Superconductivity in a two-band system with low carrier density

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We have investigated the thermodynamic properties of a two-band system with low carrier density near the superconducting-transition temperature T_c, with account taken of all possible carrier pairings. A bell-shape dependence of T_c on the electron density, and have demonstrated a possible onset of HTSC. The absolute and relative jumps of the electron heat capacity (C_S-C_N) and $(C_S-C_N)/C_N$ at the point $T=T_c$ have been calculated and the density dependence of these quantities calculated. The theory yields both small values $(C_S-C_N)/C_N<1.43$ and large ones $(C_S-C_N)/C_N>1.43$. Favorable conditions have been manifested for an experimental observation of a bend on the chemical-potential plot $\mu^{(T)}$ at the point $T=T_c$.

1. INTRODUCTION

Many theoretical papers have by now been published on various aspects of the two-band model.[1,2] The great interest in this model and in its generalizations is due, firstly, to band calculations[3,4] showing that in metal-oxide ceramics the energy bands on the Fermi surface overlap (a similar situation obtains, apparently, also in systems with heavy fermions[5]), and secondly to the possibility of using the aforementioned model to describe the properties of systems with two groups of electrons (e.g., layered compounds). Of particular interest, however, is that the use of this model to describe the properties of high-temperature ceramics can explain many superconducting-characteristics anomalies observed in experiment. In particular, by using the two-band model and assuming moderate values of the coupling constants one can obtain high T_c, two energy gaps $2\Delta_1/T_c>3.5$ and $2\Delta_2/T_c<3.5$, large values of negative $d\ln T_c/d\ln V$ (V is the volume), a positive curvature of the upper critical field near the transition temperature, and others.[6–11] Furthermore, in the two-band model it is possible to describe the decrease of T_c with increase of the oxygen disorder, as well as when copper atoms are replaced by a nonmagnetic dopant (Al, Zn, etc).[12,13]

An important role in the determination of the thermodynamic and magnetic properties of a two-band superconductor is played also by the location of the Fermi level, which is changed by doping or by introduction of oxygen. It is particularly important to take this change into account in an analysis of a many-band system with assumption of a non-phonon superconductivity mechanism. Particular interest attaches to the possibility of obtaining a bell-shaped dependence of T_c and of the heat-capacity discontinuity (C_S-C_N) at the point $T=T_c$ on the carrier density.[14] It is possible then to obtain high T_c even if all the intraband $(\lambda_{11},\lambda_{22})$ and interband (λ_{12}) interactions correspond to repulsion between carriers, but the relation $\lambda_{11}\lambda_{22}-\lambda_{12}^2<0$ is satisfied. In the three-band model with a nonphonon superconductivity mechanism it is possible to obtain the "step" which is observed for $Y_1Ba_2Cu_3O_{7-\delta}$ in the dependence of T_c on the carrier density.[15,16] An investigation by one of us, of the properties of high-temperature ceramics, based on allowance for energy-band overlap of the energy bands and for electronic topological transitions, was reviewed in Ref. 17. One can find there references to experimental research results that can be described by allowance for the singularities in the electron energy spectrum of complex systems.

An increase of the number of energy bands on the Fermi surface increases the overall electron-state density and leads to the onset of an additional interband electron-electron interaction that contributes to the onset of superconductivity. This interaction violates the universal BCS relations and leads to a substantial dependence of a number of physical characteristics on the properties of an anisotropic system.[18–20] An interesting feature of the two-band model is independence of the superconducting-transition temperature of the sign of the interband-interaction constant. This model can therefore be used for the usual electron-phonon mechanism of superconductivity as well as for a mechanism based on the repulsion between carriers. In all the references cited above, the two-band model can be used to describe the properties of superconductors for which the relation $\mu\gg T_c$ is satisfied (μ is the chemical potential). This relation is satisfied in a number of cases also in high-temperature compound. The existence of this relation between μ and T_c makes it possible to use in the calculations an approximation diagonal in the band indices,[21,22] which leads to neglect of off-diagonal parameters such as Δ_{12} and Δ_{21}.

In systems with low carrier density, however, the relation $\mu\gg T_c$ does not hold. It becomes therefore necessary to develop a superconductivity theory for two-band systems, without constraints on the Fermi energy. This is the task of the present paper. We consider simultaneously two possible superconductivity mechanisms—phonon and electron. A characteristic feature of systems with low carrier density is a substantial dependence of the chemical potential μ on the order parameter in the superconducting phase. This circumstances has been noted in many papers, and the feasibility of experimentally observing anomalies in

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the temperature dependence of the chemical potential was first suggested in Ref. 23. It was shown there, with the BCS model as the example, the $\mu(T)$ curve has an experimentally observable bend at the point $T=T_c$. We shall show below that in the two-band case this effect is enhanced by the presence of four order parameters (Δ_{nm}; n, $m=1,2$) and is manifested at μ values easier to observe in experiment.

The plan of our paper is the following:

In Sec. 2 we present a system Hamiltonian that takes into account all possible intraband and interband interactions, and obtain a self-consistent system of equations for the order parameters Δ_{nm} and the chemical potential μ.

In Sec. 3 we investigate the anomalous behavior of the chemical potential $\mu(T)$.

In Sec. 4 we investigate the system properties near the superconducting-transition temperature ($T\sim T_c$) and determine the dependence of T_c on the carrier density for different ratios N_2/N_1 of the electron state densities of the two bands.

In Sec. 5 we calculate the discontinuity of the electron heat capacity (C_S-C_N) at the point $T=T_c$ and investigate its dependence on the carrier density. We investigate also the density dependence of the relative heat-capacity discontinuity $(C_S-C_N)/C_N$.

The research results are summarized in the last section.

2. SYSTEM HAMILTONIAN AND BASIC EQUATIONS

The considered two-band system is described by the Hamiltonian

$$H=\sum_{n\mathbf{k}\sigma}[\varepsilon_n(\mathbf{k})-\mu]a^+_{n\mathbf{k}\sigma}a_{n\mathbf{k}\sigma}-\frac{1}{V}\sum_{\substack{m_1\ldots m_4\\ \mathbf{k}\mathbf{k}'}}V^{m_3m_4}_{m_1m_2}(\mathbf{k}-\mathbf{k}';-\mathbf{k}\mathbf{k}')a^+_{m_1\mathbf{k}\uparrow}a^+_{m_2-\mathbf{k}\downarrow}a_{m_3-\mathbf{k}'\downarrow}a_{m_4\mathbf{k}'\uparrow}, \tag{1}$$

where $a^+_{n\mathbf{k}\sigma}$ and $a_{n\mathbf{k}\sigma}$ are creation and annihilation operators for a band-n electron with spin σ and quasiwave vector $\mathbf{k}$, μ is the chemical potential, and $V^{m_3m_4}_{m_1m_2}$ are the intra- and interband interaction constants. Expression (1) is a generalization of the BCS-Bogolyubov model Hamiltonian to include the two-band case. Account is taken here of all possible methods of electron pairing within each band and of electron pairing from different bands. If $m_1=m_2$ and $m_3=m_4$, the Hamiltonian (1) is equal to that of the Moskalenko model,[1] which considers only intraband pairing and transitions of a Cooper pair as a whole from one band to another are considered; this model is widely used to describe the properties of high-temperature superconductors.[6-17] Examination of the more general Hamiltonian (1) uncovers additional possible onsets of superconductivity (on account of single-particle hybridization and of all interband-interaction constants) and makes possible a description of the properties of a system with a low density of states ($\mu\sim T_c$).

