

## SOME PECULIAR FEATURES OF THE NEWEST LAYERED HIGH $T_c$ SUPERCONDUCTORS\*

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Some features of the high  $T_c$  superconductors are analysed on the basis of the bisoliton theory. They are the dependence of the transition temperature  $T_c$  on the number of layers  $N$  and the anomalous current–voltage characteristics SIN contacts. By means of the exciton theory a few normal optical properties of the high  $T_c$  materials are used as well. This is a small part of the many interesting properties of high  $T_c$  superconductors.

### 1. Introduction

It is a fundamental problem in the field of high  $T_c$  cuprates to understand the underlying physics to these compound systems.<sup>1</sup> Briefly, I shall discuss some properties of copper oxide superconductors.

All new high temperature superconductors (HTSC) are characterized by a highly anisotropic behavior along the  $c$  axis and by multidimensional structures. Cuprate superconductors are of extreme type II ( $\lambda/\xi \gg 1$ ,  $\lambda$  is the coherence length,  $\xi$  is the magnetic penetration depth). They have an anomalously high  $T_c$  (critical temperature). They are antiferromagnetic (AFM) insulators before doping.

One of the fundamental problems is still the mechanism of high temperature superconductivity. We have in the present time many mechanisms under consideration.<sup>1</sup> The nature of the mechanism of high temperature superconductivity continues to be a mystery. Progress towards understanding these materials is tied to the quality of the experimental data.<sup>2</sup> In this paper we discuss some features of the layered high  $T_c$  superconductors on the basis of the conception of the bisoliton theory.<sup>3</sup> This theory as well as the BCS theory considers the properties of HTSC below  $T_c$ . The bisoliton theory does not contradict the problem of AFM insulators before doping. This review deals with some properties of optical reflection and absorption under normal temperature using the exciton theory.

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## 2. Bisoliton Theory of High $T_c$ Superconductivity

According to a bisoliton model high  $T_c$  superconductivity<sup>3</sup> in lanthanum and yttrium superconductors, containing in their unit cells a single  $\text{CuO}_2$  layer situated parallel to the  $a$ ,  $b$  planes of the crystal, is stipulated by quasi-one-dimensional condensate bisolitons.<sup>3</sup> The bisolitons are distributed periodically in the layers along the axis  $a$  or  $b$ . One bisoliton contained in each period  $aL$  is formed by two quasiparticles (usually holes). Quasiparticles are connected in singlet spin state by a local deformation field.

In a condensate moving with the velocity  $V = \hbar k/m$ , much smaller than that of longitudinal sound,  $V_0$ , two quasiparticles with effective masses  $m$  and wave numbers  $k_1 = 2k + k_F$  and  $k_2 = -k_F$  participate in the formation of bisoliton.

In the frame  $\xi = (x - Vt)/a$  moving with velocity  $V$ , in each period  $aL$  containing one bisoliton symmetric wave, the function of the condensate bisolitons has the form

$$\Psi(\xi_1, \xi_2, t) = \sqrt{2} \Phi(\xi_1) \Phi(\xi_2) \cos[k_F(\xi_1 - \xi_2)] e^{ik(\xi_1 + \xi_2) - iE_p t}. \quad (1)$$

The real periodic functions  $\Phi(\xi) = \Phi(\xi + L)$  satisfy the normalization condition

$$\int_0^L \Phi^2(\xi) d\xi = 1. \quad (2)$$

These are the solitons to a nonlinear Schrödinger equation

$$\left( \frac{\partial^2}{\partial \xi^2} + 4g\Phi^2(\xi) - \varepsilon \right) \Phi(\xi) = 0, \quad \varepsilon = E_p/J, \quad (3)$$

determining the motion of quasiparticles in the field of deformation

$$U(\xi) = -4g\Phi^2(\xi). \quad (4)$$

Here  $E_p$  is the energy of the quasiparticle,  $g = \sigma^2/2\kappa J$  is a nondimensional parameter of the interaction between a quasiparticle and the field of deformation,  $\sigma$  is the electron-phonon interaction and  $\kappa$  is the coefficient of elasticity at a chain.  $J = \hbar^2/2ma^2$  is the energy of the exchange interaction at neighboring unit cells,  $m$  is the effective mass of a quasiparticle appearing when doping the crystal and  $a$  is a lattice constant.

In the general case the periodic solution Eq. (3) is expressed by means of the elliptic Jacobi functions. Provided that the inequality  $gL \gg 1$  is fulfilled, these functions are reduced to the hyperbolic functions

$$\Phi(\xi) = \sqrt{g/2} \operatorname{sech}(g\xi). \quad (5)$$

In this case the energy of both quasiparticles in the field of deformation (4), counted from the Fermi energy  $E_F$ , has the value

$$E_p = -g^2 J. \quad (6)$$

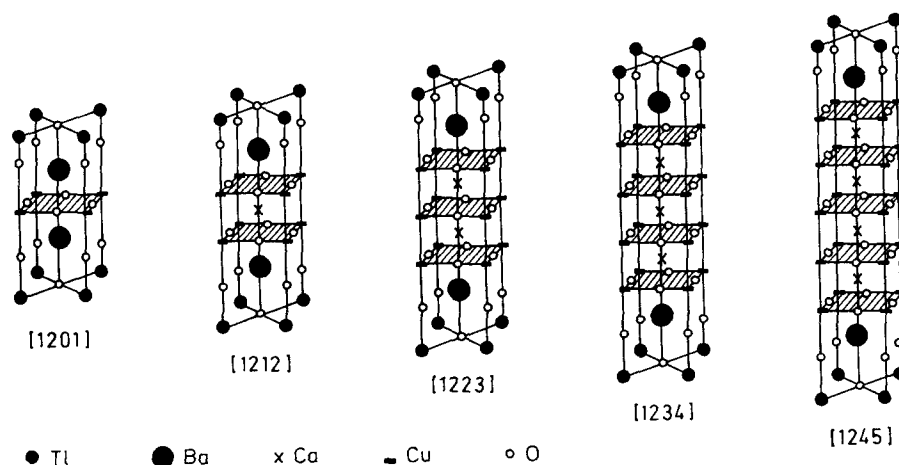


Fig. 1. The structures of the unit cells of the family of thallium oxides  $Tl_1Ba_2Ca_{N-1}CuNO_{2N+3}$  at values of  $N = 1, 2, 3, 4$ , and  $5$ .

