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Dependence of the superconducting transition temperature on the number of cuprate layers in a unit cell of high-temperature superconductors

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New bismuth and thallium high-T_c superconductors[1,2] contain several N (1, 2, 3, ...) quadratic CuO_2 planes forming sheafs between individual layers of thallium oxides. Neighboring CuO_2 layers in the sheafs are separated by Ca(Sr) ions.

The first theoretical investigation of the dependence of T_c on the number of CuO_2 layers within a sheaf was carried out by Anderson et al.[3] Birman and Lu[4] applied the Ginzburg–Landau approximation to new high-T_c superconductors. They determined the upper limit of T_c equal to 140 K for monolayer and bilayer thallium families. In several works, the dependence on the number of CuO_2 layers in a unit cell was calculated by using the microscopic formulation of the generalized BCS theory.

Eab and Tang[5,6] derived expressions for the critical temperature T_c of superconductors with N layers on the basis of the Ginzburg–Landau phenomenological model by using energy minimization. Using the experimental values of T_c for the first members of a series, the values of T_c for other members can be determined.

The theory of layered crystals with any number of interacting layers within a unit cell was developed by Jha[7] (see also Refs. 8 and 9).

In all works, it was shown that the value of T_c increases monotonically with the number of layers in sheafs and attains a constant value for $N > 10$. However, experiments carried out in 1989 by Kikuchi et al.[10] revealed that this is not true. The authors of Ref. 10 synthesized the superconductor $Tl_1Ba_2CaCu_4O_{12}$ and observed a decrease in the value of T_c upon a transition from three to four layers. They also synthesized a series of superconductors $Tl_1Ba_2Ca_{N-1}Cu_NO_{2N+3}$ with the number N varying from two to five[10] and proved that the value of T_c increases with N to $N = 4$ and then decreases for $N = 5$.

It was noted in Ref. 11 that such a decrease is also observed for $N = 6$.

In the next sections, we shall explain the experimentally observed decrease in T_c for large values of N by using the bisoliton model developed at the Institute of Theoretical Physics of the Academy of Sciences of the Ukraine.[12,15]

1. ROLE OF INTERPLANE INTERACTION IN HIGH-TEMPERATURE SUPERCONDUCTIVITY

The bisoliton condensate of thallium and bismuth high-T_c superconductors are usually investigated theoretically under the assumption that the value of T_c is determined only by CuO_2 planes.

Let us suppose that a unit cell contains N quadratic CuO_2 planes. The energy of quasiparticle pairs forming the bisoliton condensate as a result of interaction of quasiparticles with longitudinal β_{nx} (along the layers) and transverse $\xi_{n\alpha}$ displacements of the sites $a_{n\alpha}$ in a crystal is characterized by the Hamiltonian[14,15]

$$\begin{aligned}\mathcal{H} = \sum_{\alpha} \varphi_{n\alpha} \{ & -J [\varphi_{n+1,\alpha} + \varphi_{n-1,\alpha}] \\ & + [W_{\perp} + W_{\parallel} + 2\sigma_{\parallel} (\beta_{n+1,\alpha} - \beta_{n\alpha}) \varphi_{n\alpha} \\ & - \mathscr{L} (\varphi_{n,\alpha+1} + \varphi_{n,\alpha-1} + 2\sigma_{\perp} (\xi_{n\alpha} - \xi_{n\alpha+1}) \varphi_{n,\alpha+1} \\ & + (\xi_{n\alpha} - \xi_{n,\alpha-1}) \varphi_{n,\alpha-1} \} \} . \end{aligned} \tag{1}$$

The index $\alpha = 1, 2, \ldots$ labels the layers in a unit cell. The index n varies from 1 to L. The functions $\varphi_{n\alpha}$ satisfy the periodic

$$\varphi_{n\alpha} = \varphi_{n+L,\alpha} \tag{2a}$$

and the boundary conditions

$$\varphi_{n0} = \varphi_{n,N+1} = 0. \tag{2b}$$

The normalization condition

$$\sum_{n=1}^{L} \sum_{\alpha=1}^{N} \varphi_{n\alpha}^2 = 1 \tag{3}$$

indicates that each sheaf of N layers contains a bisoliton.

We shall seek the wave function of a sheaf containing N planes in the form

$$\psi(\xi) = \sum_{\alpha=1}^{N} C_\alpha \bar{\varphi}_\alpha(\xi) \tag{4}$$

with the coefficients C_α satisfying the conditions

$$C_0 = C_{N+1} = 0; \quad \sum_{\alpha=1}^{N} C_\alpha^2 = 1. \tag{5}$$

The energy $E_{bs}^{(N)}$ of a sheaf containing N layers is defined by the system of equations obtained in Refs. 14, 15:

$$\chi(N) C_\alpha - \gamma [C_{\alpha+1} + C_{\alpha-1}] - \sigma [C_{\alpha+1}^2 + C_{\alpha-1}^2] = 0, \tag{6}$$

where

$$\chi(N) = \mathscr{E}_{bs}(N) - \mathscr{E}_{bs}^0. \tag{7}$$

The second term in Eq. (6) accounts for the interaction between two adjacent CuO_2 planes separated by Ca(Sr) ions. The third term takes into account the role of variation of interplane distances.

