Structural anomalies in compounds of the type La_2CuO_4

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(Submitted 21 September 1987)
Pis'ma Zh. Eksp. Teor. Fiz. **46**, No. 10, 402–405 (25 November 1987)

The structural anomalies in $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_7$ [D. Mc K. Paul *et al.*, Phys. Rev. Lett. **58**, 1976 (1987); N. B. Brandt *et al.*, Proceedings of the All-Union Working Conference on High-Temperature Superconductivity, Sverdlovsk, 1987; A. I. Golovashkin *et al.*, JETP Lett. (in press)] are explained in terms of the presence of the Fermi surface of a van't Hoff singularity. These anomalies indicate that there is a soft mode which is not related to the structural transition.

In determining the mechanism of high-temperature superconductivity in compounds based on La_2CuO_4 attention should be focused on those effects occurring in them which are absent in ordinary superconductors. The structural anomalies which are not related to the change in the crystal symmetry and which were detected in Refs.

 0021-3640/87/220506-05$01.00

1–3 are such effects. In $La_{2-x}Sr_xCuO_4$ with $x = 0.15$ the orthorhombic distortions, which occur at 180 K as a result of a structural phase transition, decrease sharply at 70 K (Ref. 1). At $x = 0.2$ there is no transition to the orthorhombic phase, but the lattice constants c and a change drastically in the temperature interval 20–90 K. The ratio c/a reaches a minimum at the temperature of the superconducting transition.[2] The compound $YBa_2Cu_3O_7$ reveals a similar decrease in the ratio c/a in the temperature interval[3] 95–110 K. We will show below that such anomalies are a consequence of the presence of a van't Hoff singularity at the Fermi level.

The saddle point in a two-dimensional electron spectrum is accompanied by a state-density singularity

$$N(E) = \frac{1}{v_0 J} \ln \frac{1}{|E-E_0|} + \text{const}, \tag{1}$$

where v_0 is the volume of the unit cell. If the Fermi level μ is equal to E_0, the system is subjected to Peierls-type instabilities: for $\mu = \text{const}$ and $T = 0$, because of the presence of a singularity $\alpha\epsilon^2 \ln|\epsilon|$ with $\alpha > 0$ (ϵ is the distance from the singularity to the boundary of the filled states) in the thermodynamic potential Ω, the energy $\beta\epsilon^2/2$ can be used to produce a strain on the lattice which (a) removes the singularity from the Fermi level, (b) reveals a gap in it, and (c) splits the singularity into two parts.[4] In the experimental studies of Refs. 1–3 apparently case (a) is realized, since it does not require the crystal symmetry to be changed. To sustain the condition $\mu = \text{const}$, this type of instability requires a rather large constant, a "reservoir," in (1).

An increase in temperature eliminates the strain-induced instability because of the diffusion of the Fermi distribution through a second-order phase transition, since the expansion of Ω in ϵ does not contain odd powers because of the presence of local symmetry near the singularity:

$$\Omega_N(\epsilon) = \Omega_0 + A\,\frac{T-T_D}{T_D}\,\epsilon^2 + \frac{1}{2} B\,\epsilon^4 . \tag{2}$$

In case (a) we have $A = 1/2v_0 J$, $B = 7\zeta(3)/24\pi^2\, v_0 J T_D^2$, and $T_D \sim \mu e^{-\beta v_0 J}$. The strain-induced instability can also be eliminated by lowering the temperature as a result of the superconducting gap Δ if $\Delta \gtrsim \epsilon$. This condition can be satisfied in superconductors of the type La_2CuO_4 because of the large value of Δ and because of the rigid lattice. We will describe this phenomenon by using the Ginzburg-Landau expansion

$$\Omega_s(\epsilon, \Delta) = \Omega_N(\epsilon) + a(\epsilon)\,\frac{T - T_c(\epsilon)}{T_D}\,\Delta^2 + \frac{1}{2} b(\epsilon)\,\Delta^4, \tag{3}$$

whose coefficients depend on ϵ. Assuming that T_c and T_D are approximately the same, we set $a(\epsilon) = a$, $b(\epsilon) = b$, and $T_c(\epsilon) = T_c(1 - \epsilon^2/\omega^2)$ and we use expansion (2) for $\Omega_N(\epsilon)$. With allowance for the fact that the derivatives of Ω with respect to Δ and ϵ vanish, we find four sets of solutions which, by analogy with those in Ref. 5, we call the N, D, S, and SD phases:

$$N:\ \epsilon^2 = 0,\ \Delta^2 = 0; \qquad D:\ \epsilon^2 = A(1-t)/B,\ \Delta^2 = 0$$
$$S:\ \epsilon^2 = 0,\ \Delta^2 = a(t_c - t)/b;\ SD:\ \epsilon^2 = p(t^* - t),\ \Delta^2 = q(t^{**} - t), \tag{4}$$

where

$$p = (Ab - a\gamma)/(Bb - \gamma^2), \quad q = (aB - A\gamma)/(Bb - \gamma^2),$$
$$t^* = \frac{Ab - a\gamma t_c}{Ab - a\gamma},\ t^{**} = \frac{aBt_c - A\gamma}{aB - A\gamma},\ t = \frac{T}{T_D},\ t_c = \frac{T_c}{T_D},\ \text{and}\ \gamma = \frac{at_c}{\omega^2}. \tag{5}$$

For definiteness, we assume $T_D > T_c$. The reciprocal of this condition can be found by permuting ϵ and Δ. Analysis of the stability of solutions (4) leads to the following results: 1) $Bb < \gamma^2$, $Ab > a\gamma$, and $aB < A\gamma$: at $t > 1$ the N phase is stable and at $t < 1$ the D phase is stable; 2) $Bb < \gamma^2$, $Ab < a\gamma$, and $aB > A\gamma$: at $t > 1$ the N phase is stable, at $t_p < t < 1$ the D phase is stable, and at $t < t_p$ the S phase is stable; the S and D phases are metastable at $t_p < t < t^*$ and $t^{**} < t < t_p$, respectively; we use the notation

$$t_p = (t_c - A\sqrt{b}/a\sqrt{B})/(1 - A\sqrt{b}/a\sqrt{B});$$

3) $Bb < \gamma^2$, $Ab < a\gamma$, and $aB < A\gamma$: at $t > 1$ the N phase is stable and at $t < 1$ the D phase is stable; the S phase is metastable at $t < t^*$; 4) $Bb > \gamma^2$, $Ab > a\gamma$, and $aB > A\gamma$: at $t > 1$ the N phase is stable, at $t^{**} < t < 1$ the D phase is stable, and at $t < t^{**}$ the SD phase is stable; 5) $Bb > \gamma^2$, $Ab > a\gamma$, and $aB < A\gamma$: the same as in case 1); 6) $Bb > \gamma^2$, $Ab < a\gamma$, and $aB > A\gamma$: at $t > 1$ the N phase is stable, at $t^{**} < t < 1$ the D phase is stable, at $t^* < t < t^{**}$ the SD phase is stable, and at $t < t^*$ the S phase is stable.

In case 4) the behavior of the strain is the same as that in Ref. 1, in case 6) (Fig. 1a) the behavior of the strain is the same as that in Ref. 2, and in case 2) (Fig. 1b) the behavior of the strain is the same as that in Ref. 3. Strain changes the thermodynamics of superconductors appreciably: it causes the ratio $2\Delta(0)/T_c$ and the functional dependence $H_c(T)$ to change and gives rise to additional abrupt changes in the heat capacity (the anomalous heat capacity in $La_{1.85}Sr_{0.15}CuO_4$ at 80 K, which corresponds to that at T_D, was observed in Ref. 6).

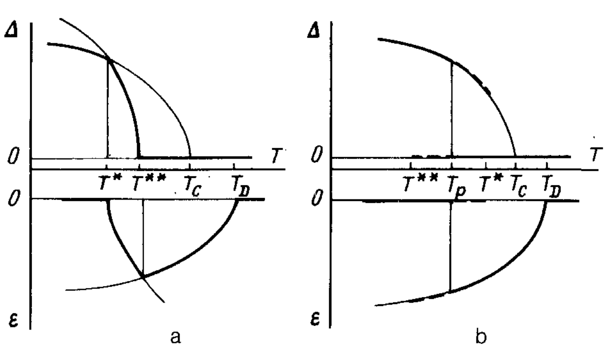

FIG. 1.

