Effect of the bistable behavior of the apical oxygen atom on the superconducting transition in $YBa_2Cu_3O_{7-\delta}$

A. P. Saĭko, V. E. Gusakov, and V. S. Kuz'min
Institute of Solid State and Semiconductor Physics, Academy of Sciences of Belarus, 220726, Minsk, Belarus

(Submitted 20 August 1992; resubmitted 23 September 1992)
Pis'ma Zh. Eksp. Teor. Fiz. **56**, No. 8, 425–428 (25 October 1992)

The bistable behavior of the apical oxygen atom in the compound $YBa_2Cu_3O_{7-\delta}$ may lead to high superconducting transition temperatures in the case of an electron–phonon pairing mechanism.

1. It was recently established experimentally[1,2] that the O(4) oxygen atoms in the high-T_c superconducting compound $YBa_2Cu_3O_{7-\delta}$ can be in two nonequivalent states—in an asymmetric two-well potential—along the crystallographic c axis. As the temperature is varied, a competition between the anharmonic contributions to the potential well would evidently have the result that metastable states of the apical oxygen atoms could become stable and vice versa; i.e., abrupt transitions would occur from one state to the other, and they would be accompanied by the hysteresis which is inherent in such cases (more on this below). In the present letter we work on the

 0021-3640/92/000367-04$03.00 © 1992 American Institute of Physics

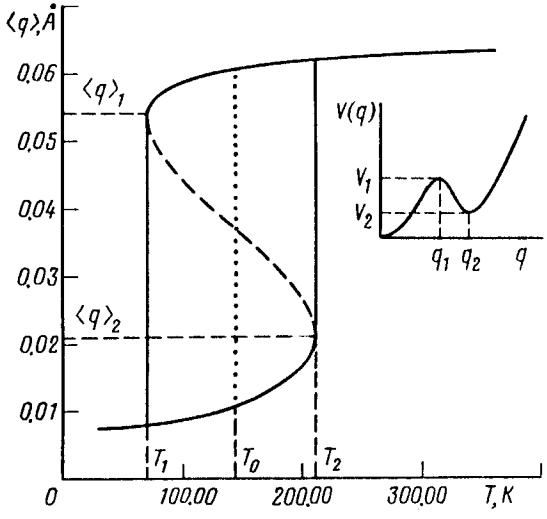

FIG. 1. Bistable behavior of the expectation value $\langle q \rangle$ of the displacement of the O(4) atom as a function of the temperature. The inset shows the model potential $V(q)$. $V_1=0.04$ eV, $q_1=0.067$ Å, $V_2=0.0045$ eV, $q_2=0.13$ Å.

basis of an electron–phonon pairing mechanism to analyze the behavior of the superconducting transition temperature T_c in the compound $YBa_2Cu_3O_{7-\delta}$. We assume that the anharmonically unstable lattice consisting of apical oxygen atoms dominates the situation. A corresponding problem was taken up in Refs. 3 and 4 (see also Ref. 5) for the case of harmonically unstable lattices.

2. We assume that the apical oxygen atoms are moving in an asymmetric two-well potential $V(q)=\alpha q^2/2-\beta q^3/3+\gamma q^4/4$ (Fig. 1), set up by the other atoms, and that these apical atoms interact with each other via harmonic long-range forces with a coupling constant f. Here q describes the instantaneous displacements of oxygen from its equilibrium position along the c axis, and the relations $\alpha, \beta, \gamma > 0$ hold.

The expression[6] for the effective electron–phonon coupling constant λ for the (dominant) lattice mode in which we are interested can be written

$$\lambda=\eta\,\mathrm{Re}[-\ll\delta q|\delta q\gg_{\omega=0}], \tag{1}$$

where $\ll\delta q|\delta q\gg_\omega$ is the Fourier transform of the two-time temperature Green's function,[7] $\delta q=q-\langle q\rangle$, $\langle q\rangle$ is the expectation value of the coordinate q, and η is the Hopfield parameter. If we treat the interaction between apical oxygen atoms in the mean-field approximation (a natural approach in the case of long-range forces), and if we deal with anharmonic effects in the approximation of self-consistent phonons,[7] we find the following expression for the Green's function which we need:

$$\begin{aligned}&\ll\delta q|\delta q\gg_\omega=[m(\omega^2-\Omega^2)]^{-1},\\ &\Omega^2\equiv[\alpha+2f-2\beta\langle q\rangle+3\gamma(\sigma+\langle q\rangle^2)]/m,\end{aligned} \tag{2}$$

where Ω is the "one-particle" frequency, renormalized by the anharmonic interactions, $\sigma=\langle q^2\rangle-\langle q\rangle^2$, and m is the mass of the oxygen atom. Using the relation between the correlation function and the Green's function,