### 3. Interlayer Effects in the Newest High $T_c$ Superconductors

New bismuth and thallium high  $T_c$  superconductors<sup>12,13</sup> contain several  $N (= 1, 2, 3 \dots)$  of quadratic  $CuO_2$  planes forming sheaves between individual layers of thallium oxides. Neighboring  $CuO_2$  layers in the sheaves are separated by  $Ca(Sr)$  ions (Fig. 1).

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.*<sup>14</sup> Birman and Lu<sup>15</sup> 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 generalized BCS theory.

Eab and Tang<sup>16,17</sup> 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 value 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 (Ref. 18, see also Ref. 19).

In all works, it was shown that the value of  $T_c$  increases monotonically with the number of layers in sheaves and attains a constant value for  $N > 10$ . However, experiments carried out in 1989 by Kikuchi *et al.*<sup>21</sup> revealed that it is not true. The authors of Ref. 21 synthesized the superconductor  $Tl_1Ba_2CaCu_4O_{12}$  and observed a decrease in the value of  $T_c$  upon a transition from three or four layers. They also synthesized a series of superconductors  $Tl_1Ba_2Ca_{N-1}CuNO_{2N+3}$ , with the number  $N$  varying from two to five, 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. 22 that such a decrease is also observed for  $N = 6$ .

The  $T_c(K)$  and the intraplanar lattice constant  $a(\text{\AA})$  dependences on the number of layers in the unit cell are given in Tables 1, 2, and 3. The highest  $T_c$  value was obtained for  $N = 4$  which has four  $\text{CuO}_2$  layers in a unit cell.<sup>21</sup>

In both single and double Tl-layered systems, the systems with the highest  $T_c$  ( $N = 4$  for the former and  $N = 3$  for the latter) have the shortest intraplanar lattice constant  $a(\text{\AA})$ . In this case too the system with the highest  $T_c$  ( $N = 3$ ) has the shortest  $a(\text{\AA})$ .

Table 1. Single Tl-layered system  $\text{Tl}_1\text{Ba}_2\text{Ca}_N\text{O}_{2N+3}$ .

$N$	1	2	3	4	5	6
$a(\text{\AA})$	—	3.8500	3.8493	3.8153	3.8469	—
$T_c(K)$	13–15	78–91	116–120	122	106	102

Table 2. Double Tl-layered system  $\text{Tl}_2\text{Ba}_2\text{Ca}_{N-1}\text{Cu}_N\text{O}_{2N+4}$ .

$N$	1	2	3	4
$a(\text{\AA})$	3.8587	3.857	3.822	—
$T_c(K)$	20–80	110	125	108–112

Table 3. Double Bi-layered system  $\text{Bi}(\text{Ca}, \text{Cr})_{N+1}\text{Cu}_N\text{O}_{2N+4}$ .

$N$	1	2	3	4
$a(\text{\AA})$	3.796	3.823	3.818	—
$T_c(K)$	12–22	85–90	110–120	90

I shall explain the experimentally observed decrease in  $T_c$  for large values of  $N$  by the following.

### 3.1. Role of interplane interaction in high temperature superconductivity

The bisoliton condensate of thallium and bismuth high  $T_c$  superconductors is usually investigated theoretically under the assumption that the value of  $T_c$  is determined only by  $\text{CuO}_2$  planes.

Let us suppose that a unit cell contains  $N$  quadratic  $\text{CuO}_2$  planes. The energy of quasiparticle pairs forming the bisoliton condensate as a result of the interaction of quasiparticles with longitudinal  $\beta_{nz}$  (along the layers) and transverse  $\xi_{n\alpha}$  displacements of the sites,  $a_{n\alpha}$ , in a crystal is characterized by the Hamiltonian<sup>5,6</sup>

$$H = \sum_{\alpha} \varphi_{n\alpha} (-J(\varphi_{n+1,\alpha} + \varphi_{n-1,\alpha}) + \{W_{\perp} + W_{\parallel} + 2\sigma_{\parallel}(\beta_{n+1,\alpha} - \beta_{n\alpha})\} \varphi_{n\alpha} - L[\varphi_{n,\alpha+1} + \varphi_{n,\alpha-1} + 2\sigma_{\perp}(\xi_{n\alpha} - \xi_{n,\alpha+1})\varphi_{n,\alpha+1} + (\xi_{n\alpha} - \xi_{n,\alpha-1})\varphi_{n,\alpha-1}]) \quad (7)$$

The index  $\alpha = 1, 2, \dots$  labels the layers in a unit cell. The index  $n$  varies from 1 to  $L$ .  $L$  is the interaction coefficient between layers. The energy of a longitudinal deformation is determined by the formulae

$$W_{\parallel} = \frac{1}{2} \kappa_{\parallel} \sum_{n\alpha} (\beta_{n+1,\alpha} - \beta_{n\alpha})^2 (\text{longitudinal}) \quad (8)$$

$$W_{\perp} = \frac{1}{2} \kappa_{\perp} \sum_{n\alpha} (\xi_{n\alpha} - \xi_{n,\alpha-1})^2 (\text{transverse}) \quad (9)$$

The functions  $\varphi_{n\alpha}$  satisfy the periodic conditions

$$\varphi_{n\alpha} = \varphi_{n+L,\alpha} \quad (10)$$

and the boundary conditions

$$\varphi_{n0} = \varphi_{n,N+1} = 0. \quad (11)$$

The normalization condition

$$\sum_{n=1}^L \sum_{\alpha=1}^N \varphi_{n\alpha}^2 = 1 \quad (12)$$

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

$$\psi(\xi) = \sum_{\alpha=1}^N C_{\alpha} \bar{\varphi}_{\alpha}(\xi), \quad (13)$$

with the coefficients  $C_{\alpha}$  satisfying the conditions

$$C_0 = C_{N+1} = 0, \quad \sum_{\alpha=1}^N C_{\alpha}^2 = 1. \quad (15)$$

The energy  $E_{bs}(N)$  of a sheaf containing  $N$  layers is defined by the system of equations obtained in Ref. 4:

$$\chi(N)C_{\alpha} - \gamma(C_{\alpha+1} + C_{\alpha-1}) - \sigma(C_{\alpha+1}^2 + C_{\alpha-1}^2)C_{\alpha} = 0, \quad (16)$$

where

$$\chi(N) = E_{bs}(N) - E_{bs}^0, \quad (17)$$

$E_{bs}^0$  being the energy of a layer,  $\gamma = L/J$ , and  $2\sigma = \delta^2/\kappa J$ .

