High-temperature superconductivity and the characteristics of the electronic energy spectrum

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The possibility is indicated of applying the theory of superconductors with overlapping energy bands to describe the thermodynamic and electromagnetic properties of the high-temperature compounds $La_{2-x}(Ba,Sr)_xCuO_4$ and $YBa_2Ci_3O_{7-\delta}$. The two-band model was used to obtain high values of T_c, two energy gaps $2\Delta_1/T_c > 3.5$ and $2\Delta_2/T_c < 3.5$, large negative values of d ln T_c/d ln V (V is the volume) in lanthanum ceramics, small values of the jump in the electron heat capacity at $T = T_c$, negative curvature of the upper critical magnetic field H_{2c} near the transition temperature, etc. Such behavior of the above quantities is observed experimentally. A description is also obtained of the decrease in T_c as the disordering of oxygen increases, and also as copper atoms are replaced by a nonmagnetic impurity (Al, Zn, etc.). The main mechanism responsible for this decrease is the interband scattering of electrons by impurities and by randomly distributed oxygen vacancies. A theory has been developed of multiband superconductors which takes into account the points of high symmetry in momentum space. On the basis of this theory one can explain the existence of a plateau in the dependence of T_c on δ for $YBa_2Cu_3O_{7-\delta}$, and also in the dependence of T_c on x for $La_{2-x}(Ba,Sr)_xCuO_4$, that has been observed in a number of experiments. Moreover this theory also explains the presence of two maxima in the dependence of T_c on pressure for $Bi_2Sr_2CaCu_2O_8$.

1. INTRODUCTION

The discovery of high-temperature superconductivity in

$La_{2-x}(Ba, Sr)_xCuO_{4-\delta}$ ($T_c \sim 40$ K), $YBa_2Cu_3O_{7-\delta}$ ($T_c \sim 90$ K)

and other ceramics has stimulated experimental research on the properties of these materials. In particular, the oxygen composition, the effect of substitution of copper atoms by other metals, and the effect of neutron irradiation on the superconducting properties of metal-oxide ceramics has been studied very intensively.

A large number of theoretical models and mechanisms have been proposed to explain this phenomenon and to explain the rich variety of magnetic and superconducting properties of these materials. Besides the usual mechanism of superconductivity based on the electron-phonon interaction,[1-5] mechanisms have been proposed based on excitons,[6] holes,[7] magnetic interactions,[8] the interference between dielectric and superconductor correlations,[9] and so on.

Band-structure calculations[10-13] show that in these compounds the Fermi surface can pass through points of high symmetry corresponding to an electronic topological Lifshits transition.[14] In addition, in these compounds several of the energy bands overlap on the Fermi surface.[13,15] For example, in $YBa_2Cu_3O_{7-\delta}$, the number of bands overlapping on the Fermi surfaces increases with the number of oxygen atoms:[15] there are two overlapping energy bands when $\delta = 1$ and three when $\delta = 0$. This suggests that metal-oxide ceramics can be described using the multiband theory of superconductivity.[16-19] An increase in the number of energy bands on the Fermi surface leads to an increase in the total density of electron states, and also to an additional interband electron-electron interaction, which favors the superconducting state. This interaction destroys the validity of the universal BCS relations, and the thermodynamic characteristics depend significantly on the properties of the anisotropic system.

An interesting feature of the two-band model is that the temperature of the superconducting transition T_c is independent of the sign of the interband electron-electron interaction constant. Hence we can use the two-band model for the usual electron-phonon mechanism of superconductivity, and also for the mechanism based on repulsive interactions between carriers belonging to different bands.

These features of the band structure explain the experimental behavior of the thermodynamic and electromagnetic characteristics of metal-oxide ceramics. In particular, assuming moderate values of the coupling constants, the two-band model predicts a high value of T_c, two energy gaps $2\Delta_1/T_c > 3.5$, $2\Delta_2/T_c < 3.5$, a large negative value of dln T_c/dln V (V is the volume), a positive curvature of the upper critical field near the transition temperature, and so on.[20-25] These properties have been observed in a number of experiments.[26-29] It has been suggested[30] that a gapless state in a pure two-band system can occur for a fairly strong interband interaction and may explain the observed linear temperature dependence of the heat capacity in high-temperature superconductors in the low-temperature region.[31] In

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addition, the two-band model can explain the decrease in T_c with increasing oxygen disorder and also with the replacement of copper atoms by a nonmagnetic impurity (Al, Zn, and so on).[23,32] In Refs. 23 and 32 it was assumed that the basic mechanism responsible for the decrease in T_c is interband scattering of electrons by randomly distributed oxygen vacancies or by impurities. Also the position of the Fermi level plays an important role in determining T_c. Alloying or the introduction of oxygen can change the position of the Fermi level and force it to pass through special critical points of the energy spectrum, leading to an electronic topological transition. The dependence of T_c on the position of the chemical potential was considered in the two-band model in Ref. 25.

The purpose of the present review article is to consider the application of the multiband model[16] to high-temperature superconductors and to extend this theory to the case when points of high symmetry in momentum space are located near the Fermi level.

The basic assumptions of the theory of superconductivity with overlapping energy bands are discussed. A model Hamiltonian is formulated describing the system and the main conclusions of the theory are presented. The differences between the basic formulas of the microscopic theory of multiband superconductors and the universal relations of the BCS–Bogolyubov theory are pointed out. These differences depend on the properties of the material and hence may explain the diversity of observed properties of superconductors, including high-temperature superconductors. Since at the present time there is no available theoretical approach capable of explaining the thermodynamic, magnetic, and superconducting properties of high-temperature superconductors from a unified point of view, it is useful to try to explain individual aspects of this many-sided problem from the point of view of the multiband mechanism of superconductivity.

We note that current theories of band spectra in complex materials can describe the band structure adequately, but not exactly. Hence the application of the multiband theory to high-temperature superconductor compounds is to a certain degree problematical. Nevertheless the existence of overlapping energy bands on the Fermi surface is certain and so it is reasonable to use this theory to explain the properties of high-temperature superconductors.

The two-band model is used in Sec. 2 to describe the thermodynamic properties of $La_{2-x}(Ba,Sr)_xCuO_4$ (one wide band and one narrow band) and $YBa_2Cu_3O_{7-\delta}$ (both bands with the same width).

The temperature dependence of the upper critical field H_{c2} in high-temperature superconductors is considered in Sec. 3 with the help of the two-band model.

The effect of oxygen disorder and impurities replacing Cu in $YBa_2Cu_3O_{7-\delta}$ is considered in Sec. 4. Interband scattering of electrons by impurities turns out to be the basic mechanism leading to the decrease of the transition temperature T_c with increasing oxygen vacancies or impurity atoms.

In Sec. 5 we consider the usual electron-phonon mechanism of superconductivity in the two-band model with strong anisotropy and extremum points in **k** space, which lead to electronic topological transitions when oxygen atoms are introduced into the system. The formation of flat regions on the Fermi surface will be considered, as well as cylindrical cavities.

The dependence of T_c on the filling of the energy bands is considered in the model of three overlapping energy bands, assuming that superconductivity is due only to the effective interband interaction of holes and that the sign of the effective interaction does not affect T_c. Then this interaction can be extended over a large part of **k** space and the integrals in the equations determining T_c can be cut off at an energy of the order of electronic energy.

2. THERMODYNAMIC PROPERTIES

The Hamiltonian describing a two-band system has the form[16]

$$H = \sum_{n,\mathbf{k},\sigma} \varepsilon_n(\mathbf{k}) a^+_{n\mathbf{k}\sigma} a_{n\mathbf{k}\sigma} - \sum_{n,m,k,k'} V_{nm}(\mathbf{k},\mathbf{k}') a^+_{n\mathbf{k}\uparrow} a^+_{n,-\mathbf{k}\downarrow} a_{m,-\mathbf{k}'\downarrow} a_{m,\mathbf{k}'\uparrow}, \tag{2.1}$$

where ε_n is the energy of electrons in the nth band ($n,m = 1,2$), V_{nm} are the effective matrix elements of the interband interaction, $a^+_{n\mathbf{k}\sigma}$ and $a_{n\mathbf{k}\sigma}$ are the creation and annihilation operators of electrons in the state $|n\mathbf{k}\sigma\rangle$. Using (2.1), we obtain a system of equations for the order parameters Δ_1 and Δ_2

$$\Delta_n = \frac{1}{2}\sum_m V_{nm} \sum_k \frac{\operatorname{th}\left(\frac{\beta E_m(k)}{2}\right)}{E_m(\mathbf{k})}, \tag{2.2}$$