If a unit cell contains only one CuO_2 layer, we must put $\gamma = \sigma = 0$ in Eq. (6).

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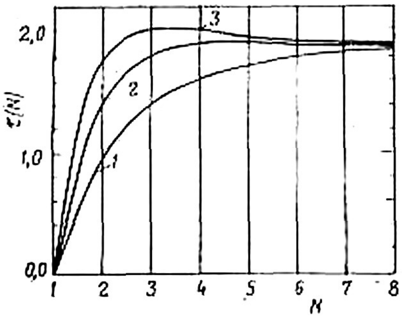

FIG. 1. Dependence of the ratio $\tau(N) = [T_c(N) - T_c(1)]/A\gamma$ for the values σ/γ = 0 (1), 0.06 (2), and 0.8 (3) on the number N of plane CuO_2 layers in unit cells of layered superconductors.

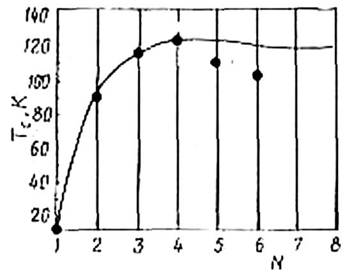

FIG. 2. Theoretical dependence (for σ/γ = 0.6) of the critical temperature T_c of a series of superconductors $Tl_1Ba_2Ca_{N-1}Cu_NO_{2N+3}$ on the number N of plane layers in unit cells. Experimental data are marked by circles.

2. ENERGY OF SHEAFS OF CuO_2 PLANES FOR A FIXED SEPARATION BETWEEN THE PLANES

If we disregard the variation of the separation between the planes in sheafs, we must put σ = 0. In this cse, Eq. (6) is reduced to

$$\varkappa(N) C_\alpha - \gamma [C_{\alpha+1} - C_{\alpha-1}] = 0 \tag{8}$$

under the additional conditions (5). Then the energy level $\mathscr{E}_{bs}^0$ of a plane splits into N sublevels due to the interaction between the layers. The roots of the equation have the following values:

$$\chi_J(N) = -2\gamma \cos[\pi J/(N+1)], \quad J = 1, N. \tag{9}$$

The energy is given by

$$\mathscr{E}_{bs}^{(J)} = \mathscr{E}_{bs}^0 - 2\gamma \cos[\pi J/(N+1)], \tag{10}$$

where $\mathscr{E}_{bs}^0$ is the energy of a layer. The superconducting state is determined by the minimum value, i.e., for J. Consequently, the critical temperature T_c of a layered superconductor is defined as

$$T_c(N) - T_c(1) = 2\gamma A \cos\frac{\pi}{N+1}, \tag{11}$$

where $T_c(1)$ is the critical temperature of a superconductor with a single plane. The coefficient A can be determined from experimental values for the first members of the series.

3. ENERGY OF A SHEAF OF CuO_2 PLANES WITH A VARYING SEPARATION

In order to calculate the energy of a sheaf of CuO_2 planes taking into account the variation of the separation between the planes, we shall, in the first approximation, make the following substitution in Eq. (6):

$$C_{\alpha+1}^2 + C_{\alpha-1}^2 \to D(N). \tag{12}$$

In this case, the system of equations (6) is transformed to

$$[\chi(N) - \sigma D(N)] C_\alpha - \gamma [C_{\alpha+1} - C_{\alpha-1}] = 0. \tag{13}$$

For a further simplification of our analysis, we shall estimate the functions $D(N)$ by using the values of C_α obtained in Sec. 2 for σ.

The critical temperature of a superconductor containing N layers is defined as

$$\tau(N) = \frac{T_c(N) - T_c(1)}{\gamma A} = 2\cos\frac{\pi}{N+1} + \frac{\sigma}{\gamma} D(N). \tag{14}$$

Figure 1 shows the $\tau(N)$ dependence for the values of σ/γ equal to 0; 0.06 and 0.8. The maximum appears on the $\tau(N)$ curve when the variation of separation between the planes is taken into account.

Using the experimental values of $T_c(N)$ for a series of $Tl_1Ba_2Ca_{N-1}Cu_NO_{2N+3}$ superconductors, we can determined the theoretical dependence of T_c on the number of CuO_2 layers in a unit cell for σ/γ = 0.6. This dependence is presented by the curve in Fig. 2. Experimental results are indicated by circles.

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