO_2 planes, the electron system which is pertinent to the superconductivity is in nearly tetragonal surroundings: The orthorhombic perturbation may be regarded as small both because of the remote CuO chains and because of the deviation of the CuO_2 lattice from a square shape [$(b-a)/a\sim 0.02$; Ref. 5, for example]. In a zeroth approximation in the orthorhombic perturbation, the superconductivity classes are thus determined by the tetragonal group D_4 (see Refs. 6 and 7, for example, regarding the classification of the superconducting states in crystals with group D_4), and for some of these classes an orthorhombic perturbation will necessarily split the superconducting transition.

For clarity we restrict the analysis to the singlet superconductivity classes, and we also omit all superconducting states in which there is a violation of the translational symmetry of the lattice. In other words, we assume that no period doubling (for example) occurs in the course of the superconducting transition (the results of the present paper could easily be extended to include that other case). The singlet superconductivity classes from group D_4, for which a transition is necessarily split by an orthorhombic perturbation, arise from the two-dimensional representation of group D_4 with basis functions of the type[4] $k_z k_y$ and $k_z k_x$; this circumstance corresponds to d pairing. In this representation, the superconductivity is described by the two-component order parameter $\vec{\eta} = (\eta_x, \eta_y)$, which consists of the complex coefficients of the basis functions in an expansion of the singlet scalar function $\psi(k) = \eta_x k_y k_z + \eta_y k_x k_z$. The Ginzburg–Landau functional which is symmetric under group D_4 is of the following form,[6] where $\tau = 1 - (T/T_c)$:

$$F = -\alpha\tau\vec{\eta}\cdot\vec{\eta}^* + \frac{1}{2}\beta_1(\vec{\eta}\cdot\vec{\eta}^*)^2 + \frac{1}{2}\beta_2|\vec{\eta}^2|^2 + \frac{1}{2}\beta_3(|\eta_x|^4 + |\eta_y|^4). \quad (1)$$

Depending on the signs of the parameters β_2 and β_3, the energy minimum will correspond to the superconductivity classes listed in Table I, where $C_{2x}, C_{2y}, C_{2(x+y)}$, and C_{2z} are the groups of rotations of π radians around the axes $x, y, x+y, z$, respectively.

When a weak orthorhombic perturbation is incorporated,

$$\tilde{F} = \tilde{\alpha}(|\eta_x|^2 - |\eta_y|^2), \quad (2)$$

TABLE I.

Parameter β	Order parameter[1)] $\vec{\eta} = (\eta_x, \eta_y)$	Superconductivity class[1)]	Symmetry of state with orthorhombic perturbation[2)]
$\beta_3 < \min(0, -2\beta_2)$	$\sim (1, 0)$	$D_2(C_{2x}) \times R$	$D_2(C_{2x}) \times R$
— " — " —	$\sim (0, 1)$	$D_2(C_{2y}) \times R$	$D_2(C_{2y}) \times R$
$\beta_2 > \max(0, -\frac{1}{2}\beta_3)$	$\sim (1, i)$	$D_4(E)$	$D_2(E)$
$\beta_3 > 0 > \beta_2$	$\sim (1, 1)$	$D_2(C_{2(x+y)}) \times R$	$C_{2z}(E) \times R$

[1)]Order parameter and classes of superconducting states from the two-dimensional representation Γ_5 of the group D_4, which minimize Ginzburg–Landau functional (1) for the specified parameters β.
[2)]The fourth column shows the symmetry of the states with the orthorhombic perturbation. For the last two states, the symmetry has been lowered to the extent that a transition to these states from the normal metal is possible only through two successive second-order phase transitions, split by a temperature interval which is proportional to the magnitude of the orthorhombic distortion of the tetragonal crystal lattice in $YBa_2Cu_3O_7$.

we find a narrow temperature interval $|\tau| \sim |\tilde{\alpha}|/\alpha$ near T_c in which $\tilde{F}$ is comparable to F. In this interval, the superconducting classes are determined by the orthorhombic group D_2, and it is specifically the one-dimensional representation $k_z k_y$ and $k_z k_x$ of this group into which the two-dimensional representation Γ_5 of group D_4 splits. With $\tau_{c1} = -|\tilde{\alpha}|/\alpha$, the metal goes from a normal state into one of these representations. If $\tilde{\alpha}>0$, the representation $k_z k_x$, which corresponds to superconductivity class $D_2(C_{2x})\times R$, will arise, while in the case $\tilde{\alpha}<0$ it will be the representation $k_z k_y$, which corresponds to the class $D_2(C_{2x})\times R$. These symmetry groups cannot be adjacent to the symmetry groups which prevail far from T_c, under the condition $|\tilde{\alpha}|/\alpha \ll \tau \ll 1$, where the orthorhombic perturbation is small, and the superconductivity classes are determined by functional (1). To cast some light on this adjacency question, we need to find the actual—not the approximate—symmetry of the states far from T_c, i.e., when we incorporate the orthorhombic perturbation. For this purpose, we need to delete those of the symmetry elements in the third column of the table which are not contained in group D_2. The lowering of the symmetry of the superconducting state far from T_c due to the orthorhombic perturbation is represented in the fourth column of the table.