where the energy of the elementary one-particle excitations has the form

$$E_m(k) = \left(\varepsilon_m^2(k) + \Delta_m^2\right)^{1/2}. \tag{2.3}$$

We will assume that the important mechanism in high-temperature superconductors is interband attractive interaction between quasiparticles. Then we can put $V_{22} = 0$ and V_{12}, $V_{11} \neq 0$ and the critical transition temperature to the superconducting state T_c has the form

$$T_c = \frac{2\gamma_e\omega_D}{\pi} e^{-\xi}, \tag{2.4}$$

where

$$\xi = \frac{[\lambda_{12}^2 + (\lambda_{11}^2/4)]^{1/2}}{\lambda_{12}^2} - \frac{\lambda_{11}}{2\lambda_{12}^2}, \tag{2.5}$$

$$\lambda_{11} = N_1 V_{11}, \quad \lambda_{12} = (N_1 N_2)^{1/2} V_{12},$$

N_1 and N_2 are the densities of electronic states on the corresponding parts of the Fermi surface. We see from (2.4) and (2.5) that interband interactions between electrons leads to important differences between these equations and the case of one-band superconductors (the BCS theory). In the approximation of weak coupling we have for the order parameters Δ_1 and Δ_2 at $T = 0$

$$\Delta_1(0) = 2\omega_0 z^{1/(1+nz^2)} e^{-\xi}, \quad \Delta_2(0) = 2\omega_0 z^{-1/[1+(1/nz^2)]} e^{-\xi}. \tag{2.6}$$

From (2.4) and (2.6) we have

$$\frac{2\Delta_1(0)}{T_c} = \frac{2\pi}{\gamma_e} z^{1/(1+nz^2)}, \quad \frac{2\Delta_2(0)}{T_c} = \frac{2\pi}{\gamma_e} z^{-1/[1+(1/nz^2)]}, \tag{2.7}$$

where

$$z = \frac{\Delta_1(0)}{\Delta_2(0)} = \frac{(\lambda_{11}/2) + [(\lambda_{11}^2/4) + \lambda_{12}^2]^{1/2}}{\sqrt{n}\,\lambda_{12}}. \quad (2.8)$$

It follows from (2.7) that the ratio $2\Delta/T_c$ is not universal, but depends on z and on the ratio of the electronic densities of states $n = N_1/N_2$.

The relative jump in the electronic heat capacity at the critical point $T = T_c$ has the form

$$C_s^e - C_n^e)/C_n^e \approx 1{,}43A_1(z^2), \quad (2.9)$$

where C_n^e is the low-temperature electronic heat capacity of a normal metal, which in the two-band model has the form

$$C_n^e = \frac{2\pi^2}{3}(N_1 + N_2)T. \quad (2.10)$$

The quantity $A_1(z^2)$ is given by[18,19,33]

$$A_1(z^2) = \frac{(n + z^{-2})^2}{(1 + n)(n + z^{-4})}. \quad (2.11)$$

Because of the factor $A_1(z^2)$ in (2.9), the relative jump in the electronic heat capacity in two-band superconductors is not universal. The factor $A_1(z^2)$ can be much less than unity and then the relative jump in the electronic heat capacity will be small.

The thermodynamic critical field $H_c(T)$ in the low-temperature region $(T/T_c \ll 1)$ and near T_c is given by[18,19,33]

$$\frac{H_c^2(T \sim 0)}{H_c^2(0)} \approx 1 - 2\chi\frac{T^2}{T_c^2}, \quad \frac{H_c(T \to T_c)}{H_c(0)} \approx 1{,}73A_3(z)\left(1 - \frac{T}{T_c}\right), \quad (2.12)$$

where

$$H_c(0) = \left(4\pi \sum_n N_n\Delta_n^2(0)\right)^{1/2}, \quad \chi = 1{,}06A_3(z), \quad (2.13)$$

$$A_2(z) = \frac{z(1 + n)}{1 + nz^2}\exp\left(-\frac{1 - nz^2}{1 + nz^2}\ln z\right),$$

$$A_3(z) = \left(\frac{n + 1/z^2}{n + 1/z^4}\right)z^{-1/(1+nz^2)}.$$

Because of the functions $A_2(z)$ and $A_3(z)$ in (2.12), the thermodynamic critical field is no longer universal, but depends significantly on the properties of the anisotropic system.

One can attempt to use the above results for the thermodynamic properties of two-band systems to describe the high-temperature superconductors $La_{2-x}M_xCuO_4$ and $YBa_2Cu_3O_x$. In the first of these compounds overlap of the two bands is possible: the first band consists of copper $d_{x^2-y^2}$ and oxygen 2p hybridized orbitals and the second band consists mainly of d_{z^2} and oxygen 2p orbitals.[20] The second band is narrow and we have $N_1 \ll N_2$ $(n \ll 1)$.

In the case of $YBa_2Cu_3O_x$, the number of bands on the Fermi surface depends on the value of x (Ref. 15). Since the bands have about the same width we can put $N_1 \approx N_2$ and $n \approx 1$ in this case. Numerical estimates of the thermodynamic characteristics using the formulas given above are listed in Tables I–III. The observed value $T_c \approx 40$°K in $La_{2-x}M_xCuO_4$ can be obtained for small, physically reasonable values of the frequency ω_0. For example, the last column of Table I for $T_c = 40$ °K corresponds to $\omega_0 = 214$, 155, and 120 °K. For the metallic ceramics $YBa_2Cu_3O_{7-\delta}$ we have $\omega_0 \approx 863$ °K and it is not difficult to obtain the observed value $T_c \approx 100$ °K using the theory presented above. The possible values of T_c for this case are given in the last column of Table III. Tables II and III show that in the weak coupling approximation $2\Delta_1/T_c$ and $2\Delta_2/T_c$ can be different, the jump in the electronic heat capacity can be small, and $H_c(T)$ can differ significantly from the prediction of the BCS theory. These features are observed in high-temperature superconductors. In particular, in a series of tunneling experiments (see Ref. 26, for example) two energy gaps were observed in $La_{2-x}(Ba,Sr)_xCuO_4$, where

$$2\Delta_1/T_c > 3{,}5 \text{ and } 2\Delta_2/T_c < 3{,}5.$$

Small values of $2\Delta_2/T_c$ have also been obtained in infrared absorption experiments (see Ref. 27 and the bibliography in Ref. 20).

The volume dependence of T_c predicted by this model is of interest. We obtain from (2.4) and (2.5)

$$\frac{d\ln T_c}{d\ln V} = \frac{d\ln\omega_0}{d\ln V} - \left(\frac{\lambda_{11}}{4\lambda_{12}^2\eta} - \frac{\lambda_{11}}{2\lambda_{12}^2}\right)\frac{d\ln\lambda_{11}}{d\ln V} - \left[\frac{1}{\eta} - \frac{2}{\lambda_{12}}\left(\eta - \frac{\lambda_{11}}{2}\right)\right]\frac{d\ln\lambda_{12}}{d\ln V}, \quad (2.14)$$

where $\eta = (\lambda_{12}^2 + 1/4\lambda_{11}^2)^{1/2}$. The dependence of $d\ln T_c/d\ln V$ on T_c is shown in Fig. 1 for

$$\frac{d\ln\omega_0}{d\ln V} = -1, \quad \frac{d\ln\lambda_{11}}{d\ln V} = \frac{d\ln\lambda_{12}}{d\ln V} = -2$$

and for $\omega_0 = 181$, 360, 500 °K (curves 1–3, respectively). It follows from Fig. 1 that $d\ln T_c/d\ln V$ can be large and negative, as observed experimentally in $La_{2-x}M_xCuO_4$ compounds.[28] It is not necessary to assume anomalously large values of the derivatives with respect to volume of the parameters of the theory ω_0, λ_{11}, λ_{12}; physically reasonable values can be used.

We note that the behavior of the quantity $d\ln T_c/d\ln V$

TABLE I. Dependence of $T_c/1.14\omega_0$ on the two interaction parameters λ_{11} and λ_{12}.

λ_{12}:	0,1	0,2	0,3	0,4	0,5
$\lambda_{11} = 0{,}1$	0,002	0,02	0,059	0,11	0,164
0,3	0,048	0,082	0,127	0,177	0,226
0,5	0,146	0,173	0,210	0,25	0,291

TABLE II. The case $n = 0.1$ in $La_{2-x}(Ba,Sr)_xCuO_4$.