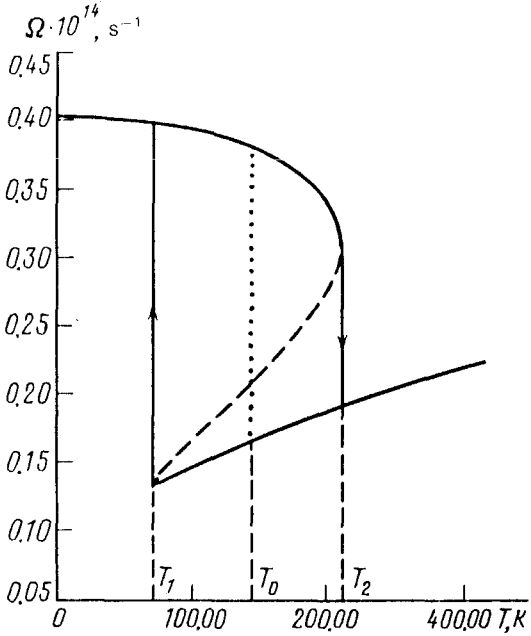

FIG. 2. Temperature dependence of the vibration frequency Ω of the O(4) atom, renormalized by anharmonic interactions.

$$\sigma=\int_0^\infty d\omega\ \coth(\omega/2\theta)\left[-\frac{1}{\pi}\,\mathrm{Im}\ \ll\delta q\,|\,\delta q\gg_{\omega+i\epsilon}\right],$$

along with the condition that the average force is zero $[(\partial/\partial t)\langle p(t)\rangle=0$, where p is the momentum which is the conjugate of the coordinate $q]$, we find two equations for a self-consistent determination of the expectation values $\langle q\rangle$ and σ:

$$\sigma=(1/2m\Omega)\coth(\Omega/2\theta),$$
$$(\beta-3\gamma\langle q\rangle)\sigma=\alpha\langle q\rangle-\beta\langle q\rangle^2+\gamma\langle q\rangle^3. \tag{3}$$

An examination of the bifurcation properties of Eqs. (3) reveals that for certain values of the parameters α, β, γ, and f there is a hysteresis loop (Fig. 1) near the critical temperature T_0, with a discontinuity of the first kind in the average displacement $\langle q\rangle$ at the temperature T_2 (during heating) and T_1 (during cooling). The temperatures T_1 and T_2 determine the width of the loop; i.e., the system of interacting anharmonic oscillators becomes unstable at the points $(\langle q\rangle_1, T_1)$ and $(\langle q\rangle_2, T_2)$. If Maxwell's rule holds, a discontinuity of the first kind occurs at T_0 without a hysteresis. The behavior of σ is similar. A bistable behavior is characteristic of the effective frequency Ω (Fig. 2) and also of other statistical-thermodynamic parameters of the system. In the $YBa_2Cu_3O_{7-\delta}$ system, a hysteretic behavior has been seen[8–11] experimentally for such parameters as the shear modulus, the thermal conductivity, and the lattice constants, with boundaries $T_1\sim 70$ and $T_2\sim 200$ K.