Consider the one-particle temperature Green's functions (normal and anomalous)

$$G^{\sigma\sigma'}_{nm}(\mathbf{k}\mathbf{k}',\tau\tau')=-\langle Ta_{n\mathbf{k}\sigma}(\tau)a^+_{m\mathbf{k}'\sigma'}(\tau')\rangle,$$
$$F^{\sigma\sigma'}_{nm}(\mathbf{k}\mathbf{k}',\tau\tau')=-\langle Ta_{n\mathbf{k}\sigma}(\tau)a_{m\mathbf{k}'\sigma'}(\tau')\rangle, \tag{2}$$

and also the matrix Green's functions $\hat{G}$ and $\hat{F}$ made up of the Green's functions (2)

$$\hat{G}=\begin{pmatrix}G_{11}&G_{12}\\G_{21}&G_{22}\end{pmatrix};\quad \hat{F}=\begin{pmatrix}F_{11}&F_{12}\\F_{21}&F_{22}\end{pmatrix}. \tag{3}$$

Applying the Green's-function method[24] to the Hamiltonian (1) we obtain in the $n\mathbf{k}w$ representation a matrix equation for the Green's-function components

$$\begin{pmatrix}i\hat{W}-\hat{\varepsilon}&\hat{\Delta}\\\hat{\Delta}&i\hat{W}+\hat{\varepsilon}\end{pmatrix}\begin{pmatrix}\hat{G}(\omega)\\\hat{F}^+(\omega)\end{pmatrix}=\begin{pmatrix}\mathbf{1}\\0\end{pmatrix}, \tag{4}$$

$$\begin{pmatrix}i\hat{W}-\hat{\varepsilon}&-\hat{\Delta}^t\\-\hat{\Delta}^t&i\hat{W}+\hat{\varepsilon}\end{pmatrix}\begin{pmatrix}\hat{F}(\omega)\\\hat{G}^t(-\omega)\end{pmatrix}=\begin{pmatrix}0\\\mathbf{1}\end{pmatrix}. \tag{5}$$

The superscript "t" labels here the transpose of a matrix

$$\hat{W}=\begin{pmatrix}\omega&0\\0&\omega\end{pmatrix},\quad \hat{\varepsilon}=\begin{pmatrix}\varepsilon_1-\mu_1&0\\0&\varepsilon_2-\mu_2\end{pmatrix},$$
$$\hat{\Delta}=\begin{pmatrix}\Delta_{11}&\Delta_{12}\\\Delta_{21}&\Delta_{22}\end{pmatrix},\quad \mathbf{1}=\begin{pmatrix}1&0\\0&1\end{pmatrix},$$
$$\mu_n=\mu+A_n,\quad A_n=\sum_{\mathbf{k}m}(2V^{nm}_{mn}-V^{mn}_{mn})\langle a^+_{m\mathbf{k}\uparrow}a_{m\mathbf{k}\uparrow}\rangle, \tag{6}$$

A_n is a quantity that renormalizes the chemical potential in the self-consistent-field approximation. Simple matrix transformations based on (4) and (5) yield for the Green's functions $G_{nm}(\omega)$ and $F_{nm}(\omega)$

$$G_{11}(z)=\frac{1}{D(z)}[(z+\bar{\varepsilon}_1)(z^2-\xi_2^2)-\Delta_{12}\Delta_{21}(z+\bar{\varepsilon}_2)], \tag{7}$$

$$G_{12}(z)=\frac{\Delta_{12}}{D(z)}[\Delta_{11}(z+\bar{\varepsilon}_2)+\Delta_{22}(z+\bar{\varepsilon}_1)], \tag{8}$$

$$F_{11}(z)=-\frac{\Delta_{11}}{D(z)}\left[z^2-\xi_2^2+\frac{\Delta_{12}\Delta_{21}}{z_{(12)}}\right], \tag{9}$$

$$F_{12}(z)=\frac{-\Delta_{12}}{D(z)}\frac{z_{(13)}}{z_{(14)}}[\Delta_{11}\Delta_{22}-\Delta_{12}\Delta_{21}+(z+\bar{\varepsilon}_1)\times(z+\bar{\varepsilon}_2)], \tag{10}$$

where

$$\xi_n^2=\bar{\varepsilon}_n^2+\Delta_{nn}^2,\quad \bar{\varepsilon}_n=\varepsilon_n-\mu_n,$$
$$z_{(12)}=\Delta_{11}/\Delta_{22},\quad z_{(13)}=\Delta_{11}/\Delta_{12},\quad z_{(14)}=\Delta_{11}/\Delta_{21}, \tag{11}$$

$$D(z)=(z^2-\xi_1^2)(z^2-\xi_2^2)+2\Delta_{12}\Delta_{21}(\varepsilon_1\varepsilon_2-z^2)+(\Delta_{11}\Delta_{22}-\Delta_{12}\Delta_{21})^2-\Delta_{12}^2\Delta_{21}^2. \tag{12}$$

The Green's functions G_{22}, G_{21}, F_{22}, and F_{21} are easily obtained from Eqs. (7)–(12) by interchanging the subscripts 1 and 2. We obtain then for the order parameters Δ_{np} the set of equations

$$\Delta_{np}=\frac{1}{\beta V}\sum_{\mathbf{k}\omega}\sum_{lr}V_{np}^{lr}F_{lr}(i\omega)$$

$$=\frac{1}{\beta V}\sum_{\mathbf{k}w}[V_{np}^{11}F_{11}(i\omega)+V_{np}^{22}F_{22}(i\omega)+V_{np}^{12}F_{12}(i\omega)$$

$$+V_{np}^{21}F_{21}(i\omega)]. \qquad (13)$$

In the case Δ_{12}, $\Delta_{21}\ll\Delta_{11}$, Δ_{22} (this condition is satisfied in ordinary superconductors in which[21,22] $\mu\gg T_c$) expression (13) goes over into the known result of the model of Ref. 1. Substituting expressions (9) and (10) in (13) and summing over w, we reduce the set of equations for the order parameters Δ_{np} to the form

$$\Delta_{np}=\frac{1}{4V}\sum_{\substack{\mathbf{k}lr\\ r\neq l}}V_{np}^{ll}\Delta_{ll}\left[\left(\frac{\xi_l^2-\xi_r^2+2\Delta_{12}\Delta_{21}(1+1/z_{(12)})}{d}+1\right)\right.$$