λ_{11}	λ_{12}	z	$\frac{2\Delta_1}{T_c}$	$\frac{2\Delta_2}{T_c}$	$\frac{C_s^e - C_n^e}{C_n^e}$	χ	$A_3(z)$
0,1	0,3	3,73	6,07	1,63	0,365	2,58	0,734
0,1	0,4	3,58	6,12	1,71	0,388	2,42	0,741
0,1	0,5	3,49	6,15	1,76	0,403	2,33	0,743
0,3	0,2	6,32	5,06	0,80	0,202	5,28	0,771
0,3	0,3	5,12	5,50	1,07	0,171	4,08	0,743
0,3	0,5	4,25	5,86	1,38	0,304	2,96	0,733

as a function of T_c in the two-band model is similar to the behavior of this quantity in the theory of two-dimensional superconductivity,[28,34] in which the logarithmic singularity in the electronic density of states is taken into account.

Therefore the features of the density of electron states such as overlapping energy bands and electronic topological transitions can be crucial to the thermodynamic properties of high-temperature superconductors. It may be necessary to take into account these features simultaneously.

3. UPPER CRITICAL FIELD

The properties of two-band superconductors near the upper critical field can be studied using the generalized Ginzburg–Landau equations.[35-37]

Putting $V_{22} = 0$, the expression for H_{c2} in the low-temperature region ($T \to 0$) reduces to the form[38]

$$\frac{H_{c2}(T\to 0)}{H_{c2}(0)} = 1 + \frac{16\gamma_e}{\pi^2 e_0^2}\left(\frac{T}{T_c}\right)^2 \Phi(T)\exp(\nu(\lambda) - \nu(1)), \tag{3.1}$$

$$H_{c2}(0) = \frac{\pi^2 T_c^2 e_0^2}{2\gamma_e e \vartheta_1 \vartheta_2}\exp(\nu(1) - \nu(\lambda)), \tag{3.2}$$

$$\Phi(T) = (\lambda\gamma^- + \frac{1}{\lambda}\gamma^+)[\xi'(2) + \frac{1}{2}\xi(2)(2\ln\frac{T}{T_c} + 2\ln\frac{4}{\pi e_0} + \nu(\lambda) - \nu(1) + \ln\lambda)],$$

$$\nu(\lambda) = \left[\left(\ln\lambda + \frac{\lambda_{11}}{\lambda_{12}^2}\right)^2 + \frac{4}{\lambda_{12}^2}\right]^{1/2},$$

$$\gamma^{\pm} = \frac{1}{2}\left[1 \pm \left(\frac{\ln\lambda + \lambda_{11}\lambda_{12}^{-2}}{\nu(\lambda)}\right)\right]; \tag{3.3}$$

where $\lambda = \vartheta_1/\vartheta_2$, with ϑ_1 and ϑ_2 being the velocities of electrons in the corresponding cavity of the Fermi surface, e_0 is the base of natural logarithms, and e is the charge of the electron.

For temperatures close to the superconducting transition temperature T_c we obtain[18,38]

$$\frac{H_{c2}(T\sim T_c)}{H_{c2}(0)} = \frac{8\gamma_e\vartheta_1\vartheta_2}{e_0^2[\vartheta_1^2\eta_1 + \vartheta_2^2\eta_2]}\exp(\nu(\lambda) - \nu(1))\cdot\frac{6}{7\xi(3)} \times\left(1 - \frac{T}{T_c}\right) \times\left\{1 + \left(1 - \frac{T}{T_c}\right)\left[\frac{\frac{\vartheta_1^2}{\vartheta_2^2}\eta_1 + \frac{\vartheta_2^2}{\vartheta_1^2}\eta_2}{\left(\frac{\vartheta_1}{\vartheta_2}\eta_1 + \frac{\vartheta_2}{\vartheta_1}\eta_2\right)^2}\frac{31}{10}\xi(5)\left(\frac{6}{7\xi(3)}\right)^2 - \frac{3}{2}\right]\right\}, \tag{3.4}$$

where

$$\eta_{1,2} = (1 \pm \eta)/2, \quad \eta = \lambda_{11}/\lambda_{12}^2\nu(1). \tag{3.5}$$

Putting $\vartheta_1 = \vartheta_2$ in (3.1)–(3.4), we obtain the corresponding relations for an ordinary one-band superconductor:[39,40]

$$\frac{H_{c2}(T\to 0)}{H_{c2}(0)} = 1 + \frac{16\gamma_e}{\pi^2 e_0^2}\left(\frac{T}{T_c}\right)^2\left\{\xi(2)\ln\frac{T}{T_c} + \xi'(2) + \xi(2)\ln\frac{4}{\pi e_0}\right\}, \tag{3.6}$$

$$\frac{H_{c2}(T\to T_c)}{H_{c2}(0)} = \frac{8\gamma_e}{e_0^2}\frac{6}{7\xi(3)}\left(1 - \frac{T}{T_c}\right)\left\{1 + \left(1 - \frac{T}{T_c}\right) \times\left[\frac{31}{10}\xi(5)\left(\frac{5}{7\xi(3)}\right)^2 - \frac{3}{2}\right]\right\} \tag{3.7}$$

TABLE III. The case $n = 1$ in $YBa_2Cu_3O_x$.

λ_{11}	λ_{12}	z	$\frac{2\Delta_1}{T_c}$	$\frac{2\Delta_2}{T_c}$	$\frac{C_s^e - C_n^e}{C_n^e}$	χ	$A_3(z)$	T_c, K (for $\omega_0 =$ 863 K)
0,1	0,3	1,18	3,75	3,18	1,39	0,76	0,994	58
0,2	0,3	1,39	3,91	2,82	1,30	0,89	0,978	89
0,4	0,1	4,24	3,78	0,89	0,794	1,77	0,951	93
0,4	0,3	1,87	4,02	2,15	1,09	1,15	0,949	165
0,5	0,5	1,62	4,0	2,47	1,19	1,02	0,961	286

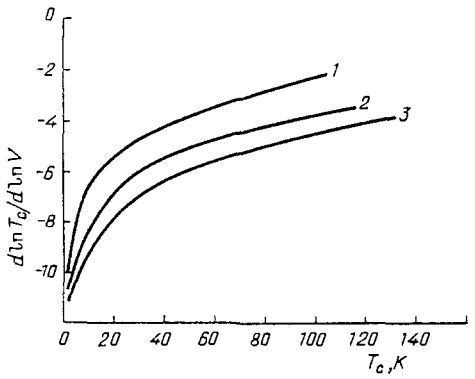

FIG. 1. Dependence of the quantity d ln T_c/d ln V (V is the volume) on T_c.

Letting $H_{c2}^0(0)$ and T_{c0} be the upper critical field and critical temperature of a low-temperature one-band superconductor, we obtain from (3.2)

$$H_{c2}(0)/H_{c2}^0(0) = (T_c/T_{c0})^2 \frac{\vartheta_1}{\vartheta_2} \cdot \exp(\nu(1) - \nu(\lambda)). \quad (3.8)$$

Numerical estimates based on (3.8) show that the upper critical field for two-band superconductors at $T = 0$ can be two or three orders of magnitude larger than $H_{c2}(0)$ for ordinary superconductors. The quantity $H_{c2}(0)$ is large because of the high value of T_c and the fact that $\vartheta_1/\vartheta_2 > 1$ or $\gg 1$.

Figure 2 shows the dependence $H_{c2}(T)/H_{c2}(0)$ obtained from (3.1) and (3.4) for $T \sim 0$ and $T \sim T_c$, respectively and the extrapolation of these functions. We see that the curvature of this dependence changes as ϑ_1/ϑ_2 increases. The curvature of curves *3* and *4* is observed experimentally. We see that if the second band contains heavy carriers (small velocity on the Fermi surface) then the two-band model qualitatively describes the behavior of H_{c2} as a function of temperature.