The second term in Eq. (16) accounts for the interaction between two adjacent  $\text{CuO}_2$  planes separated by  $\text{Ca}(\text{Sr})$  ions. The third term takes into account the role of variation of interplane distances.

If a unit cell contains only one  $\text{CuO}_2$  layer, we must put  $\gamma = \sigma = 0$  into Eq. (16).

### 3.2. Energy of sheaves of $\text{CuO}_2$ planes for a fixed separation between the planes

If we disregard the variation of the separation between the planes in sheaves, we must put  $\sigma = 0$ . In this case, Eq. (16) is reduced to

$$\chi(N)C_\alpha - \gamma(C_{\alpha+1} - C_{\alpha-1}) = 0 \quad (18)$$

under the additional conditions (15). Then the energy level  $E_{\text{bs}}^0$  of a plane splits into  $N$  sublevels due to the interaction between the layers. The roots of the equation have the following values:

$$\chi(N) = -2\gamma \cos[\pi J/(N+1)], \quad J = 1, N. \quad (19)$$

The energy is given by

$$E_{\text{bs}}^{(J)} = E_{\text{bs}}^0 - 2\gamma \cos[\pi J/(N+1)], \quad (20)$$

where  $E_{\text{bs}}^0$  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

$$T_c(N) - T_c(1) = 2\gamma A \cos \frac{\pi}{N+1}, \quad (21)$$

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.

### 3.3. Energy of sheaves of $\text{CuO}_2$ planes with a varying separation between the planes

In order to calculate the energy of a sheaf of  $\text{CuO}_2$  planes taking into account the variation of the separation between the planes, we shall, in the first approximation, make the following substitution into Eq. (16):

$$C_{\alpha+1}^2 + C_{\alpha-1}^2 \rightarrow D(N). \quad (22)$$

In this case, the system of equations (16) is transformed to

$$[\chi(N) - \sigma D(N)]C_\alpha - \gamma(C_{\alpha+1} - C_{\alpha-1}) = 0. \quad (23)$$

For a further simplification of our analysis, we shall estimate the functions  $D(N)$  by using the values of  $C$  obtained in Sec. 3.1. The critical temperature of a superconductor containing  $N$  layers is defined as<sup>4</sup>

$$t(N) = \frac{T_c(N) - T_c(1)}{\gamma A} = 2 \cos \frac{\pi}{(N+1)} + \frac{\sigma}{\gamma} D(N). \quad (24)$$

The dependences of the functions  $2\cos[\pi/(N+1)]$  and  $D(N)$  on  $N$  are shown in Table 4.

Table 4. Dependence of the functions  $2\cos[\pi/(N+1)]$  and  $D(N)$  on  $N$ .

$N$	2	3	4	5	6	7	10	12	15
$2\cos[\pi/(N+1)]$	1.0	1.41	1.62	1.73	1.80	1.85	1.90	1.94	1.96
$D(N)$	1.0	0.66	0.55	0.30	0.17	0.10	0.08	0.02	0.01

Table 5. Dependence of  $t(N)$  on the number  $N$  of sublevel in the sandwich.

$\sigma/\gamma$	$N$					
	2	3	4	5	6	7
0.6	1.60	1.80	1.95	1.91	1.90	1.91
0.8	1.80	2.15	1.06	1.97	1.93	1.93

The functions  $D(N)$  is described by the average distribution of the probability of the presence of one bisoliton on a single layer sandwich. Naturally the value  $D(N)$  is diminished when the number  $N$  of sublevels in the sandwich is increased.

Using the values of Table 4 we obtain the function  $t(N)$  which is proportional to  $T_c$ . The values of  $t(N)$  for two values of  $\sigma/\gamma$ , 0.6 and 0.8, are shown in Table 5 as a function of the number of layers ( $N$ ).

According to Eq. (24) the maximal value  $t(N)$  corresponds to the maximal critical temperature and minimal average value of the intraplanar lattice constant  $a(\text{\AA})$ . These theoretical results correspond to the experimental data shown in Tables 1, 2, and 3.

In Fig. 2 the dependence of  $t(N)$  on  $N$  is shown for the values of  $\sigma/\gamma$  equal to 0, 0.6, and 0.8. The presence of the maximum value on the curve of  $t(N)$  is an obvious consequence of taking into account the displacement of the intraplanar distance in the sandwich.

Using the experimental values of  $T_c(N)$  for the family of superconductors  $\text{Ti}_1\text{Ba}_2\text{Ca}_{N-1}\text{Cu}_N\text{O}_{2N+3}$  one can obtain at  $\sigma/\gamma = 0.6$  the theoretical dependence of  $T_c$  on the number of  $\text{CuO}_2$  layers in the unit cell. This dependence is shown by the curve in Fig. 3. The experimental values are indicated by circles.