$$\times\frac{\operatorname{th}\dfrac{\beta E_1}{2}}{E_1}-\left(\frac{\xi_l^2-\xi_r^2+2\Delta_{12}\Delta_{21}(1+1/z_{(12)})}{d}-1\right)$$

$$\left.\times\frac{\operatorname{th}\dfrac{\beta E_2}{2}}{E_2}\right]+\frac{1}{4V}\sum_{\mathbf{k}}\left(V_{np}^{12}\Delta_{12}\frac{z_{(13)}}{z_{(14)}}+V_{np}^{21}\Delta_{21}\frac{z_{(14)}}{z_{(13)}}\right)\Gamma, \qquad (14)$$

where

$$E_{1,2}=\sqrt{\frac{a\pm d}{2}},\quad a=\xi_1^2+\xi_2^2+2\Delta_{12}\Delta_{21},$$

$$d^2=(\xi_1^2-\xi_2^2)^2+4\Delta_{12}\Delta_{21}[(\bar{\varepsilon}_1-\bar{\varepsilon}_2)^2+(\Delta_{11}+\Delta_{22})^2], \qquad (15)$$

$$\Gamma=\left[\frac{(\bar{\varepsilon}_1-\bar{\varepsilon}_2)^2+(\Delta_{11}+\Delta_{22})^2}{d}+1\right]\frac{\operatorname{th}\dfrac{\beta E_1}{2}}{E_1}$$

$$-\left[\frac{(\bar{\varepsilon}_1-\bar{\varepsilon}_2)^2+(\Delta_{11}+\Delta_{22})^2}{d}-1\right]\frac{\operatorname{th}\dfrac{\beta E_2}{2}}{E_2}. \qquad (16)$$

The system (14) determines the order parameters Δ_{11} and Δ_{22} of an ordinary superconductor (and can be simplified in this case by putting $\Delta_{12}=\Delta_{21}=0$), as well as of a superconductor with low carrier density $\mu\sim T_c$.

3. ANOMALOUS BEHAVIOR OF CHEMICAL POTENTIAL

We supplement the system (14) with the expression

$$N_0=\frac{2}{\beta V}\sum_{\mathbf{k}w}[G_{11}(\mathbf{k},\omega)+G_{22}(\mathbf{k},\omega)]e^{i\omega 0+}. \qquad (17)$$

Substituting in (17) the definition (7) of the Green's functions and summing over w, we obtain

$$N_0=\sum_{\mathbf{k}nm,n\neq m}\left[1-\left(\frac{\bar{\varepsilon}_n+\bar{\varepsilon}_m}{2}+\frac{\bar{\varepsilon}_n-\bar{\varepsilon}_m}{2}\frac{\xi_1^2-\xi_2^2}{d}\right)\frac{\operatorname{th}\dfrac{\beta E_n}{2}}{E_n}\right]. \qquad (18)$$

The self consistent set of Eqs. (14) and (18) determines the order parameters Δ_{np} and the chemical potential μ for a specified temperature T and a carrier density N_0. A characteristic feature of the ground state in *a* system with low carrier density is a substantial change of the position of the Fermi level following the onset of the superconducting gap. The order parameters Δ_{np} become of the same order as the chemical potential $\mu(\mu\sim\Delta_{np})$. This leads to an anomalous behavior of the chemical potential as a function of temperature. In particular, in the single-band BCS model[23] and in the Hubbard model[25] the chemical potential has in rarefied systems a kink at the point $T=T_c$. As first noted by Van der Marel,[23] this kink is observable in experiment and consequently its observation can help explain the superconductivity mechanism. Van der Marel[23] has demonstrated the possibility of a kink at $\mu\leqslant 2$ meV, which is the lower limit of present-day accuracy.[26] Since the overlap of the energy bands plays a major role in the explanation of the properties of high-temperature superconductors, it is of interest to investigate the anomalous behavior of the chemical potential in a two-band model with low carrier density, and the possible onset of a kink at values of μ more conducive to experimental observation. We represent the order parameter Δ_{nm} near the superconducting transition temperature $T\sim T_c$ in the form

$$\Delta_{nm}=c_{nm}(\beta-\beta_c)^{1/2}+c_{nm}^{(1)}(\beta-\beta_c)^{3/2}+\dots. \qquad (19)$$

The expression for the chemical potential μ near T_c is now

$$\mu(T)=\mu_0(T)-R_0\Delta_{11}^2, \qquad (20)$$

where $\mu_0(T)$ is the chemical potential of the normal phase, and R_0 is determined from the constancy of the carrier density in the superconducting and normal phases. Substituting (19) in (20) we readily obtain a jumplike change of $d\mu/dT$. Contributions to this change are made by all the order parameters Δ_{nm}, so that the results can differ from those for the case of one band.[23]

4. SELF-CONSISTENT SYSTEM OF EQUATIONS FOR $T=T_c$

To investigate the properties of a two-band system near the superconducting-transition temperature we expand in Eqs. (14) and (18) in terms of the small parameters Δ_{nm} and Δ_{mn} with account taken of expansions (19) and (20).

We introduce the dispersion law of the nth band

$$\varepsilon_n(\mathbf{k})=-\zeta_n-\frac{k_x^2+k_y^2}{2m_n}, \qquad (21)$$

and change in these equations from summation over $\mathbf{k}$ to integration over the energy in accordance with the dispersion law (21) ($\bar{\varepsilon}_{n0}=\varepsilon_n-\mu_{0n}$, $\mu_{0n}=\mu_0-A_n$):

$$\frac{1}{V}\sum_{\mathbf{k}}\Phi(\varepsilon_n-\mu_{0n})=2N_n\int_{-D_n}^{D_{cn}}dx\Phi(-x), \qquad (22)$$

where $N_n=m_nk_{zn}^0/2(2\pi)^2$ is the density of the electron states in the nth band.

The integration limits are chosen to be able to consider simultaneously two possible superconductivity mechanisms: the values of $D_n=\eta_{0n}-\zeta_n\leqslant\omega_{D_n}$ and $D_{cn}=\omega_{D_n}$

(ω_{D_n} is the phonon cutoff frequency in the nth band) correspond to the phonon mechanism of superconductivity, and the quantities $D_n=\eta_{0n}-\zeta_n$ and $D_{cn}=\xi_{cn}-\eta_{0n}$ (ξ_{cn} is a cutoff energy of the order of that of the electron; $\eta_n=-\mu_{0n}$ corresponds to the hole mechanism.