4. EFFECT OF OXYGEN VACANCIES OR IMPURITIES ON THE TRANSITION TEMPERATURE IN HIGH-TEMPERATURE SUPERCONDUCTORS

Here the two-band model is used to attempt to understand the experimentally observed decrease in T_c with a decrease in the concentration of oxygen or with the disordering of oxygen vacancies in $YBa_2Cu_3O_{7-\delta}$. Disordering appears here as a nonmagnetic decoupling factor of superconducting pairs. We start from the Hamiltonian describing two-band superconductors

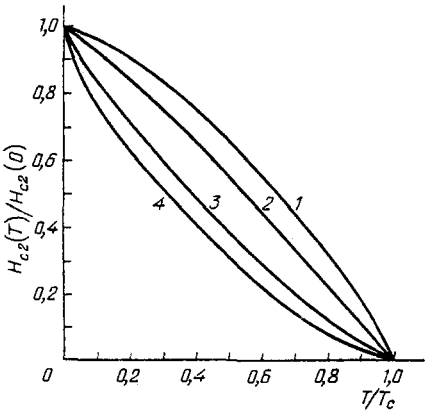

FIG. 2. Temperature dependence of $H_{c2}(T)/H_{c2}(0)$ for $\lambda_{11} = 0.2$, $\lambda_{12} = 0.3$ and $\vartheta_1/\vartheta_2 = 1$, 10, 20, and 40 (curves *1–4*, respectively).

$$H = H_0 + H_1, \quad (4.1)$$

where H_0 is the Hamiltonian (2.1) of a pure two-band material and H_1 has the form

$$H_1 = \frac{1}{V} \sum_{\sigma} \sum_{n,\mathbf{k}} \sum_{n',\mathbf{k}'} a^+_{n\mathbf{k}\sigma} a_{n'\mathbf{k}\sigma} \rho(\mathbf{k} - \mathbf{k}') U_{nn'}(\mathbf{k} - \mathbf{k}'), \quad (4.2)$$

$$\rho(\mathbf{k} - \mathbf{k}') = \sum_j \exp\left[-i(\mathbf{k} - \mathbf{k}')\mathbf{r}_j\right]. \quad (4.3)$$

Hence we assume that the metallic phase of $YBa_2Cu_3O_7$ with the maximum superconducting transition temperature $T_c \approx 90$ °K corresponds to the two-band Hamiltonian H_0. A decrease in the number of oxygen atoms (increase in δ) leads to a disordering of the system, and the additional term (4.2) in the Hamiltonian describes the interaction of electrons with lattice defects ($U_{nn'}$ is the potential energy describing the scattering of electrons by oxygen vacancies). The sum in (4.3) is taken over the randomly distributed oxygen vacancies.

Hence the effect of the oxygen composition (or disordering) on T_c reduces formally to the problem of determining the effect of a nonmagnetic impurity on the superconducting transition temperature in two-band superconductors.[41,42] A decrease in the number of oxygen atoms (increase in δ) corresponds to an increase in the concentration of impurities. The critical temperature of the two-band superconductor is found as the eigenvalue of the equation for a bound state of a pair of electrons or holes with zero binding energy. This equation is obtained starting from the Dyson equation for the two-particle Green's function of the system (4.1). Averaging it over the randomly distributed oxygen vacancies, we obtain a linearized system of equations for the superconductor order parameters Δ_1 and Δ_2 (Refs. 41 and 42):

$$\Delta_1 = \left[\lambda_{11}\xi - (\lambda_{12} - jn^{1/2}\lambda_{12})\left(1 + \frac{\tau_{12}}{\tau_{21}}\right)^{-1} J_2(\tau_{12})\right]\Delta_1 + \left[\lambda_{12}\frac{1}{\sqrt{n}}\xi + (\lambda_{11} - jn^{1/2}\lambda_{12})\left(1 + \frac{\tau_{12}}{\tau_{21}}\right)^{-1} J_2(\tau_{12})\right]\Delta_2,$$

$$\Delta_2 = [\xi n^{1/2}\lambda_{12} - \lambda_{12}n^{1/2}J_2(\tau_{12})\left(1 + \frac{\tau_{12}}{\tau_{21}}\right)^{-1}]\Delta_1 + n^{1/2}\lambda_{12}J_2(\tau_{12})\left(1 + \frac{\tau_{12}}{\tau_{21}}\right)^{-1}\Delta_2, \quad (4.4)$$

where

$$\lambda_{11} = N_1 V_{11}, \quad \lambda_{12} = (N_1 N_2)^{1/2} V_{12}, \quad j = \frac{\tau_{12}}{\tau_{21}}\frac{N_2}{N_1} = \frac{\tau_{12}}{\tau_{21}}\frac{1}{n},$$

$$\xi = \ln\frac{2\gamma\omega}{\pi T}, \quad n = \frac{N_1}{N_2}, \quad (4.5)$$

$$J_2 = \int_0^\infty \frac{\text{th}\left(\frac{\beta y}{4}\right)\left(\tau_{12}^{-1} + \tau_{21}^{-1}\right)dy}{y(y^2+1)} = \Psi\left(\frac{1}{2} + \frac{\beta}{4\pi}\left(\frac{1}{\tau_{12}} + \frac{1}{\tau_{21}}\right)\right) - \Psi\left(\frac{1}{2}\right), \quad (4.6)$$

N_1 and N_2 are the densities of electron states in the corresponding cavity of the Fermi surface, V_{11} and V_{12} are the effective electron-electron intraband and interband interactions, and τ_{12} is the relaxation time of interband scattering by oxygen vacancies.

In obtaining (4.4) we assumed that the important mechanism for high-temperature superconductivity is interband attractive interactions between electrons. Then we can put $V_{22} \ll V_{12}$ and neglect electron-electron interactions within the second band.

The condition for a nontrivial solution of (4.4) determines ξ and hence T_c and has the form

$$a\xi_c^2 - b\xi_c + c = 0, \tag{4.7}$$

where

$$a = -\lambda_{12}^2, \quad \xi_c = \ln\frac{2\omega_0\gamma}{\pi T_c}, \quad b = \lambda_{11} - \lambda_{12}^2 J_2(\tau_{12}), \tag{4.8}$$

$$c = 1 + \lambda_{11}\left(1 + \frac{\tau_{12}}{\tau_{21}}\right)^{-1} J_2(\tau_{12}) - \lambda_{12} n^{1/2}(1 + j)\left(1 + \frac{\tau_{12}}{\tau_{21}}\right)^{-1} J_2(\tau_{12}).$$

Of the two solutions of (4.7), we choose the physically reasonable solution satisfying the condition $T_c \to 0$ when λ_{11}, $\lambda_{12} \to 0$. This solution has the form

$$\ln\frac{T_c}{T_{c0}} = -\alpha\left[\Psi\left(\frac{1}{2} + \frac{\beta}{4\pi}\left(\frac{1}{\tau_{12}} + \frac{1}{\tau_{21}}\right)\right) - \Psi\left(\frac{1}{2}\right)\right], \tag{4.9}$$

where

$$\alpha = \frac{1}{2}\left\{1 - \frac{\lambda_{11} - 2[\lambda_{11} - \lambda_{12} n^{1/2}(1 + j)](1 + jn)^{-1}}{(\lambda_{11}^2 + 4\lambda_{12}^2)^{1/2}}\right\}. \tag{4.10}$$

It follows from (4.9) that the critical temperature T_c decreases with increasing concentration of oxygen vacancies (an increase in the factor $1/\tau_{12} + 1/\tau_{21}$). The rate of decrease depends very strongly on the coefficient α given by (4.10). In turn, α depends on the electron-electron interaction constants λ_{11} and λ_{12}, on the ratio N_1/N_2, and on the parameter j determining the difference between the cavities in the Fermi surface ($j = 1$ for spherically symmetric cavities). Since $\alpha < 1$, the decrease in T_c is not as sharp as in the case of a superconductor with a paramagnetic impurity.[43]

For low concentrations of oxygen vacancies

$$\frac{\beta_c}{2}\left(\frac{1}{\tau_{12}} + \frac{1}{\tau_{21}}\right) \ll 1$$

(4.9) reduces to

$$T_c = T_{c0} - \frac{\pi\alpha}{8\tau_{12}}(1 + nj). \tag{4.11}$$

The temperature T_c decreases linearly with increasing τ_{12}^{-1}.

In the other limiting case

$$\frac{\beta_c}{2}\left(\frac{1}{\tau_{12}} + \frac{1}{\tau_{21}}\right) \gg 1$$

we have

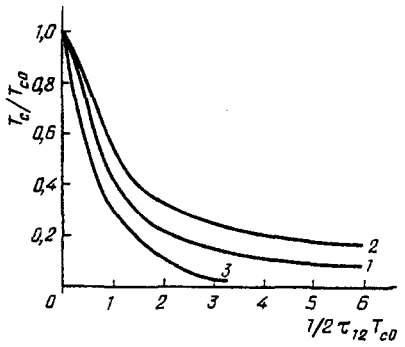

FIG. 3. Superconducting transition temperature T_c as a function of the quantity $1/2\tau_{12}T_{c0}$ for $\lambda_{11} = 0.4$, $\lambda_{12} = 0.1$ and different values of n and j: 1) $\alpha = 0.51$ ($n = 2, j = 0.5$), 2) $\alpha = 0.375$ ($n = 1, j = 2$), 3) $\alpha = 0.673$ ($n = 1, j = 0.5$).

$$T_c = T_{c0}^{1/(1-\alpha)}\left[\frac{\gamma}{\pi\tau_{12}}(1 + jn)\right]^{\alpha/(\alpha-1)} \tag{4.12}$$

In this expression $T_c \to 0$ only when the concentration of impurities becomes infinite. This means that there is no critical concentration of impurities for which $T_c = 0$. Hence interband scattering of electrons by oxygen vacancies in $YBa_2Cu_3O_{7-\delta}$ significantly suppresses superconductivity. The dependence of T_c/T_{c0} on $1/\tau_{12}T_{c0}$ is shown in Fig. 3 for different values of the parameters of the theory.