We should note that the coefficients  $A$  and  $\gamma$  will be different for various materials, so we define the distribution for each material. This dependence is phenomenological because  $A$  and  $\gamma$  are defined from experiment for the first two points (Table 1). In Fig. 3  $T_c(N)$  agrees with the experimental data well but for  $N = 5$  and 6 we have a deviation. This deviation may be explained by the fact that we used the first approach. To obtain more exact dependence it is necessary to use the next approaches. In Refs. 4 and 5 we have shown that the observed nonmonotonic dependence with the maximum at some layers can be explained if one takes into

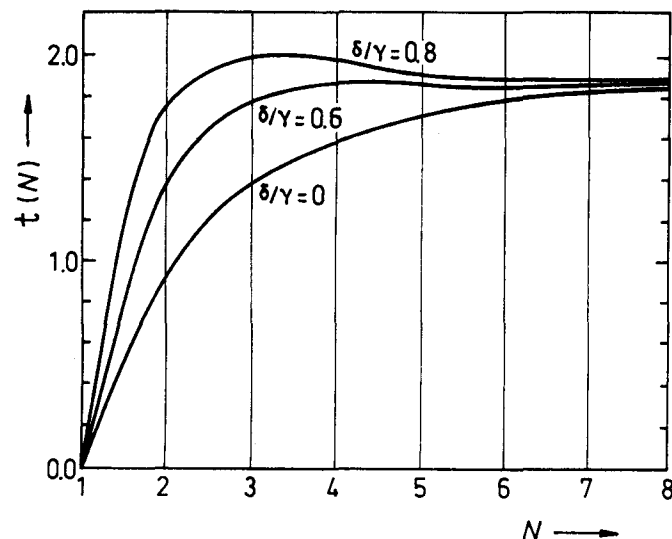


Fig. 2. Dependence of the ratio  $t(N) = [T_c(N) - T_c(1)]/A\gamma$  for the values of  $\sigma/\gamma = 0(1)$ ,  $0.6(2)$ , and  $0.8(3)$  on the number  $N$  of plane  $\text{CuO}_2$  layers in the unit cells of layered superconductors.

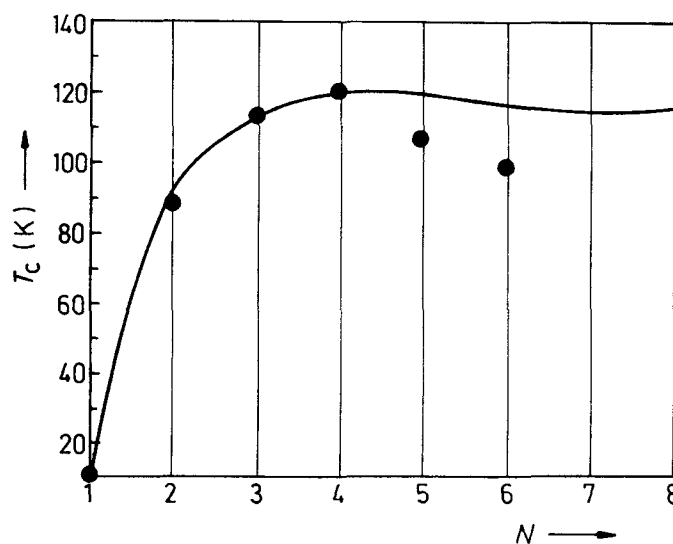


Fig. 3. Theoretical dependence for  $\sigma/\gamma = 0.06$  of the critical temperature  $T_c$  of a series of superconductors  $\text{Tl}_1\text{Ba}_2\text{Ca}_{N-1}\text{Cu}_N\text{O}_{2N+3}$  on the number  $N$  of plane layers in unit cells. Experimental data are marked by circles.



account the changing of intraplanar distances, arising with the generation of bisolitons. Another explanation for nonmonotonic dependence  $T_c(N)$  is given in Ref. 32 in the framework of the plasmon mechanism of superconductivity.

This paper obtains actual with the creation of the compound  $(\text{Ca}_{1-x}\text{S}_{2x})_{1-y}\text{CuO}_2$  with an “infinite” number of  $\text{CuO}_2$  layers.<sup>23</sup>

#### 4. Anomalous Current–Voltage Characteristics SIN Contacts

This section deals with the following peculiarities of SIN contacts of IVC and explains them in terms of a bisoliton HTSC theory:

- (i) A direct result of such states of the superconductor is the asymmetry of the current–voltage dependences in tunneling systems with respect to the sign of the applied field (the dependence of the superconducting transition dielectric gap on the direction of current in the tunneling metal–insulator–superconductor systems.<sup>24,25</sup>
- (ii) Substructures of current–voltage dependences.<sup>24,25</sup>

##### 4.1. Superconducting gaps

In Ref. 6 superconducting gaps were calculated:

$$\Delta = \frac{4E_F}{\nu} \sinh^{-1}(1/\lambda), \quad \lambda = N(E_F)G, \quad (25)$$

where  $G = \sigma^2/\kappa$  is the parameter characterizing the electron–phonon interaction. In soliton theory  $G$  determines the nonlinearity of the system,  $\nu$  is the number that determines the relative part of carriers participating in the creation of the superconductivity condensate,  $\nu = 1, 2, 3 \dots$  and satisfies equation  $k_F L = 2\pi\nu$ , where  $L$  is the period bisoliton condensate.

The energy spectrum of particles is divided into two bands (Fig. 4):

$$E_{1,2}(k) = \frac{\varepsilon(k) - \varepsilon(k - 2k_F) - 2E_F}{2} \pm \sqrt{\left(\frac{\varepsilon(k) + \varepsilon(k - 2k_F)}{2}\right)^2 + \Delta^2}. \quad (26)$$

The upper band is empty and the lower one is occupied by electrons. As shown in (6) in a quasi-one-dimensional system,  $\Delta$  is a function of the wave factor  $k_F = mG/8\pi\hbar^2$ , or  $\lambda = 0, 5$  (Fig. 5).