Integrating next over the energy and equating the coefficients of equal powers in the difference $(\beta-\beta_c)$, we obtain for c_{nm} and $c_{nm}^{(1)}$ the set of equations

$$c_{nm}=-\sum_l c_{ll}N_lJ_lV_{nm}^{ll}-(c_{12}V_{nm}^{21}+c_{21}V_{nm}^{12})\sum_{lp,p\neq l}\frac{N_lI_{lp}}{1+b_{lp}}, \tag{23}$$

$$\begin{aligned}c_{nm}^{(1)}=&-\sum_l c_{ll}^{(1)}N_lJ_lV_{nm}^{ll}-(c_{12}^{(1)}V_{nm}^{21}+c_{21}^{(1)}V_{nm}^{12})\sum_{lp,p\neq l}\frac{N_lI_{lp}}{1+b_{lp}}\\&-\sum_l c_{ll}N_lV_{nm}^{ll}\left(-\frac{\theta_l}{\beta}+(\beta c_{ll})^2\bar F_l\right)\\&-(c_{12}V_{nm}^{21}+c_{21}V_{nm}^{12})\left(\frac{1}{\beta}\sum_{lp,p\neq l}\frac{N_lT_{lp}}{1+b_{lp}}+(\beta c_{11})^2\Gamma\right).\end{aligned} \tag{24}$$

Here

$$J_l=J^0(-\beta D_{cl})-J^0(\beta D_l);\quad I_{lp}=I_{lp}^0(-\beta D_{cl})-I_{lp}^0(\beta D_l). \tag{25}$$

The quantities $\bar F_l$, T_{lp}, and Γ are analogously differences of type (25), where

$$J^0(x)=\int_0^x\frac{\operatorname{th}\frac{y}{2}}{y}dy,\quad I_{lp}^0(x)=\int_0^x\frac{\operatorname{th}\frac{y}{2}}{y-\frac{r_l}{1+b_{lp}}}dy,\quad r_l=\beta t_l,$$

$$t_l=\bar\xi_{3-l}-b_{l3-l}\bar\xi_l-\eta_0(1-b_{l3-l}),\quad \bar\xi_l=\xi_l+A_l;\quad b_{lp}=\frac{m_l}{m_p},$$

$$\theta_l=\operatorname{th}\frac{\beta D_{cl}}{2}-\operatorname{th}\frac{\beta D_l}{2},\quad T_{lp}^0(x)=\int_0^x\frac{dy}{\operatorname{ch}^2\frac{y}{2}}\frac{y}{y-\frac{r_l}{1+b_{lp}}}, \tag{26}$$

$$\begin{aligned}\bar F_n^0(x)=&F^0(x)+\frac{R_0}{\beta}z_{(1n)}^2\frac{\operatorname{th}\frac{x}{2}}{x}+(1+1/z_{(n3-n)})\\&\times\sum_{lp,p\neq l}\frac{N_l}{2r_lN_n}[D_{lp}^1(x)-D_{lp}^2(x)]+\frac{z_{(1n)}^2}{z_{(13)}z_{(14)}}\\&\times\left[\sum_{lp,p\neq l}\frac{N_l[2B_{lp}(x)+(-1)^{l+p}\alpha_{lp}^1(x)]}{N_n(1+b_{lp})^2}\right.\\&\left.-\sum_{r,r\neq n}\frac{1-b_{nr}}{(1+b_{nr})^2}2B_{nr}(x)\right],\end{aligned}$$

$$F^0(x)=\int_0^x\frac{y-\operatorname{sh}y}{4y^3\operatorname{ch}^2\frac{y}{2}}dy,$$

$$B_{lp}(x)=\int_0^x\frac{y-\operatorname{sh}y}{4y^2\operatorname{ch}^2\frac{y}{2}}\frac{dy}{y-\frac{r_l}{1+b_{lp}}},$$

$$\alpha_{lp}^i(x)=\frac{\operatorname{th}\frac{x}{2}}{x\left(x-\frac{r_l}{1+b_{lp}}\right)^i},$$

$$D_{lp}^j(x)=\int_0^x\frac{\operatorname{th}\frac{y}{2}}{y}\frac{dy}{y-\frac{r_l}{b_{lp}-(-1)^j}},\quad i,j=1,2,$$

$$\Gamma^0(x)=\sum_{lp,p\neq l}Y_{lp}^0(x),$$

$$\begin{aligned}Y_{lp}^0(x)=&\frac{N_lB_{lp}(x)}{1+b_{lp}}\left[\frac{1}{z_{(1l)}^2}+\left(\frac{1}{z_{(l2)}^2}-\frac{1}{z_{(1l)}^2}\right)\frac{1}{1+b_{lp}}\right.\\&\left.+\frac{4}{z_{(13)}z_{(14)}}\frac{b_{lp}}{(1+b_{lp})^2}\right]+\frac{N_l\alpha_{lp}^1(x)}{(1+b_{lp})^2}\\&\times\left[\frac{1-b_{lp}}{1+b_{lp}}\frac{1}{z_{(13)}z_{(14)}}-\frac{1}{2}\left(\frac{1}{z_{(l2)}^2}-\frac{1}{z_{(1l)}^2}\right)\right]\\&+\frac{N_l}{2r_l}[D_{lp}^1(x)-D_{lp}^2(x)]\left(\frac{1}{z_{(12)}}+\frac{1}{2z_{(1l)}^2}\right.\\&\left.+\frac{1}{2z_{(l2)}^2}\right)+\frac{R_0}{\beta}\frac{N_lQ_{lp}(x)}{1+b_{lp}(x)}\\&+\frac{N_l}{z_{(13)}z_{(14)}}\frac{r_l}{(1+b_{lp})^4}[\alpha_{lp}^2-2b_{lp}H_{lp}(x)],\end{aligned} \tag{27}$$

$$Q_{lp}(x)=\frac{\operatorname{th}\frac{x}{2}}{x}\left(1+\frac{2r_l}{1+b_{lp}}\right)-\frac{1-b_{lp}}{1+b_{lp}}\left[D_{lp}^1(x)+\frac{2r_lB_{lp}(x)}{1+b_{lp}}\right],$$

$$\begin{aligned}H_{lp}(x)=&\frac{x-\operatorname{sh}x}{4x^2\operatorname{ch}^2\frac{x}{2}}\frac{1}{x-\frac{r_l}{1+b_{lp}}}+\int_0^x\frac{dy}{y-\frac{r_l}{1+b_{lp}}}\\&\times\left(\frac{y-\operatorname{sh}y}{2y^2\operatorname{ch}^2\frac{y}{2}}+\frac{\operatorname{sh}y}{2y(\operatorname{ch}y+1)^2}\right).\end{aligned}$$