We next consider the densities of electron states of disordered two-band superconductors. The ratio $N_n(\omega)/N_n$ ($n = 1,2$) is given by[44,45]

$$\frac{N_n(\omega)}{N_n} = \mathrm{Im}\frac{u_n(\omega)}{\left(1 - u_n^2(\omega)\right)^{1/2}} = \mathrm{Re}\frac{u_n(\omega)}{\left(u_n^2(\omega) - 1\right)^{1/2}}, \tag{4.13}$$

where $u_1(\omega)$ and $u_2(\omega)$ satisfy the system of equations

$$\frac{\omega}{\Delta_1} = u_1(\omega) + \alpha_1\frac{u_1(\omega) - u_2(\omega)}{\left(1 - u_2^2(\omega)\right)^{1/2}}, \quad \alpha_1 = \frac{1}{2\tau_{12}\Delta_1},$$
$$\frac{\omega}{\Delta_2} = u_2(\omega) + \alpha_2\frac{u_2(\omega) - u_1(\omega)}{\left(1 - u_1^2(\omega)\right)^{1/2}}, \quad \alpha_2 = \frac{1}{2\tau_{12}\Delta_2}. \tag{4.14}$$

For completeness we note that the order parameters Δ_1 and Δ_2 are determined from the following system of equations at arbitrary temperature:

$$\Delta_n = \frac{\pi}{\beta}\sum_m V_{nm}N_m\sum_m \frac{1}{\left(u_m^2(\Omega) + 1\right)^{1/2}}, \quad \Omega = (2n + 1)\frac{\pi}{\beta},$$
$$\frac{\Omega}{\Delta_1} = u_1(\Omega) + \alpha_1(\Omega)\frac{u_1(\Omega) - u_2(\Omega)}{\left(1 + u_2^2(\Omega)\right)^{1/2}}\frac{\omega}{\Delta_2} \tag{4.15}$$
$$= u_2(\Omega) + \alpha_2(\Omega)\frac{u_2(\Omega) - u_1(\Omega)}{\left(1 + u_1^2(\Omega)\right)^{1/2}}.$$

It is not difficult to show that the density of electron states and also the order parameters Δ_1 and Δ_2 of the superconducting phase depend significantly on the relaxation times of interband scattering of electrons by oxygen vacancies. An analytical method of calculating the density of electron states has been given by one of the authors.[45] It yields a

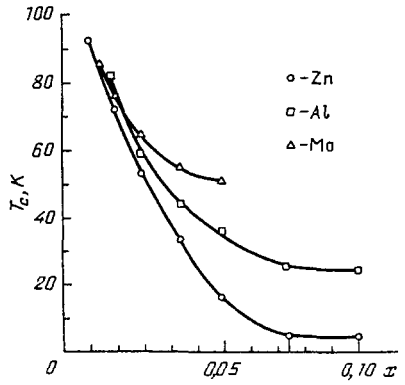

FIG. 4. Superconducting transition temperature T_c of $YBa_2(Cu_{1-x}M_x)_3O_{7-\delta}$ for M = Al, Mo, and Zn as a function of x (Ref. 46).

nonanalytic dependence of the density of states on the small concentration of impurities (oxygen vacancies) in the frequency regions near the order parameters Δ_n and uses an expansion in the small parameters of the theory in the region far from the order parameters. Numerical calculations of the densities of states based on (4.13) for different values of the parameters of the theory were also discussed in Ref. 45.

The energy gap of a two-band superconductor corresponds to the highest frequency at which the density of states is still equal to zero. In spite of the fact that a pure two-band superconductor has two energy gaps, the addition of impurities (disorder) leads to a single energy gap in the two-band model because of mixing of states belonging to different cavities of the Fermi surface by the impurity (oxygen vacancies). A proof of this statement is the fact that both densities of electron states become nonzero simultaneously.[45] The decrease in the number of energy bands with decreasing number of oxygen atoms in $YBa_2Cu_3O_{7-\delta}$ is an interesting question and can be understood assuming that oxygen vacancies lead to a decoupling because of interband scattering of carriers by the vacancies. The result is a single hybridized band instead of two overlapping bands. We note that the above theory can also be used to describe the behavior of T_c as a function of the concentration of impurities x in $YBa_2(Cu_{1-x}M_x)_3O_{7-\delta}$, where M = Al, Mo, Zn. In this case τ_{12} is determined by interband scattering of conduction electrons from the randomly distributed impurities. The dependence of T_c on $1/\tau_{12}$ obtained in Fig. 3 is qualitatively consistent with the observed dependence of T_c on the concentration of impurities[46] (Fig. 4).

5. TWO-BAND MODEL AND ELECTRONIC TOPOLOGICAL TRANSITIONS

Recently an interesting feature has been observed in the experimental dependence of the superconducting transition temperature of $YBa_2Cu_3O_{7-\delta}$ as a function of δ and also in $(La_{1-x}Sr_x)_2CuO_4$ as a function of x. The transition temperature T_c is practically constant (step-like) in the region $0.2 \lesssim \delta \lesssim 0.6$ in $YBa_2Cu_3O_{7-\delta}$ (Ref. 47) and in the region $0.05 \lesssim x \lesssim 0.08$ in $(La_{1-x}Sr_x)_2CuO_4$ (Ref. 48).

In Secs. 5 and 6 we use the theory of superconductors with overlapping energy bands and electronic topological transitions to obtain the dependence of T_c on the position of the chemical potential μ and to understand the origin of the step-like behavior of T_c.

In the present Section we consider the dependence of the superconducting transition temperature in the two-band model assuming the phonon mechanism of superconductivity and taking into account the Van Hove–Lifshits features in the electronic energy spectrum. The case of a topological transition in two-band superconductors with the formation of elliptical cavities in the Fermi surface was considered in Refs. 49 and 50. Here we will consider strongly anisotropic (quasi-one-dimensional and quasi-two-dimensional) three-dimensional systems. The presence of singular points in momentum space of anisotropic systems of this kind leads to electronic topological transitions accompanied by the formation of flat areas on the Fermi surface or cylindrical cavities when the Fermi level passes through special critical points ε_{kn}.

The formation of flat areas on the Fermi surface in a one-band system has been studied in a number of papers,[51–53] and has been confirmed by numerous experiments in the intermetallic compound $AuGa_2$.

The electronic topological transitions considered here can be observed in high-temperature superconductors where the atoms are clearly arranged in chains (one-dimensional) or in a plane (two-dimensional). The possibility of topological transitions in high-temperature ceramics was discussed in Refs. 30 and 54. We start from the Hamiltonian (2.1) with $V_{nm} \neq 0$ $(n,m = 1,2)$, which corresponds to including intraband and interband interactions.

1. We consider first the formation of flat areas on the Fermi surface. We assume a strongly anisotropic system where the trajectories of the electrons are nearly one-dimensional in a certain region of momentum space. Near the critical points the energy of an electron in the nth band can be written in the form

$$\varepsilon_n(p) = \varepsilon_{kn} + \frac{p_z^2}{2m}; \tag{5.1}$$

where m_n is the effective mass of the electron.