##### 4.2. Superconducting current

In a superconductor with a current ( $Q \neq 0$ ), the energy spectrum is deformed, and the symmetry relative to the sign inversion of the momentum is violated (see Fig. 2). Such an asymmetric electron distribution is responsible for the emergence of a nonattenuation superconducting current  $I_s$  given by

$$I_s = \sum_k \frac{eh}{2mi} \left( \Psi_k \frac{\partial \Psi_k^*}{\partial x} - \Psi_k^* \frac{\partial \Psi_k}{\partial x} \right), \quad (27)$$

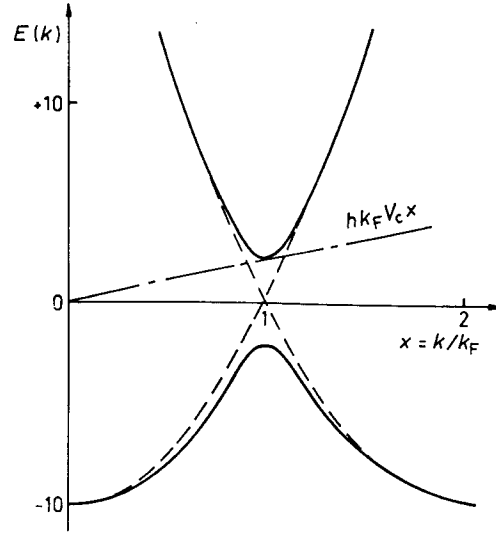


Fig. 4. Energy structure of one-particle spectrum in the superconducting state; the dot-dashed line corresponds to the normal state.  $\mu = 10$ ,  $\Delta = 2$  in relative units.

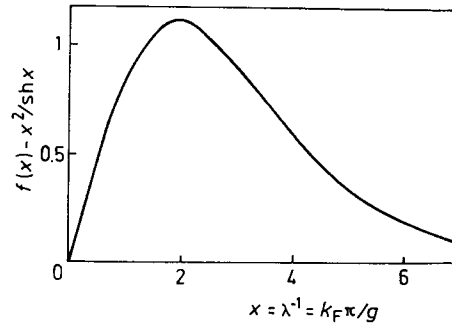


Fig. 5. Dielectric gap  $\Delta$  as a function of the wave number  $\pi k_F / g$ .

where the wave function  $\psi_k(x)$  is defined in Ref. 7. This current oscillates with time at a frequency  $\omega = \hbar k_F Q / m$ . According to Ref. 7, its mean value is

$$\langle I_s \rangle = \lim_{T \rightarrow \infty} \int_{-T/2}^{T/2} I(t) dt = \frac{e V k_F}{\pi} (1 - \Delta / E_F). \quad (28)$$

As the superconducting current increases in proportion to the velocity of bisolitons, the top of the lower band (filled with electrons) is raised and the bottom of the upper (empty) band is lowered. When they reach the same level, a fraction of electrons go over to the unfilled band, and the system acquires a resistance. Consequently, such a system offers no resistance to the current only when

$$\Delta_{\text{eff}} = E_{\text{up}}(k = -|k_F| + Q/2) - E_l(k = |k_F| + Q/2) > 0. \quad (29)$$

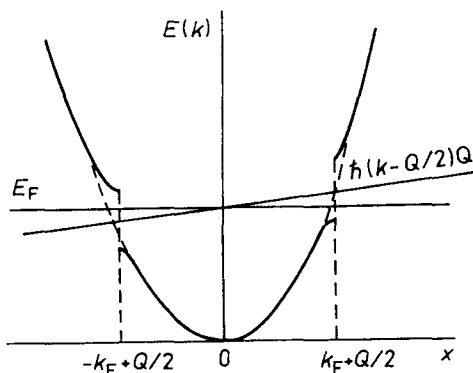


Fig. 6. The energy structure of the one-particle spectrum of a bisoliton in the superconducting state with a current ( $Q \neq 0$ ).

Following Ref. 7 we obtain

$$\Delta_{\text{eff}} = \Delta - 2\hbar k_F V > 0 \quad (30)$$

( $\Delta_{\text{eff}}$  characterizes the effective dielectric gap width in a superconductor with a current). Thus, we can derive the following expressions for the critical velocity  $V_{\text{er}}$  and the critical current ( $I_{\text{er}}$ ):

$$\begin{aligned} V < V_{\text{er}} &= \frac{\Delta}{2\hbar k_F}, \\ \langle I_s \rangle < \langle I_{\text{er}} \rangle &= \frac{e\Delta}{2\pi\hbar} \left( 1 - \frac{\Delta}{k_F} \right). \end{aligned} \quad (31)$$

In a system with a current  $I < I_{\text{er}}$  in the superconducting state, there is no scattering of charge carriers which would not violate the asymmetry of energy bands. The same situation holds at finite temperature below the critical value. In this case, the charge carriers generated by thermal excitations are in equilibrium and do not participate in the transport of current. Thus, we arrive at the two-component Fermi gas, one component of which is superconducting and the other is normal. A drift of the normal component is accompanied by energy dissipation and liberation of Joule heat.

The superconducting gaps expression is

$$2\Delta = \frac{8k_F^2 J}{\nu(1 - Q^2/4k_F^2)} \sinh^{-1} \left( \frac{k_F \pi}{g} \right). \quad (32)$$

Let us give the comparison with experiment. If  $Q = 0$ , the current is absent, and the formula describes the dependence of  $k_F$  (see Fig. 5) which agrees with the experimentally observed dependence of the gap on the doping concentration.<sup>3</sup> The dependence on  $\nu$  is well described by the simplified formula (multigap

superconductivity<sup>30</sup>)  $\Delta = (\Delta_0/\nu)(\nu = 1, 2, 3 \dots)$ . Two energy gaps with the values  $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$ , observed simultaneously in Ref. 30 during point contact spectroscopy of  $2\Delta_1 = 13.3$  MeV and  $2\Delta_2 = 26$  MeV, correspond to the values  $\nu = 1$ ,  $\nu = 2$ , and  $\Delta_2/\Delta_1 = 2$  in the above model of superconductivity. According to the tunnel measurement<sup>31</sup> a multigap pattern is also observed in superconducting  $\text{LaSrCuO}$  film with gap width equal to 20, 30, and 60, respectively. This relation between the gaps can be compared with the values  $\nu = 3, 2$ , and 1. We can observe the dependence on  $Q$  by the displacement  $\sigma$  which characterizes the asymmetric JVC included in the next section.