Equation (18) for the carrier density is transformed into

$$N_0=2\sum_l N_l\left[D_{cl}+D_l-\frac{2}{\beta}\ln\frac{\operatorname{ch}\frac{\beta D_{cl}}{2}}{\operatorname{ch}\frac{\beta D_l}{2}}\right]$$

$$+2\sum_{lp,p\neq l}N_l\left[R_0\Delta_{11}^2\theta_l-\frac{\Delta_{12}\Delta_{21}\beta}{1+b_{lp}}\chi_{lp}-\frac{\Delta_{ll}^2\beta}{2}\varkappa_l\right], \tag{28}$$

where θ_l is defined in (26), while χ_{lp} and $\varkappa_l$ are differences of the type (25), where

$$\varkappa_l^0(x)=\frac{\operatorname{th}\frac{x}{2}}{x},$$

$$\chi_{lp}^0(x)=\frac{\operatorname{th}\frac{x}{2}}{x}+\frac{2r_l}{(1+b_{lp})^2}\alpha_{lp}^1(x)-\frac{1-b_{lp}}{1+b_{lp}}\left[D_{lp}^1(x)+\frac{2r_l}{1+b_{lp}}B_{lp}(x)\right]. \tag{29}$$

We introduce quasiband indices in accord with the rule

$$11\to(1),\quad 22\to(2),\quad 12\to(3),\quad 21\to(4), \tag{30}$$

and also the symbols:

$$V_{nm\ pr}^{pr}\to V_{nm\ pr}\to U_{(n')(m')},\quad n',m'=1-4,$$

$$N_{(3)}J_{(3)}=\frac{z_{(13)}}{z_{(14)}}\sum_{lp,p\neq l}\frac{N_lI_l}{1+b_{pl}},$$

$$N_{(4)}J_{(4)}=\frac{z_{(14)}}{z_{(13)}}\sum_{lp,p\neq l}\frac{N_lI_l}{1+b_{lp}},$$

$$N_{(3)}\bar F_{(3)}=\frac{z_{(13)}}{z_{(14)}}\Gamma,\quad N_{(4)}\bar F_{(4)}=\frac{z_{(14)}}{z_{(13)}}\Gamma, \tag{31}$$

$$N_{(3)}\theta_{(3)}=-\frac{z_{(13)}}{z_{(14)}}\sum_{lp,p\neq l}\frac{N_lT_l}{1+b_{lp}},$$

$$N_{(4)}\theta_{(4)}=-\frac{z_{(14)}}{z_{(13)}}\sum_{lp,p\neq l}\frac{N_lT_l}{1+b_{lp}}.$$

Equations (23) and (24) take formally in the "pseudoband" representation (30) and (31) the form of the "fourband" model:[18]

$$c_{(n)}=-\sum_{(m)=1}^{4}N_{(m)}U_{(n)(m)}c_{(m)}, \tag{32}$$

$$c_{(n)}^{(1)}=-\sum_{(m)=1}^{4}N_{(m)}U_{(n)(m)}c_{(m)}^{(1)}-\sum_{(m)=1}^{4}\Phi_{(m)}U_{(n)(m)}, \tag{33}$$

where

$$\Phi_{(m)}=\left(-\frac{\theta_{(m)}}{\beta}+(\beta c_{(m)})^2\bar F_{(m)}\right)N_{(m)}.$$

We omit hereafter the parentheses of the pseudoband subscripts. Changeovers to the true band indices will be specially stipulated. It is convenient to rewrite Eqs. (32) and (33) in the matrix form

$$D_0c=0 \tag{32a}$$

$$D_0c^{(1)}=-\Phi, \tag{33a}$$

where c, $c^{(1)}$, and Φ are single-column matrices in the indices 1 to 4, and

$$D_0=\begin{pmatrix}1+N_1J_1U_{11} & N_2J_2U_{12} & N_3J_3U_{13} & N_4J_4U_{14}\\ N_1J_1U_{12} & 1+N_2J_2U_{22} & N_3J_3U_{23} & N_4J_4U_{24}\\ N_1J_1U_{31} & N_2J_2U_{32} & 1+N_3J_3U_{33} & N_4J_4U_{34}\\ N_1J_1U_{41} & N_2J_2U_{42} & N_3J_3U_{43} & 1+N_4J_4U_{44}\end{pmatrix}. \tag{34}$$

From the condition that the system (32a) have a solution, we obtain an equation for the critical temperature T_c:

$$\|D_0\|=0, \tag{35}$$

where $\|...\|$ designates the determinant of a matrix. It follows from the system (33a) that

$$c_1^{(1)}=\|D_1\|/\|D_0\|. \tag{36}$$

Since $\|D_0\|=0$, we get

$$\|D_1\|=0, \tag{37}$$

where D_1 is a 4×4 matrix that differs from D_0 in that the first column is replaced by the elements of the matrix Φ.

The condition (37) leads to the relation

$$\sum_{n=1}^{4}c_nN_n\left(-\frac{\theta_n}{\beta}+(\beta c_n)^2\bar F_n\right)\frac{f_n}{z_{1n}}=0, \tag{37a}$$

where θ_n and $\bar F_n$ are defined in (25)–(27).

$$\frac{1}{z_{1n}}=\frac{\|L_n\|}{\|A_0\|},\quad n=2-4,\quad \frac{1}{z_{11}}=1, \tag{38a}$$

A_0 is the cofactor of the first diagonal element of the matrix D_0, and L_n are matrices that differ from the matrix A_0 in that the $(n-1)$st column is replaced by the column

$$N_1J_1\begin{pmatrix}U_{21}\\U_{31}\\U_{41}\end{pmatrix},$$

and

$$f_n=\frac{\|X_n\|}{\Phi_n\|L_n\|}, \quad n=2-4; \quad f_1=1, \tag{38b}$$

where X_n is the cofactor of the "nn" diagonal element of the matrix D_1.

We have on the basis of (37a)

$$c_1^2=\frac{1}{\beta_c^3}\frac{\sum_{n=1}^{4} N_n\theta_n f_n/z_{1n}^2}{\Sigma_{n=1}^4 N_n\bar{F}_n f_n/z_{1n}^4}=\frac{\overline{c_1^2}}{\beta_c^3}. \tag{39}$$

Assuming the particle number N_0 to be fixed and using the expansion (19) for the chemical potential near T_c we obtain

$$\mu(T)=\mu_0(T)-\frac{R_0}{\beta}\overline{c_1^2}(T_c-T), \tag{20a}$$

where

$$\frac{R_0}{\beta}=\frac{\Sigma_{lp,p\neq l}N_l[\varkappa_l/2z_{(1l)}^2+\chi_{lp}/(1+b_{lp})/z_{(13)}z_{(14)}]}{\Sigma_l N_l\theta_l}, \tag{40}$$

and μ_0 is determined from the equation

$$N_0=2\sum_l\left[D_{c_l}+D_l-\frac{2}{\beta}\ln\frac{\operatorname{ch}\frac{\beta D_{c_l}}{2}}{\operatorname{ch}\frac{\beta D_l}{2}}\right]. \tag{28a}$$

Expressions (39) and (40) obtained for c_1^2 and R_0 as well as (20a) and (28a) for the chemical potential μ and for μ_0 complete, in a self-consistent manner, the set of equations (32)–(34) for the order parameters Δ_{np} near T_c. It is therefore possible to calculate the dependence of the superconducting temperature T_c on the carrier density N_0 for all values of the interaction constants $\lambda_{nm}=N_m U_{nm}$ ($n,m=1-4$), and also the temperature dependence of the chemical potential $\mu(T)$.