With the help of the modified Hamiltonian (2.1) and the dispersion law (5.1), we obtain the following system of equations for the order parameters Δ_n near the transition temperature $(T \approx T_c)$:

$$\begin{aligned} \Delta_1 &= A_1 V_{11} I_1(\beta, \varepsilon'_{k1})\Delta_1 + A_2 V_{21} I_2(\beta, \varepsilon'_{k2})\Delta_2, \\ \Delta_2 &= A_1 V_{12} I_1(\beta, \varepsilon'_{k1})\Delta_1 + A_2 V_{22} I_2(\beta, \varepsilon'_{k2})\Delta_2, \end{aligned} \tag{5.2}$$

where

$$I_n(\beta, \varepsilon'_{kn}) = \int_0^{\omega_D} \frac{d\varepsilon}{(\varepsilon + \varepsilon'_{kn})^{1/2}} \theta(\varepsilon + \varepsilon'_{kn}) \frac{\operatorname{th}\left(\frac{\beta\varepsilon}{2}\right)}{\varepsilon}, \tag{5.3}$$

$$\varepsilon'_{kn} = \mu - \varepsilon_{kn}, \quad A_n = N_n \varepsilon_F^{1/2} \alpha_n,$$

$$N_n = \frac{m_n p_{Fn}}{2\pi^2}, \quad \alpha_n = \frac{2}{\pi} \frac{\left(\int\int dp_x dp_y\right)_n}{4p_{Fn}^2}. \tag{5.4}$$

The transition temperature T_c is obtained from the condition that the determinant of the system (5.2) must vanish:

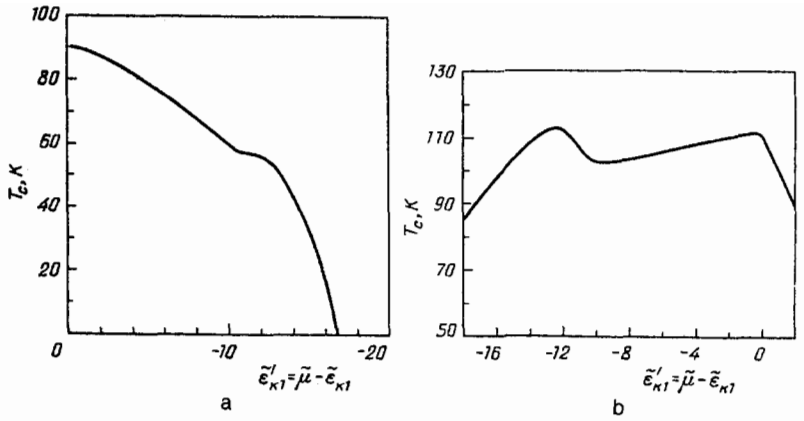

FIG. 5. Superconducting transition temperature T_c as a function of the parameter $\tilde{\varepsilon}'_{k1} = \tilde{\mu} - \varepsilon_{k1}$ in the case of formation of flat areas on the Fermi surface: a $-\lambda_{11} = 0.4$, $\lambda_{12} = 0.2$, $\lambda_{22} = 0.1$, $\alpha_1 = \alpha_2 = 0.18$, $\tilde{\varepsilon}_{k2} = \tilde{\varepsilon}_{k1} + 12$, $\tilde{\omega}_D = 43$, $\tilde{\varepsilon}_F = 500$. b $-\lambda_{11} = 0.125$, $\lambda_{12} = 0.3$, $\lambda_{22} = 0.1$, $\alpha_1 = 0.5$, $\alpha_2 = 0.1$, $\tilde{\varepsilon}_{k2} = \tilde{\varepsilon}_{k1} + 12$, $\tilde{\omega}_D = 40$, $\tilde{\varepsilon}_F = 500$.

$$\lambda_{11}\tilde{\varepsilon}_F^{1/2}\alpha_1 I_1(\tilde{\beta}_c, \tilde{\varepsilon}'_{k1}) + \lambda_{22}\tilde{\varepsilon}_F^{1/2}\alpha_2 I_2(\tilde{\beta}_c, \tilde{\varepsilon}_{k2}) - (\lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21}) I_1(\tilde{\beta}_c, \tilde{\varepsilon}'_{k1}) I_2(\tilde{\beta}_c, \tilde{\varepsilon}'_{k2})\tilde{\varepsilon}_F\alpha_1\alpha_2 - 1 = 0, \tag{5.5}$$

where

$$I_n(\beta_c, \varepsilon'_{kn}) = \int_0^{\tilde{\omega}_D} \frac{1}{\left(x + \tilde{\varepsilon}'_{kn}\right)^{1/2}}\theta(x + \tilde{\varepsilon}'_{kn})\frac{\operatorname{th}\left(\frac{\beta_c x}{2}\right)}{x},$$

$$\beta_c = \frac{T_0}{T_c}, \quad \tilde{\varepsilon}'_{kn} = \frac{\varepsilon'_{kn}}{2T_0}, \quad \tilde{\varepsilon}_F = \frac{\varepsilon_F}{2T_0}, \tag{5.6}$$

$$\tilde{\omega}_{Dn} = \frac{\omega_{Dn}}{2T_0}, \quad \lambda_{nm} = (N_n N_m)^{1/2} V_{nm}.$$

T_0 is an arbitrary temperature introduced to obtain dimensionless quantities in (5.5).

Figure 5 shows the dependence of the superconducting transition temperature T_c on the parameter $\tilde{\varepsilon}'_{k1} = \tilde{\mu} - \tilde{\varepsilon}_{k1}$, which varies because of the introduction of oxygen (change in the concentration of impurities) or because of pressure. These results were obtained from the solution of (5.5).

In Fig. 5a note that T_c varies only slightly in the region $-12 < \tilde{\varepsilon}'_{k1} < -10$. Therefore the topological transitions considered here can lead to a step-like dependence of T_c on the concentration of oxygen in $YBa_2Cu_3O_{7-\delta}$ (Fig. 6) or on the concentration of impurities in $(La_{1-x}Sr_x)_2CuO_4$ (Ref. 48). Topological transitions accompanied by the formation of flat areas on the Fermi surface can lead to a double maximum in the dependence of T_c on $\tilde{\varepsilon}'_{k1}$ (Fig. 5b). Scattering by impurities would lead to a broadening of these maxima.[51-53] We note that this form of the dependence of T_c on pressure was observed in $Bi_2Sr_2CaCu_2O_8$ (Ref. 55).

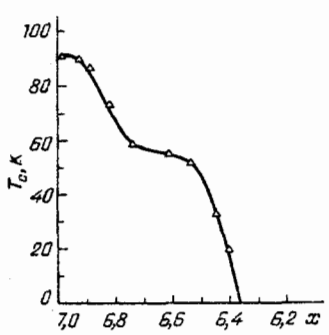

FIG. 6. Experimental dependence of T_c in $YBa_2Cu_3O_x$ on the oxygen content x (Ref. 47).

2. We next consider electronic topological transitions accompanied by the formation of flat areas on the Fermi surface (because of one-dimensional motion of electrons in the first band) and the formation of a cylindrical cavity in the Fermi surface (because of two-dimensional motion of electrons in the second band).

The dispersion laws near the critical points ($\nabla\varepsilon_m = 0$) are written in the form

$$\varepsilon_1(p) = \varepsilon_{k1} + \frac{p_z^2}{2m_1}, \qquad \varepsilon_2(p) = \varepsilon_{k2} + \frac{1}{2m_2}(p_x^2 + p_y^2). \tag{5.7}$$

In this case the temperature of the superconducting transition is determined from the equation

$$\lambda_{11}\tilde{\varepsilon}_F^{1/2}\alpha_1 I_1(\tilde{\beta}_c, \tilde{\varepsilon}'_{k1}) + \lambda_{22} I'_2(\beta_c, \tilde{\varepsilon}'_{k2}) - (\lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21})\tilde{\varepsilon}_F^{1/2}\alpha_1 I_1(\beta_c, \tilde{\varepsilon}'_{k1}) I'_2(\tilde{\beta}_c, \tilde{\varepsilon}'_{k2}) - 1 = 0; \tag{5.8}$$

where

$$N_z = \frac{m_2(\int dp_z)_2}{2\pi^2}, \quad I'_2(\tilde{\beta}_c, \tilde{\varepsilon}'_{k2}) = \int_{\tilde{\varepsilon}_{k2}}^{\tilde{\omega}_D} dx \frac{\operatorname{th}\left(\frac{\beta_c x}{2}\right)}{x}. \tag{5.9}$$

The dependence of T_c on $\tilde{\varepsilon}'_{k1} = \tilde{\mu} - \tilde{\varepsilon}_{k1}$ obtained by solving (5.8) is shown in Fig. 7 for the case

$$\lambda_{11} = 0{,}25, \quad \lambda_{12} = 0{,}1, \quad \lambda_{22} = 0{,}3, \quad \alpha_1 = 0{,}3,$$

$$\tilde{\varepsilon}'_{k2} = \tilde{\varepsilon}'_{k1} + 30, \quad \tilde{\omega}_D = 43, \quad \tilde{\varepsilon}_F = 500.$$

In this case superconductivity is possible near both points $\varepsilon'_{k1} = 0$ and $\varepsilon'_{k2} = 0$.