#### 4.3. Current–voltage characteristics

The deformation of the energy spectrum by a superconducting current leads to peculiarities in the current–voltage characteristics of metal–insulator–superconductor systems, which can be observed experimentally. The current through a metal–insulator–superconductor junction is determined with the help of the barrier transmission coefficient which has a constant value<sup>7</sup>:

$$I = \frac{e}{2\pi\hbar} \rho \int P[f_1(E) - f_2(E)]d\xi + \langle I_s \rangle \quad (33)$$

( $\rho$  is the density of electrons incident on barriers in the metal and  $f_{1,2}(E)$  are the Fermi distribution functions for electrons in the metal and superconductor, respectively). The component  $\langle I_s \rangle$  in formula (33) is due to the possibility of tunneling through a barrier directly from the lower band of the superconductor to a state in the metal below the Fermi level (and in the opposite direction for the reverse current) in the bisoliton theory of superconductivity (in view of the violation of symmetry in the electronic distribution). Such a tunneling resembles the Josephson current in a superconductor–insulator–superconductor system. The current in the outer layer of the metal is normal.

In Ref. 7 we calculated the current–voltage characteristics. Figure 7 shows the current  $I$  (curve 1) and conductivity  $dI/d\varphi$  (curve 2) as functions of the applied voltage  $\varphi$  at temperature  $k_B T/\Delta = 0.1$ . In the temperature region near  $T = 0$ , we obtain the following expression for  $\Delta_{\pm}$  at  $\varphi = 0$ :

$$\begin{aligned} \Delta_+ &= \Delta - Jk_F Q a^2, & \Delta_- &= \Delta + Jk_F Q a^2, \\ \sigma &= \Delta_+ - \Delta_- = 2Jk_F Q a^2 = 2\alpha\Delta. \end{aligned} \quad (34)$$

#### 4.4. Substructures of current–voltage dependences

The superconducting band substructure revealed in a good deal of experiments in HTSC has not yet been explained unambiguously. It is apparent that the comprehension of the reasons inducing the substructure is associated with the peculiarities of the superconductivity mechanism. As was noted in Refs. 23 and 24, the multi-band structure may arise in the bisoliton theory, and this is caused by the existence of a periodic structure of the bisoliton.

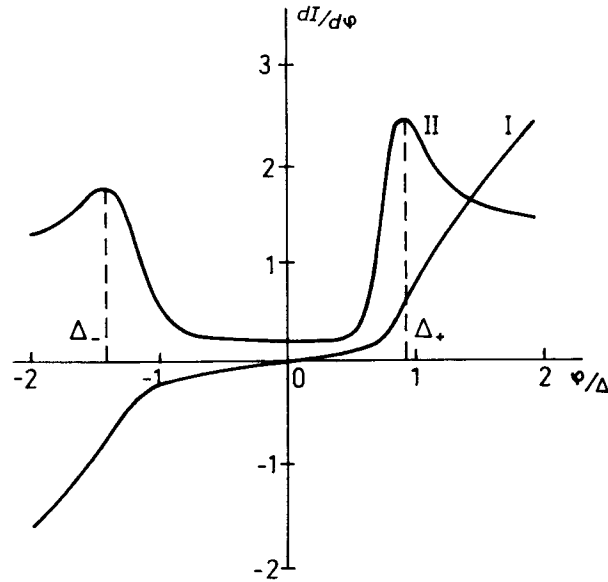


Fig. 7. Characteristic (curve I) and dependence of conductivity  $dI/d\varphi$  on voltage  $\varphi$  (curve II) for superconducting current.

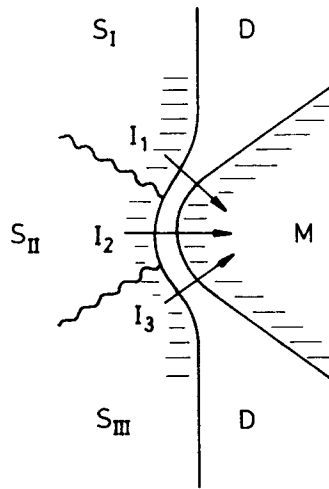


Fig. 8. The metal-dielectric-superconductor structure.

We consider the system composed of the metal in the normal state, the dielectric barrier, and superconductor (Fig. 8). When the contact is formed between the metal needle and the superconductor surface the latter in the near surface region can be characterized by the different concentration values of carriers and the parameter

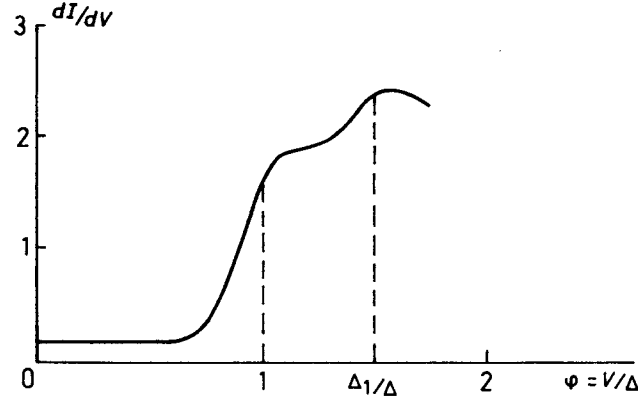


Fig. 9. The conductivity dependence on the external potential for the inhomogeneous superconductor with  $\Delta_2/\Delta_3 = 3/2$ .

$\nu$  in each of the regions  $S_i$ . As the concentration changes the gap value changes continuously, the  $\nu$  variation leads, according to Ref. 6, to the jumplike change of the gap.

As is suggested in Ref. 7 the total current in such a system can be represented as a sum of tunneling currents from each superconductor region to the metal contact. Thus, the total current that runs through a system is determined by

$$I = \sum I_i, \quad (35)$$

where  $I_i$  is determined by (I).