Figure 1 shows the dependence of the superconducting temperature T_c on the carrier density $N_0/2N_1$ for different degrees of hybridization: a) weak: $\lambda_{11}=\lambda_{22}=0.2$, $\lambda_{12}=\lambda_{21}=\lambda_{33}=\lambda_{44}=0.01$, $\lambda_{34}=\lambda_{43}=0.105$, the remaining ones: $\lambda_{nm}=0.001$ ($n, m=1-4$); b) strong $\lambda_{11}=\lambda_{22}=0.2$, $\lambda_{12}=\lambda_{21}=\lambda_{33}=\lambda_{44}=0.1$, $\lambda_{34}=\lambda_{43}=0.15$, the remaining ones $\lambda_{nm}=0.01$ ($n, m=1-4$).

Calculations are performed for the following values of the parameter

$$\zeta_1=0 \text{ eV}, \quad \zeta_2=0.03 \text{ eV}, \quad \zeta_{c1}=0.05 \text{ eV}, \quad \zeta_{c2}=0.08 \text{ eV}.$$

It follows from Fig. 1 that one can obtain a bell-shaped dependence of T_c on N_0 (curves *1–3*). Inclusion of strong hybridization lowers T_c. The character of the dependence of the transition temperature T_c on the carrier density N_0 is strongly influenced by the relation between the electronic-state densities of the different bands. Lowering the ratio N_2/N_1 slows down the growth of T_c with increase of N_0 (for case b) and accelerates the decrease for both cases (a, b).

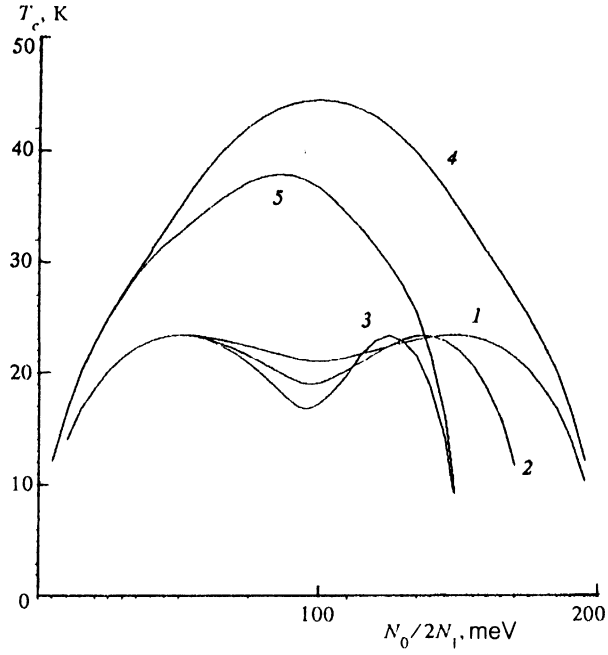

FIG. 1. Dependence of T_c on the carrier density $N_0/2N_1$ in the case of weak (*1–3*) and strong (curves *4*, *5*) hybridization for $N_2/N_1=1$ (curves *1* and *4*); 0.75 (*2*); 0.5 (*3*, *5*).

In the case of weak hybridization (curves *1–3*) the T (N_0) plot acquires two maxima. The degree to which then become pronounced, given the parameters λ_{mn}, is determined by the electron state-density ratio N_2/N_1. The presence of weakly pronounced maxima (curve *1*) corresponds to the case N_1 and N_2, and more strongly pronounced maxima (curves *2* and *3*) appear at N_1/N_2 and are determined by the anisotropy of the system (by the difference between the bands). Each of these maxima is connected with the occupation of the corresponding band. In the absence of interband interaction (energy-band overlap) the plot would consist of two nonoverlapping curves. The onset of interband interactions produces simultaneous superconductivity in both bands, with a single superconducting temperature determined by all the interaction constants λ_{nm}. With increase of the interband-interaction constants ($\lambda_{34},\lambda_{43}\sim\lambda_{11},\lambda_{22}$) the contribution due to the overlap of the two bands begins to predominate over the individual contribution of each band, so that the $T_c(N_0)$ plot is a single bell-shaped curve (*4*, *5*).

Figure 2 shows the temperature dependence of $\eta=-\mu$ for a non-phonon superconductivity mechanism at various carrier densities N_0 and with weak hybridization. We see that this plot has at $T=T_c$ (curves *1–3*) a kink that becomes less peaked with increase of the carrier density and vanishes at $\eta\sim 8$ meV (curve *4*). The behavior of $\eta(T)$ under strong hybridization is similar. The anomaly of the temperature dependence of the chemical potential $\eta=-\mu$ at the point $T=T_c$ is due to the appearance, on the Fermi surface, of a superconducting gap that does not differ excessively from the chemical potential. This gap influences substantially the chemical potential f at $T<T_c$, since the

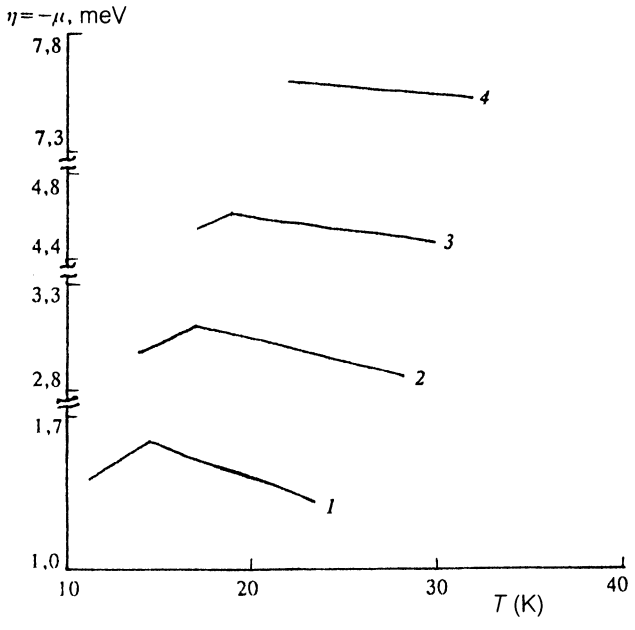

FIG. 2. Temperature dependence of the chemical potential ($\eta=-\mu$) for various values of the carrier density N_0. Curve *1* corresponds to $N_0/2N_1=0.01$; *2*—0.015; *3*—0.02; *4*—0.03.

values of η and Δ_{nm} are self-consistently determined from the set of equations (14) and (18).

Allowance for the energy-band overlap leads to a kink on the temperature dependence of the chemical potential at $T=T_c$ for the sufficiently high values $\eta\leqslant 8$ meV ($\eta\leqslant 2$ meV in the single band case[23]), which undoubtedly facilitates experimental verification of this effect.