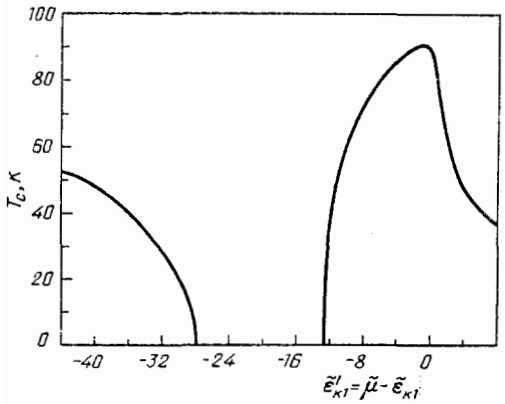

FIG. 7. Dependence of T_c on the parameter $\tilde{\varepsilon}'_{k1}=\tilde{\mu}-\tilde{\varepsilon}_{k1}$ (the case of a flat area and cylindrical cavity on the Fermi surface).

6. OVERLAP OF THREE ENERGY BANDS ON THE FERMI SURFACE

We consider a crystal with strong electron-phonon and Coulomb interactions and assume that repulsive interaction between electrons (holes) dominates. Superconductivity could not occur in this case in a system with one energy band. In multiband superconductors, where two or more energy bands overlap on the Fermi surface, a system with repulsive interaction between electrons (holes) becomes unstable to superconducting pairing. The cause of superconductivity in this case is interband repulsion between electrons (holes). We start with the Hamiltonian (2.1), where the first term corresponds to the kinetic energy of the electrons of the n bands and the second term determines the interband repulsion between carriers ($-V_{nm}>0$ for $n\neq m$) with opposite momenta and spins. Because of the interband interaction, the migration of a pair from one band to another and back always leads to a net attractive interaction between the pairs and therefore even when all the interaction constants are repulsive, interband interactions can lead to a net attraction[16-25] (see Sec. 2). As noted above, this is a qualitative difference between the multiband theory and the one-band theory. Therefore in this Section we consider the interband interaction explicitly. In a more rigorous treatment it would be necessary to take into account repulsive interaction between electrons inside each band ($-V_{nn}>0$), which negatively affects superconductivity. Estimates of the critical temperature T_c in the two-band model[16,22] (Sec. 2) with $-V_{nm}>0$ show that the observed T_c in high-temperature superconductors can be obtained even when $|V_{nm}|<|V_{nn}|$ by extending the interaction region to a large part of momentum space and by introducing a cut-off energy in determining T_c.

Three energy bands overlap on the Fermi surface in the yttrium ceramic $YBa_2Cu_3O_{7-\delta}$ for $\delta=0$ (Ref. 15). Therefore $n,m=1$–3 for this compound. Using the method of Green's functions,[56] we obtain from (2.1) a system of equations for the three order parameters

$$\Delta_n=\sum_{m,\mathbf{k}}V_{nm}\frac{\operatorname{th}\left(\frac{\beta E_m(\mathbf{k})}{2}\right)}{E_m(\mathbf{k})}\Delta_m, \tag{6.1}$$

$$E_m=[(\varepsilon_m-\mu)^2+\Delta_m^2]^{1/2}. \tag{6.2}$$

Near the superconducting transition temperature we have

$$\Delta_1=\sum_{\mathbf{k}}V_{12}\frac{\operatorname{th}\left[\frac{\beta(\varepsilon_2-\mu)}{2}\right]}{\varepsilon_2-\mu}\Delta_2+\sum_{\mathbf{k}}V_{13}\frac{\operatorname{th}\left[\frac{\beta(\varepsilon_3-\mu)}{2}\right]}{\varepsilon_3-\mu}\Delta_3,$$

$$\Delta_2=\sum_{\mathbf{k}}V_{21}\frac{\operatorname{th}\left[\frac{\beta(\varepsilon_1-\mu)}{2}\right]}{\varepsilon_1-\mu}\Delta_1+\sum_{\mathbf{k}}V_{23}\frac{\operatorname{th}\left[\frac{\beta(\varepsilon_3-\mu)}{2}\right]}{\varepsilon_3-\mu}\Delta_3,$$

$$\Delta_3=\sum_{\mathbf{k}}V_{31}\frac{\operatorname{th}\left[\frac{\beta(\varepsilon_1-\mu)}{2}\right]}{\varepsilon_1-\mu}\Delta_1+\sum_{\mathbf{k}}V_{32}\frac{\operatorname{th}\left[\frac{\beta(\varepsilon_2-\mu)}{2}\right]}{\varepsilon_2-\mu}\Delta_2. \tag{6.3}$$

Examining the electronic superconductivity, we write the dispersion law for the nth band in the form

$$\varepsilon_n=-E_n-\frac{\hbar}{2m_n}(k_x^2+k_y^2),\quad m_n>0. \tag{6.4}$$

This equation is an expansion of the energy near the critical energy E_n ($\nabla\varepsilon_n=0$) corresponding to a topological transtransition.[14] Such points always exist in an energy band, but they normally do not affect the properties of metals, but show up in the presence of impurities or pressure. According to band calculations,[10-13] they also exist in high-temperature superconductors. A change in the oxygen composition in an yttrium ceramic changes the position of the Fermi level so that the relation $E_n=\mu$ is satisfied, which favors the formation of cylindrical cavities in the Fermi surface. The two-dimensional nature of the band spectrum is determined by the CuO_2 plane.

In (6.3) we transform the series over $\mathbf{k}$ to integrals with respect to energy with the help of the dispersion law (6.4). Let

$$J(a,b)=\int_a^b\frac{\operatorname{th}\left(\frac{\beta_c x}{2}\right)}{x}\,dx. \tag{6.5}$$

Then the system of equations (6.3) takes the form

$$\begin{aligned}\Delta_1&=N_2V_{12}J(\eta-E_2,\eta-E_{c2})\Delta_2\\&\quad+N_3V_{13}J(\eta-E_3,\eta-E_{c3})\Delta_3,\\ \Delta_2&=N_1V_{21}J(\eta,\eta-E_{c1})\Delta_1+V_{23}N_3J(\eta-E_3,\eta-E_{c3})\Delta_3,\\ \Delta_3&=N_1V_{31}J(\eta,\eta-E_{c1})\Delta_1+N_2V_{32}J(\eta-E_2,\eta-E_{c2})\Delta_2,\end{aligned} \tag{6.6}$$

where

$$\eta=-\mu,\quad N_n=\frac{k_z}{(2\pi)^2}\cdot\frac{m_n}{\hbar^2},$$

E_{cn} ($n=1,2,3$) are the cut-off energies in the corresponding bands. From the condition for a nontrivial solution of the system (6.6) we obtain an equation for the superconducting transition temperature $T_c=1/\beta_c$

$$\begin{aligned}1-\lambda_{23}\lambda_{32}&J(\eta-E_2,\eta-E_{c2})J(\eta-E_3,\eta-E_{c3})-\lambda_{12}\lambda_{21}\\&\times J(\eta,\eta-E_{c1})J(\eta-E_2,\eta-E_{c2})\\&-\lambda_{13}\lambda_{31}J(\eta,\eta-E_{c1})J(\eta-E_3,\eta\end{aligned}$$

$$- E_{c3}) - \lambda_{13}\lambda_{21}\lambda_{31}J(\eta, \eta - E_{c1})J(\eta - E_2,$$
$$\eta - E_{c2})J(\eta - E_3, \eta - E_{c3})$$
$$- \lambda_{31}\lambda_{12}\lambda_{23}J(\eta, \eta - E_{c1})J(\eta - E_2, \eta - E_{c2})$$
$$J(\eta - E_3, \eta - E_{c3}) = 0; \qquad (6.7)$$

here $\lambda_{mn} = (N_m N_n)^{1/2} V_{nm}$; $m,n = 1,2,3$.

We simplify the problem by assuming that only the interband interactions (1,2) and (2,3) are important, i.e. we put $\lambda_{13} = \lambda_{31} = 0$. Then

$$1 - \lambda_{12}\lambda_{21}J(\eta, \eta - E_{c1})J(\eta - E_2, \eta - E_{c2})$$
$$- \lambda_{23}\lambda_{32}J(\eta - E_2, \eta - E_{c2})$$
$$\times J(\eta - E_3, \eta - E_{c3}) = 0. \qquad (6.8)$$

The condition $\lambda_{13} = \lambda_{31} = 0$ can be satisfied when the symmetries of the wave functions of bands 1 and 3 such that direct transitions are forbidden. However, transitions through the intermediate band are possible and are taken into account. In this way, all three bands are active. In a model with a large number of parameters, an assumption of this kind simplifies the analysis without losing the effect of participation of all the bands. In principle, the more complicated equation (6.7) could be considered without difficulty.