The dependence of the conductivity  $\sigma = dI/dV$  on the magnitude of the applied voltage for the case of homogeneous superconductors composed of two regions with  $\Delta_2/\Delta_3 = 3/2$  at  $k_B T/\Delta = 0.1$ ,  $I_{02}/I_{03} = 0.75$  is shown in Fig. 9. The current-voltage dependences of this type are observed for many HTSC.<sup>24,26</sup> It should be noted that the values of  $\Delta$  obtained experimentally are well described by the empirical function  $\Delta_n = \Delta_0/n$ ,  $n = 1, 2, 3, \dots$

### 5. Interlayer Interaction in the Reflection Spectra of Bismuth HTSC Crystals

In this section we consider normal properties of HTSC. We explain interesting experiments of the reflection spectra<sup>27</sup> of bismuth crystals. We follow Refs. 9–11. Considerable efforts are focused on studying the optical properties of  $\text{Bi}_2\text{Sr}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_{2n+4}$  compounds. In particular, there is a great interest on how the  $\text{Bi}_2\text{O}_2$  layers affect essentially the physical properties, optical ones induced, of these crystals. The fact that peculiarity of  $E \sim 4$  eV in  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$  and  $\text{Bi}_2\text{Sr}_2\text{CuO}_6$  crystals consists of several peaks and forms relatively intensive and

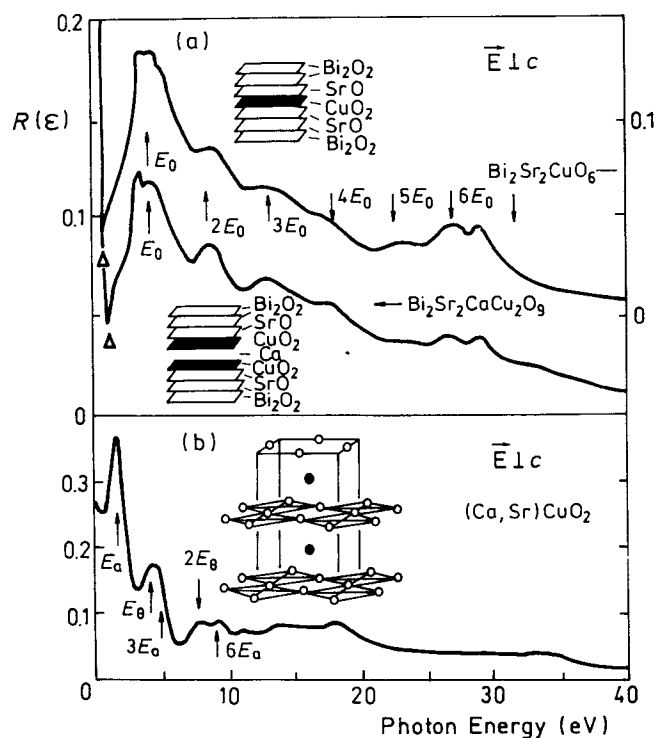


Fig. 10. Experimental reflection spectra  $R(\epsilon)$  for the crystals: (a)  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  and  $\text{Bi}_2\text{Sr}_2\text{CuO}_6$ , (b)  $(\text{Ca},\text{Sr})\text{CuO}_2$ .

wider reflection band than in  $(\text{Ca},\text{Sr})\text{CuO}_2$  (Figs. 10(a) and (b)) implies that excitations in  $\text{CuO}_2$  layer, as in  $\text{Bi}_2\text{O}_2/\text{SrO}$  layers, give probably the total contribution to this wide reflection peak. Generally speaking, the  $\text{Bi}_2\text{O}_2/\text{SrO}$  layers can also be isolating and have no direct relation to superconductivity.

### 5.1. Model of crystal

According to experimental data we shall assume the conducting planes and nonconduction  $\text{Bi}_2\text{O}_2/\text{SrO}$  layers to be isolated and the excitations, effected in them, to be preserved well enough in zero approximation. Thus, such a crystal can be regarded as a unidimensional molecular crystal where the above planes interacting between themselves play the role of molecules. One can use here the approach well known in the theory of molecular crystals,<sup>28</sup> having noted one important point: not all layers involved in the unit cell are identical. Frequencies of the transitions in them are specified somewhat different so that this situation is more close to the case of combined Fermi–Davydov resonance<sup>28</sup> where the frequencies in a single molecule can be different.

Let the number of frequencies in the unit cell of crystal be  $\sigma$ , then the wave functions of the ground  $\psi^0$  and excited  $\psi$  states, and also the Hamiltonian operator of such layered crystal, can be written as

$$\psi^0 = \prod_{n=1}^{\sigma V} \varphi_{n\alpha}^0, \quad (36)$$

$$\psi = \sum c_{n\alpha} \varphi_n, \quad (37)$$

$$H = \sum_{n=1}^{\sigma N} H_{n\alpha} + \frac{1}{2} \sum_{n\alpha \neq m\beta} V_{n\alpha, m\beta},$$

$$H_{n\alpha} = E_{n\alpha} \varphi_{n\alpha}, \quad H_{n\alpha} \varphi_{n\alpha}^0 = E_{n\alpha}^0 \varphi_{n\alpha}^0. \quad (38)$$

Here  $N$  enumerates the number of unit "layered" cells in the main region of the crystal cycle,  $\varphi_{n\alpha}^0$  and  $\varphi_{n\alpha}$  are the wave functions of an isolated layer in the ground and excited states, respectively,  $H_{n\alpha}$  is the Hamiltonian of an isolated layer,  $V_{n\alpha, m\beta}$  is the interaction operator of  $n\alpha$  and  $m\beta$  layers, and  $a_{n\alpha}$  are the probability amplitudes because of the fact that the excitation obeying the normalization condition arises in the layer. The excitation energy of the crystal, containing  $\sigma$  molecules in the unit cell, is determined by the standard expression which after the Fourier transformation takes the form

$$\Delta H = \sum_{\kappa\alpha} a_{\kappa\alpha}^* a_{\kappa\alpha} (\Delta\varepsilon_\alpha + D_\alpha) + \sum_{\kappa\alpha\beta} a_{\kappa\alpha}^* a_{\kappa\beta} M_{\alpha\beta}(\kappa), \quad (39)$$

$$\Delta\varepsilon_{n\alpha} = \Delta\varepsilon_\alpha, \quad D_{n\alpha} = D_\alpha, \quad M_{\alpha\beta}(\kappa) = \sum_m H_{n\alpha, m\beta} e^{i\kappa(m-n)}. \quad (40)$$

Here  $\kappa$  is one-dimensional wave vector directed perpendicularly to the layers, i.e. along the crystal axis.