5. HEAT-CAPACITY JUMP AT THE POINT $T=T_c$

In the preceding section we changed over to the pseudo-band representation, which allowed us to write down Eqs. (32) and (33), as it were, for a four-band model.

It can also be shown that the difference between the free energies in the superconducting and normal phases in the pseudoband representation generalizes the corresponding expression of the Moskalenko two-band model.[1,18] We obtain

$$\frac{\Psi_S-\Psi_N}{V}=\sum_{nmp}\int_0^{\Delta_p}\Delta_n\Delta_m\frac{(\delta U^{-1})_{nm}}{\delta\Delta_p}\delta\Delta_p, \qquad (41)$$

where n, m, and p are the pseudoband numbers (n, m, $p=1$–4), and U^{-1} is the inverse of the interaction matrix U (31). We expand, in the pseudoband formalism, the set of Eqs. (14) for the order parameters Δ_n in powers of the small quantity $(\beta\Delta_n)^2$ in the vicinity of the critical temperature T_c:

$$\Delta_m=-\sum_n N_n U_{nm}(J_n+(\beta\Delta_n)^2\bar{F}_n+\ldots), \qquad (42)$$

where J_n and $\bar{F}_n$ are defined in (25)–(27).

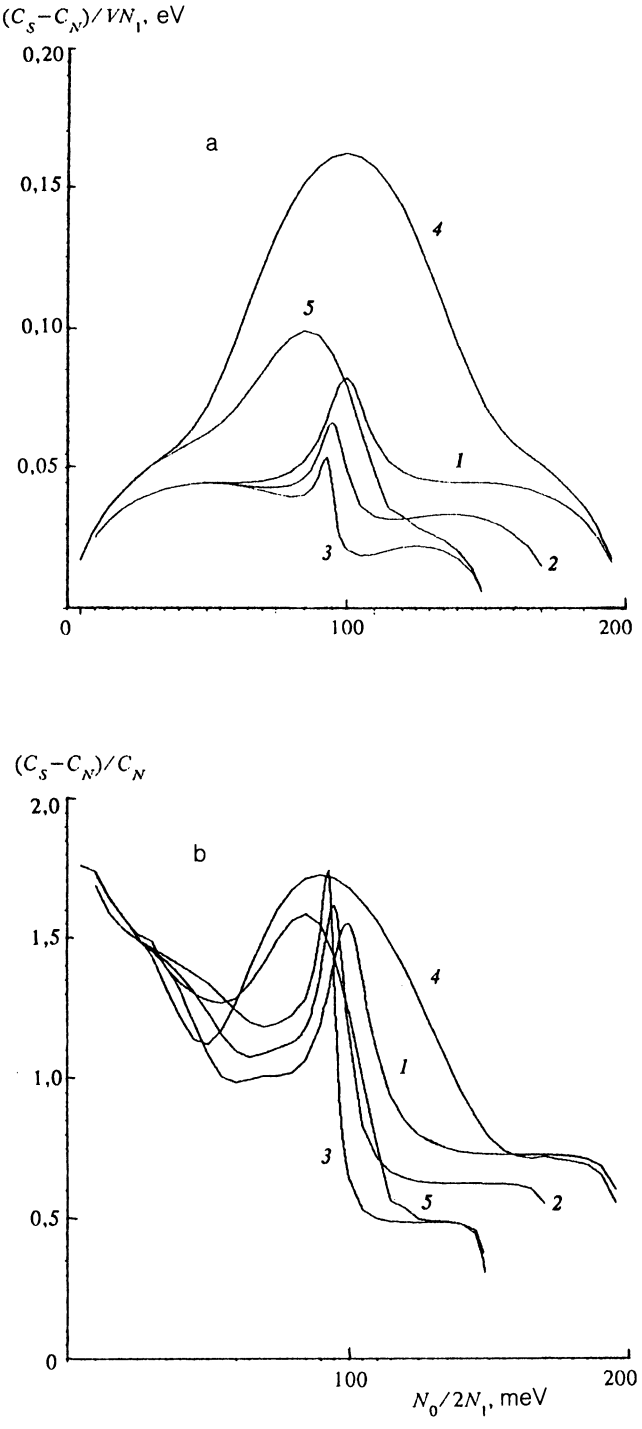

FIG. 3. Dependences of the absolute $(C_S-C_N)/VN_1$ and relative $(C_S-C_N)/C_N$ electron-temperature jumps on the carrier density $N_0/2N_1$. The curves labels are the same as in Fig. 1.

Using the calculation method of Refs. 18 and 14 for Eqs. (41) and (42), we obtain for the heat-capacity jump at the point $T=T_c$

$$\frac{C_S-C_N}{V}=-T\frac{\partial^2}{\partial T^2}\frac{\Psi_S-\Psi_N}{V}=\beta_c^5\sum_{n=1}^{4}N_n\bar{F}_n c_n^4. \qquad (43)$$

Substituting expression (39) in this equation, we get

$$\frac{C_S-C_N}{V}=T_c\left[\frac{\Sigma_{n=1}^4 N_n\theta_n f_n/z_{1n}^2}{\Sigma_{n=1}^4 N_n\bar{F}_n f_n/z_{1n}^4}\right]^2\sum_{n=1}^4\frac{N_n\bar{F}_n}{z_{1n}^4}. \quad (44)$$

The equation for the electronic heat capacity in the normal phase is[14]

$$C_N=4T\sum_{n=1}^2 N_n\varphi_n(\eta), \quad (45)$$

where

$$\varphi_n(\eta)=\int_{-\beta(\eta-\zeta_{cn})}^{\infty}\frac{x^2dx}{(1+e^x)(1+e^{-x})}. \quad (46)$$

In accordance with Eqs. (44) and (45) we have for the relative heat-capacity jump

$$\frac{C_S-C_N}{C_N}=\left[\frac{\Sigma_{(n)=1}^4 N_{(n)}\theta_{(n)}f_{(n)}/z_{(1n)}^2}{\Sigma_{(n)=1}^4 N_{(n)}\bar{F}_{(n)}f_{(n)}/z_{(1n)}^4}\right]^2 \times\frac{\Sigma_{(n)=1}^4 N_{(n)}\bar{F}_n/z_{(1n)}^4}{4\Sigma_{n=1}^2 N_n\varphi_n(\eta)}. \quad (47)$$

Using the rules (30) and (31) for the change to the usual band representation, we can obtain on the basis of Eqs. (25)–(27), (38a,b), and (45) analytic expressions for the absolute and relative jumps of the electron heat capacity at the point $T=T_c$.

Figure 3 shows the dependences of these quantities on the carrier density N_0, obtained by numerical methods using the equations given above. The numbers of the curves in these figures are the same as in Fig. 1.