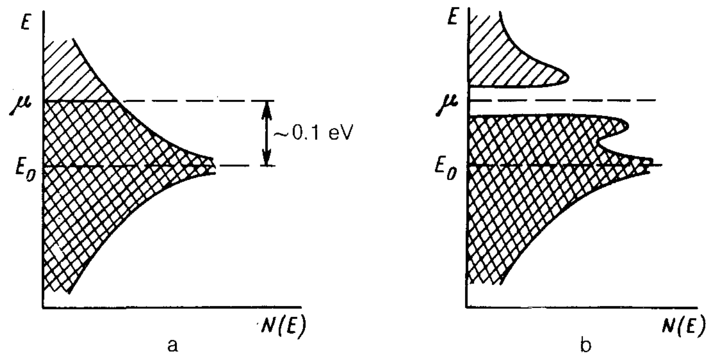

FIG. 2.

Calculations of the band structure of La_2CuO_4 show[7] that the Fermi level lies at the center of a quasi-two-dimensional 4-eV-wide band, which is described well by a strong-coupling approximation whose slight asymmetry accounts for the fact that the van't Hoff singularity lies ~ 0.1 eV below the Fermi level (Fig. 2a). The Fermi level in $La_{2-x}Sr_xCuO_4$ also falls at $x \sim 0.1$ and goes through the van't Hoff singularity: Accordingly, the $T_c(x)$ curve reveals a maximum at[8] $x = 0.15$. The interpretation of this behavior is complicated because of the presence of orthorhombic distortions which give rise to a conversion to a dielectric spectrum and to an additional maximum in $N(E)$ (Fig. 2b), which can be used to account for the maximum in $T_c(x)$ (Ref. 5). However, since at $x = 0.2$ there are no orthorhombic distortions, and since T_c differs only slightly from its maximum value, we can draw the conclusion that the van't Hoff singularity plays the key role. The results of Ref. 3 show that $YBa_2Cu_3O_7$ has a van't Hoff singularity.

Estimating a and b in $La_{2-x}Sr_xCuO_4$ from the heat capacity jump,[9] $\Delta C \sim 5$ mJ/cm^{3}K, and from the BCS ratio, $\Delta = 3.06\sqrt{T_c(T_c - T)}$, and determining from the spectrum[7] $J \approx 5$ eV, we can satisfy the inequalities for cases 4) and 6) for the appropriate choice of ω. Assuming $T^* = 20$ K, $T^{**} = 40$ K, and $T_D = 80$ K for $x = 0.2$ and $T_D = 70$ K for $x = 0.15$, we find $\omega \sim 500$ K and $\omega \gtrsim 700$ K, respectively, in reasonable agreement with the estimate based on the BCS theory:

$$\omega = T_c \left[8\pi^2 \ln \frac{\mu}{T_c} \Big/ 7\zeta(3) \right]^{1/2} \sim 400\,\mathrm{K}.$$

The foregoing discussion clearly shows that the proximity of the van't Hoff singularity to the Fermi level not only increases the state density but also produces a soft photon mode. In $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_7$ the frequency of this mode vanishes at 70–90 K and 110 K, respectively. The proximity of these temperatures to T_c tends to increase the electron-photon coupling constant.

I wish to thank V. V. Moshchalkov, A. I. Golovashkin, and K. V. Mitsen for the opportunity to review the experimental results of their work and for a discussion.

[1]D. Mc K. Paul *et al.*, Phys. Rev. Lett. **58**, 1976 (1987).
[2]N. B. Brandt *et al.*, Proceedings of the All-Union Working Conference on High-Temperature Supercon-

ductivity, Sverdlovsk, 1987.
[3]A. I. Golovashkin *et al.*, Pis'ma Zh. Eksp. Teor. Fiz. (in press).
[4]T. M. Rice and C. K. Scott, Phys. Rev. Lett. **35**, 120 (1975).
[5]Yu. V. Kopaev *et al.*, Zh. Eksp. Teor. Fiz. **58**, 1012 (1970) [Sov. Phys. JETP **31**, 1884 (1970)]; Zh. Eksp. Teor. Fiz. **65**, 1984 (1973) [Sov. Phys. JETP **38**, 991 (1974)].
[6]B. D. Dunlap *et al.*, Phys. Rev. B **35**, 7210 (1987).
[7]L. F. Mattheiss, Phys. Rev. Lett. **58**, 1028 (1987).
[8]R. B. van Dover *et al.*, Phys. Rev. B **35**, 5337 (1987).
[9]B. Batlog *et al.*, Phys. Rev. B **35**, 5340 (1987).

Translated by S. J. Amoretty