### 5.3. Dielectric function of crystal

To study the spectral distribution within the transitions it is convenient to go over the second quantization representation. According to the known procedure (see, e.g. Ref. 28) the excitation energy operator of the crystals conserves, in Heitler-London approximation, the previous form,<sup>28</sup> where the values  $a_{\kappa\alpha}^+$  and  $a_{\kappa\alpha}$  can now be regarded as the Bose operators.

The dielectric function is expressed through the dipole moment operators:<sup>28</sup>

$$\varepsilon_{xx}(\kappa\omega) = \varepsilon_{0xx} - \frac{4\pi}{\nu} \sum_{\alpha\beta} d_\alpha d_{\beta\alpha} \langle\langle (a_{\kappa\alpha} + a_{\kappa\alpha}^+)_{\tau}, (a_{-\kappa\beta} + a_{\kappa\beta}^+) \rangle\rangle_{\omega}. \quad (41)$$

Here  $\nu = ls$  is the unit cell volume,  $l$  is the dimension along the axis, and  $s$  is the layer area. In the layer axis  $|x, y|$  the crystal lattice is square, thus  $\varepsilon_{0x} \Rightarrow \varepsilon_0$ , and  $d_\alpha$  is dipole moment of layer  $\alpha$ . Green's function was calculated in Refs. 9 and 10.



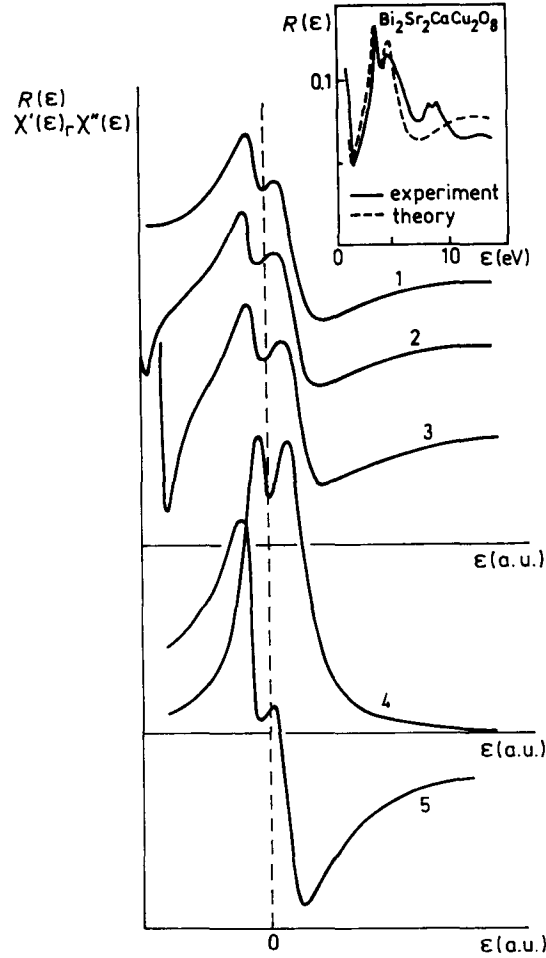


Fig. 11. The spectral dependence of the reflection coefficient  $R(\omega)$  in the region of mixed  $\text{CuO}_2\text{Bi}_2\text{O}_2/\text{SrO}$  transition for the four-layered crystal under varying interaction parameter of the layers of different origin ( $\chi'$ ,  $\chi''$  — real part and imaginary part of the dielectric function).

#### 5.4. Reflection coefficient

The reflection coefficient is determined by the following equation:<sup>9</sup>

$$R(\omega) = \left| \frac{n(\omega) - 1}{n(\omega) + 1} \right|^2 = \frac{(n - 1)^2 + \kappa^2}{(n + 1)^2 + \kappa^2}, \quad (42)$$

where the complex refractive index  $n(\omega) = n + i\kappa$  is connected with the dielectric permeability function

$$\varepsilon(\omega) = \varepsilon' + i\varepsilon'' = n^2(\omega) = (n + i\kappa)^2. \quad (43)$$

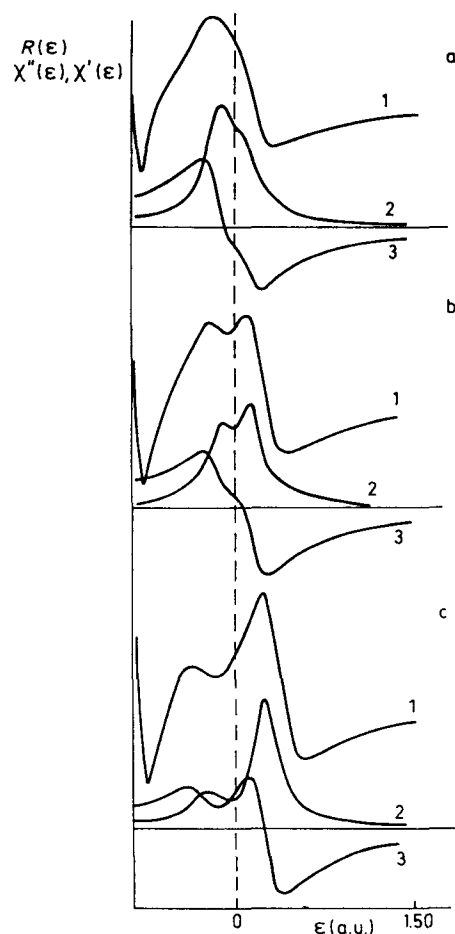


Fig. 12. Change in the reflection spectrum  $R(\omega)$  for the three-layered crystal under varying parameter  $a$ : (a)  $a = 0$ , (b)  $a = 0.05$ , (c)  $a = 0.15$ .

As is shown in Fig. 11, the calculations based on this model give good results and represent the experimental data quite well. It can also be seen in Fig. 12 that the parameter  $a$  which defines the matrix element of interaction of Cu plane with Bi plane plays a very important role. The approach based on the molecular crystals correlates with the Freeman conclusions<sup>29</sup> about the possible important role of excitons arising in the layers separating the  $\text{CuO}_2$  layers for HTSC crystals.

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