3. We describe the superconducting transition temperature T_c by the standard formula[12]

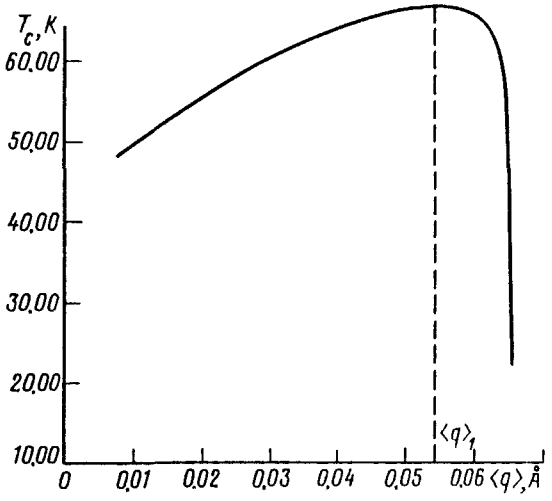

FIG. 3. Superconducting transition temperature T_c as a function of the expectation value of the position of the O(4) atom in a bistable potential.

$$k_B T_c = 0.26\,\Omega[e^{2/\lambda}-1]^{-1/2}, \quad \lambda = \eta/m\Omega^2. \tag{4}$$

It is clear from (4) that the similarities in the behavior of T_c are determined by the bistable behavior of Ω. Figure 3 shows a plot of T_c versus the expectation value $\langle q\rangle$ of the position of the apical oxygen atom. We see that T_c increases with increasing $\langle q\rangle$ in the bistability region. At the point $\langle q\rangle_1$—the "supercooled" phonon mode—the maximum value $T_c^{\max}$ is reached (as is the minimum value of Ω).

For some numerical estimates of T_c, we assign values to parameters of our model, α, β, γ, f, and η, in the following way. From experimental data[1] on Raman scattering in the $YBa_2Cu_3O_{7-\delta}$ system we find a seed frequency $\sqrt{\alpha/m} \simeq 600\ \text{cm}^{-1}$ for the apical oxygen atom. The coefficients β and γ are determined completely by the quantities q_1 and q_2 (Fig. 1). The experimental values of q_2 are in the interval[13] 0.1–0.13 Å. We have $q_1 \simeq q_2/2$, $f = 10^{-3}\,\alpha$ (weakly coupled oscillators) and a Hopfield parameter $\eta = 4$ eV/Å. For these parameter values, the values of T_c are in the liquid-nitrogen region ($T_c^{\max} > 70$ K), indicating that the high superconducting transition temperature can be explained on the basis of an ordinary electron–phonon mechanism for electron pairing involving a bistable lattice mode.

[1] L. V. Gasparov, V. D. Kulakovskiĭ, V. B. Timofeev, and E. Ya. Sherman, Zh. Eksp. Teor. Fiz. **100**, 1681 (1991) [Sov. Phys. JETP **73**, 929 (1991)].
[2] Yu. M. Baikov and S. L. Shokhor, Physica C **185–189**, 1589 (1991).
[3] N. M. Plakida, V. L. Aksenov, and S. L. Drechsler, Europhys. Lett. **4**, 1309 (1987).
[4] T. Galbaatar, S. L. Drechsler, N. M. Plakida, and G. M. Vujicic, Physica C **185–189**, 1529 (1991).
[5] J. R. Hardy and T. W. Flocken, Phys. Rev. Lett. **60**, 2191 (1988).
[6] J. C. K. Hui and P. B. Allen, J. Phys. F **4**, L42 (1974).
[7] N. M. Plakida, in *Statistical Physics and Quantum Field Theory* (ed. N. N. Bogolyubov), Nauka, Moscow, 1973.
[8] A. Jezowski, J. Klamut, R. Horyn, and K. Rogacki, Supercond. Sci. Technol. **1**, 296 (1989).
[9] M. F. Xu, A. Schenstrom, Y. Hong *et al.*, IEEE Trans. Magn. **25**, 2414 (1989).
[10] S. A. Gridnev, O. N. Ivanov, O. V. Dybova, Sverkhprovodimost' (KIAE) **3**(7), 1449 (1990) [Superconductivity **3**(7), 1135 (1990)].

[11] A. I. Golovashkin, O. M. Ivanenko, G. I. Leĭtus *et al.*, Pis'ma Zh. Eksp. Teor. Fiz. **46**, 325 (1987) [JETP Lett. **46**, 410 (1987)].
[12] V. Z. Krezin, Phys. Lett. A **122**, 434 (1987).
[13] J. Ranninger, Z. Phys. B **84**, 167 (1991).

Translated by D. Parsons