It is of interest to study the dependence of T_c on the parameter $\eta = -\mu$ determining the position of the chemical potential. We assume $a,b \gg T_c$ in the integral (6.5). Putting $E_1 = 0$, $E_2 < E_3 < E_{c1} < E_{c2} < E_{c3}$, we obtain from (6.8)

1. $\eta < E_2$:

$$T_c = \frac{2\gamma}{\pi}\eta^{1/2}(E_{c1} - \eta)^{1/2}(E_{c3} - \eta)^{\alpha}(E_3 - \eta)^{-\alpha}$$
$$\times \exp\left\{g - \frac{1}{2\varkappa_{12}\ln\left[\frac{(E_{c2} - \eta)}{(E_2 - \eta)}\right]}\right\}. \qquad (6.9)$$

2. $\eta = E_2$:

$$T_c = \frac{2\gamma}{\pi}(E_{c1} - E_2)E_2^{1/4}(E_{c2} - E_2)^{-1/4}$$
$$\times (E_{c3} - E_2)^{\alpha/2}(E_3 - E_2)^{-\alpha/2}$$
$$\times \exp\left\{-\frac{1}{2}\left[\ln^2\frac{E_2^{1/2}(E_{c3} - E_2)^{\alpha}}{(E_{c2} - E_2)^{1/2}(E_3 - E_2)^{\alpha}} + \frac{2}{\varkappa_{12}}\right]^{1/2}\right\}. \qquad (6.10)$$

3. $E_2 < \eta < E_3$:

$$T_c = \frac{2\gamma}{\pi}\eta(E_{c1} - \eta)(\eta - E_2)(E_{c2} - \eta)]^{1/4}$$
$$\times (E_{c2} - \eta)^{\alpha/2}(E_3 - \eta)^{-\alpha/2}$$
$$\times \exp\left\{-\frac{1}{2}\left[\ln^2\frac{(\eta - E_2)(E_{c2} - \eta)^2(E_3 - \eta)^{2\alpha}}{(E_{c1} - \eta)^2(E_{c3} - \eta)^{2\alpha}} + \frac{1}{\varkappa_2}\right]^{1/2}\right\}. \qquad (6.11)$$

4. $\eta = E_3$:

$$T_c = \frac{2\gamma}{\pi}(E_{c1} - E_3)^{1/4(1+\alpha)}$$
$$\times (E_3 - E_2)^{1/4}(E_{c2} - E_3)^{1/4}(E_{c3} - E_3)^{\alpha/2(1+\alpha)}E_3^{1/4(1+\alpha)}$$
$$\times \exp\left\{-\frac{1}{2}\left[\frac{1}{4}\ln^2\frac{(E_3 - E_2)(E_{c2} - E_3)}{E_3^{1/(1+\alpha)}(E_{c1} - E_3)^{1/(1+\alpha)}(E_{c3} - E_3)^{2\alpha/(1+\alpha)}} + \frac{1}{(\alpha + 1)\varkappa_{12}}\right]^{1/2}\right\}. \qquad (6.12)$$

5. $E_3 < \eta < E_{c1}$:

$$T_c = \frac{2\gamma}{\pi}(E_{c2} - \eta)^{1/4}$$
$$\times (\eta - E_2)^{1/4}\left[(E_{c1} - \eta)^{1/2}\eta^{1/2}(E_{c3} - \eta)^{\alpha}(\eta - E_3)^{\alpha}\right]^{1/\alpha(1+2\alpha)}$$
$$\times \exp\left\{\frac{-1}{4(1 + 2\alpha)}\left[\ln^2\frac{(E_{c2} - \eta)^{1+2\alpha}(\eta - E_2)^{1+2\alpha}}{(E_{c1} - \eta)(E_{c3} - \eta)^{2\alpha}\eta(\eta - E_3)^{2\alpha}} + \frac{4(1 + 2\alpha)}{\varkappa_{12}}\right]^{1/2}\right\}, \qquad (6.13)$$

where

$$\varkappa_{12} = \lambda_{12}\lambda_{21}, \quad \varkappa_{23} = \lambda_{23}\lambda_{32}, \quad \alpha = \frac{\varkappa_{23}}{2\varkappa_{12}}.$$

The dependence of T_c on the filling of the energy bands $\eta = -\mu$ obtained from (6.9)–(6.13) is shown in Fig. 8.

For $YBa_2Cu_3O_{7-\delta}$ we can assume that when the Fermi level intersects all three energy bands ($\delta = 0$) the transition temperature reaches a maximum $T_c \approx 90$ °K. As η decreases (δ increases) T_c drops and around $T = 50$ °K the dependence of T_c on η (or δ) becomes weaker; the corresponding region in η is $1.2 \lesssim \eta \lesssim 1.9$ eV for curve 2. This dependence is

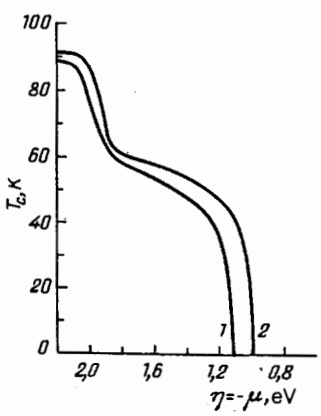

FIG. 8. Dependence of the superconducting transition temperature T_c on the filling of the energy bands $\eta = -\mu$ (overlap of three energy bands): *1)* $E_2 = 1.1$ eV, $E_3 = 2.0$ eV, $E_{c1} = E_{c2} = E_{c3} = 3.0$ eV, $\varkappa_{12} = 0.0077$, $\varkappa_{23} = 0.0025$; *2)* $E_2 = 1.0$ eV, $E_3 = 2.0$ eV, $E_{c1} = 2.5$ eV, $E_{c2} = 3$ eV, $E_{c3} = 3.5$ eV, $\varkappa_{12} = 0.008$, $\varkappa_{23} = 0.0028$.

qualitatively consistent with the experimental curve of T_c as a function of δ (Ref. 47); compare Fig. 6. We note that the step-like dependence of T_c on δ was obtained in Ref. 57 in the two-band model with repulsive interactions assuming that in a certain region μ does not change with a change in the concentration of oxygen.

7. CONCLUSION

We have summarized papers using the theory of superconductors with overlapping bands to describe the properties of high-temperature superconductors. We have also considered the effect of the Van Hove–Lifshits features of the density of electron states. We have considered the formation of flat areas and cylindrical cavities in the Fermi surface, which is typical of anisotropic systems such as superconducting ceramics.

As noted above, in multiband systems superconductivity can occur even when all the constants of the effective electron-electron interaction are repulsive. Hence the analytical results in Secs. 2–5 can be used for $V_{nm} > 0$ or $V_{nm} < 0$. The numerical estimates of the thermodynamic quantities in these Sections are given for electron-phonon interaction with $V_{nm} > 0$ (see (2.1)).

Even in the weak coupling approximation the two-band approach predicts a high value of T_c, a significant difference between $2\Delta_1/T_c$ and $2\Delta_2/T_c$, a small value of the jump in the electronic heat capacity, and so on (see Tables I and II). Note particularly the possibility of large negative values of $d\ln T_c/d\ln V$, which have been observed experimentally in lanthanum ceramics, and which represent an important test of the validity of the theory.

It is interesting that the step-like dependence of T_c on δ in $YBa_2Cu_3O_{7-\delta}$ (Ref. 47) and also the two maxima in the pressure dependence of T_c in $Bi_2Sr_2CaCu_2O_8$ (Ref. 55) can be obtained assuming the electron-phonon mechanism of superconductivity, if the overlap of the energy bands and topological transitions are taken into account.

The three-band model considered in Sec. 6 gives still better agreement with the experimental dependence of T_c on δ in $YBa_2Cu_3O_{7-\delta}$. In Sec. 6 the basic cause of superconductivity was assumed to be interband repulsive interactions between holes and in the equation determining T_c the integrals were cut off at energies of the order of the electron energy.

The results presented here show that the features of the band structure (overlapping energy bands and topological transitions) play a crucial role in determining the thermodynamic and electromagnetic properties of high-temperature superconductors.

The model considered here takes into account the overlap of the energy bands on the Fermi surface associated with the carriers in oxygen, which is supported by NMR studies in yttrium ceramics (see Ref. 58, for example). The NMR results show that the carriers in oxygen and in copper are two weakly coupled subsystems which can be treated as independent in the first approximation. We considered Coulomb repulsion in oxygen in the mean-field approximation. This approximation is standard and Coulomb interaction is normally not taken into account, or where it is taken into account the Hartree–Fock theory is used.[7,59]

The important question of p–d hybridization is not completely understood. The experiments that stimulated the current research and which were compared to theory for $YBa_2Cu_3O_{7-\delta}$ suggest that such hybridization is not very significant.

The results obtained here are qualitative, since electron correlations were not taken into account rigorously.

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