We see from this table that the symmetry of the first two states does not change. It corresponds to those superconductivity classes which may arise directly in a transition from the normal state. Accordingly, if $\beta_3 < \min(0, -2\beta_2)$, there will be a continuous crossover from a superconductivity from group D_4 far from T_c to a superconductivity from group D_2 near T_c, without a phase transition. The other two classes, $D_2(E)$ and $C_{2z}(E)\times R$, are subgroups of the groups $D_2(C_{2x})\times R$ and $D_2(C_{2y})\times R$, which prevail near T_c, so these low-symmetry states can arise only through an additional second-order phase transition at $\tau_{c2} \sim |\tilde{\alpha}|/\alpha$.

Under the conditions $\beta_2 < 0$ and $\beta_3 > 0$, there are two successive superconducting transitions: normal metal $\rightarrow D_2(C_{2x})\times R \rightarrow C_{2z}(E)\times R$ at $\tilde{\alpha}<0$ or normal metal $\rightarrow D_2(C_{2y})\times R \rightarrow C_{2z}(E)\times R$, in the case $\tilde{\alpha}>0$. The temperature of the second transition, τ_{c2}, and the form of the order parameter in each of the two superconducting phases, $D_2(D_{2x})\times R$ and $C_{2z}(E)\times R$ (for definiteness, we have chosen $\tilde{\alpha}<0$), are as follows:

$$\vec{\eta} = \begin{cases} \left(\left(\dfrac{\alpha(\tau - \tau_{c1})}{\beta_1 + \beta_2 + \beta_3} \right)^{1/2}, 0 \right) & \text{for } \tau_{c1} < \tau < \tau_{c2} = \dfrac{|\tilde{\alpha}|}{\alpha} \dfrac{2\beta_1 + 2\beta_2 + \beta_3}{\beta_3} \\ \left(\left(\dfrac{\alpha(\tau + \tau_{c2})}{2\beta_1 + 2\beta_2 + \beta_3} \right)^{1/2}, \left(\dfrac{\alpha(\tau - \tau_{c2})}{2\beta_1 + 2\beta_2 + \beta_3} \right)^{1/2} \right) & \text{for } \tau_{c2} < \tau . \end{cases} \quad (3a)$$

The ratio of the jumps in the heat capacity at the transitions,

$$\frac{\Delta C_1}{\Delta C_2} = \frac{2\beta_1 + 2\beta_2 + \beta_3}{\beta_3}, \quad (3b)$$

does not depend on the parameter $\tilde{\alpha}$, which is a measure of the orthorhombic perturbation.

In precisely the same way, two successive transitions [normal metal $\rightarrow D_2(C_{2x})\times R\rightarrow D_2(E)$, with $\tilde{\alpha}<0$] occur in the case $\beta_2>\max(0, -1/2\,\beta_3)$, with an order parameter of the following form for the $D_2(C_{2x})\times R$ and $D(E)$ phases:

$$\vec{\eta}=\begin{cases}\left(\left(\dfrac{\alpha(\tau-\tau_{c1})}{\beta_1+\beta_2+\beta_3}\right)^{1/2},\ 0\right)\text{ for }\ \tau_{c1}<\tau<\tau_{c2}=\dfrac{|\tilde{\alpha}|}{\alpha}\ \dfrac{2\beta_1+\beta_3}{2\beta_2+\beta_3}\\ \left(\left(\dfrac{\alpha(\tau+\tau_{c2})}{\beta_3+2\beta_1}\right)^{1/2},\ i\left(\dfrac{\alpha(\tau-\tau_{c2})}{\beta_3+2\beta_1}\right)^{1/2}\right)\text{ for }\ \tau_{c2}<\tau\end{cases}\tag{4a}$$

$$\frac{\Delta C_1}{\Delta C_2}=\frac{2\beta_1+\beta_3}{2\beta_2+\beta_3}\ .\tag{4b}$$

In the second transition, time reversal is violated: The order parameter becomes complex, as is witnessed by the appearance of an orbital ferromagnetism.

In conclusion, if an orthorhombic nature is indeed involved in the splitting of a superconducting transition, then (first) the splitting, $\tau_{c2}\sim\tau_{c1}\sim|\tilde{\alpha}|/\alpha$, should decrease with decreasing extent of the orthorhombic distortion, $b-a$, and (second) the split states should have null lines on the Fermi surface.

Note added in proof (21 June 1988). A splitting of the transition in $YBa_2Cu_3O_{6,9}$ was also reported by R. A. Butera [Phys. Rev. **B37**, 5909 (1988)], who asserted that the transition from the normal state is a first-order phase transition, while the subsequent transition is of second order.

Those results do not contradict the theory presented above: If we incorporate fluctuations of the electromagnetic field in accordance with the paper by B. I. Halperin, T. C. Lubensky, and S.-K. Ma [Phys. Rev. Lett. **32**, 292 (1974)], we conclude that the first transition should be of first order, because of electromagnetic fluctuations, while the second should remain of second order since the electromagnetic field has acquired a mass in the course of the first transition, so its fluctuations do not change the nature of the second phase transition.

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