As seen from Fig. 3a, the dependence of $(C_S - C_N)_{T=T_c}$ on N_0 has a maximum. At the same time, this dependence does not duplicate the behavior of $T_c(N_0)$. This circumstance indicates that a substantial contribution to the dependence of $(C_S - C_N)_{T=T_c}$ on N_0 is made not only by T_c but also by the complicated function in the right-hand side of (44). Analysis of the curves of Fig. 3 shows that the charater of the plot of $(C_S - C_N)_{T=T_c}$ versus N_0 is determined by the type of hybridization (strong or weak) and by the ratio N_2/N_1 of the electron-state densities. It is possible for T_c and $(C_S - C_N)_{T=T_c}$ to have maxima at one and the same value of N_0 (curves *4* and *5*). This situation is observed in experiment, for example in $La_{2-x}Sr_xCu_2O_4$ (Ref. 27).

The possibility of obtaining small $(C_S-C_N)/C_N < 1.43$, as well as large $(C_S-C_N)/C_N > 1.43$ values of the relative jump of the electron specific heat is demonstrated by Fig. 3b. This picture is observed in low-temperature ceramics.[28–31] The complicated dependence of the relative electron-heat-capacity jump, shown in Fig. 3b, is determined by the competition between the behavior of the difference C_S-C_N shown in Fig. 3a as a function of N_c, on the one hand, and the quantity C_N which increases as N_0 increases. Just as for single-band superconductors, in our case the ratio $(C_S-C_N)/C_N > 1.43$ is governed to a considerable degree by the smallness of C_N in the region in question compared with the case of fast metals (or by the faster increase of C_S-C_N than that of C_N as N_0 increases).

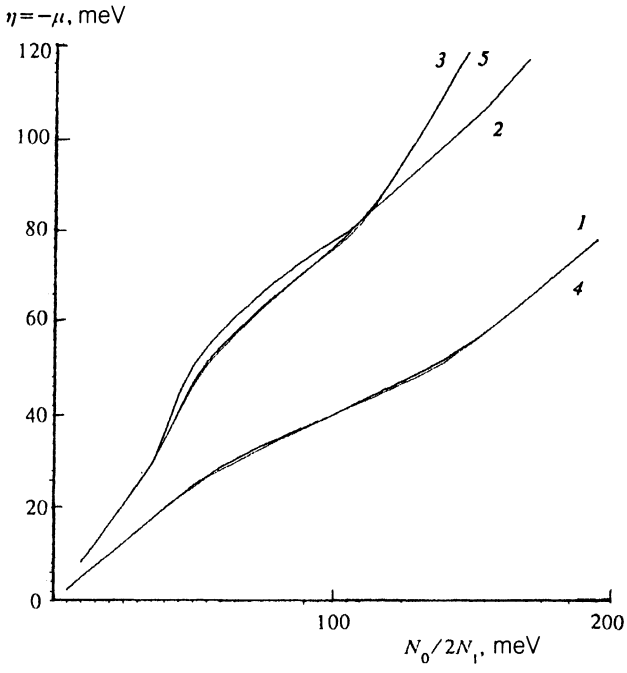

FIG. 4. Dependence of the chemical potential ($\eta=-\mu$) on the carrier density $N_0/2N_1$. The numbering of the plots corresponds to the same N_0/N_1 as in Fig. 1.

We have considered in the present study quasi-two-dimensional systems with a simple dispersion law (21). This approach is dictated, in particular, by the lower dimensionality of a number of high-temperature ceramics. Since, however, the electron-state densities $N_n(\varepsilon)$, $n=1, 2$ have no singularities for the dispersion law (21), we obtain the very same equations also for a three-dimensional system. Only the values of N_n will differ. Just as in the case of single-band semiconductors,[23] in our case the ratio $C_S-C_N/C_N > 1.43$ is governed to a considerable degree by the small C_N in the considered range of N_0 compared with the case of ordinary metals (or by the faster increase of C_S-C_N with increase of N_0 compared with the increase of C_N.

Note that our investigations were made in the mean-field approximation, and it is in this approximation that the proposed superconductivity theory, with two overlapping energy bands, describes the properties of the system for an arbitrary ratio of T_c to N_0. The mean-field approximation itself, however, may turn out to be insufficient when very low carrier densities are considered. It becomes necessary here to take into account the fluctuations of the order parameters near the superconducting transition temperature. Our numerical calculations were made mainly for values $T_c/\varepsilon_F \sim 10^{-1}$–$10^{-2}$ (cf. the data of Figs. 4 and 1), and in this respect we can be assumed to have a physical picture that is qualitatively close to the real one. To be sure, we are still faced here with the question of the nature of the superconductivity, namely, will it be based on the Cooper-

pair production mechanism or will it be determined by the Bose condensate. Good results in the ground state are obtained in the BCS theory for $\Delta \ll |\mu|$, but a condensate of nonineractiong bosons is produced in the opposite limit. Analysis of the intermediate region at finite temperature is still an unsolved problem, and our results are an interpolation of the BCS mechanism to this intermediate region. The nature of superconductivity in systems with low carrier density has been the subject of many studies (see, e.g., Refs. 23 and 32–35).

6. CONCLUSION

We have developed a superconductivity theory for a system with two overlapping energy bands on the Fermi surface. This theory is valid in the weak-field approximation for any carrier density, including a low one ($\mu \sim T_c$).

The main results are the following.

1. We have introduced a system Hamiltonian (1) which can account for superconducting pairing of electrons both within each band and from different bands. A system of self-consistent equations was derived for the order parameter Δ_{nm} (14) and for the chemical potential μ (18).

2. We have used a sub-band representation, in which the basic equations at temperatures close to critical can be expressed as the set (32)–(35) for the four-band model. This set can be used to consider both the phonon and non-phonon superconductivity mechanisms and can be used to describe superconductivity in a system with low carrier density ($\mu \sim T_c$). The low carrier density notwithstanding, this system can lead to rather high T_c in view of the inclusion of more interband interactions than in Ref. 1, which are connected with formation of superconducting pairs of electrons from different bands.

3. Our model offers more possibilities of describing various two-band systems, since a major role is played in the theory by the ratio N_2/N_1 of state densities of electrons from different bands, as well as by interaction constants λ_{nm} ($n, m = 1$–4). The foregoing is in fact clearly demonstrated in Figs. 1 and 3a which show respectively the dependences of the critical temperature T_c and of the electronic heat capacity $(C_S - C_N)_{T=T_c}$ on the carrier density for a nonphonon superconductivity mechanism and strong (curves *4–5*) hybridization.

4. The plot of the chemical potential of a superconductor with low carrier density versus temperature has at the point $T = T_c$ a sharp kink that becomes less peaked and vanishes when the carrier density is increased. It vanishes at $\mu \approx 2$ meV in the BCS model[23] and at $\mu \approx 8$ meV in the two-band case (Fig. 2). Overlap of the energy band produces thus favorable conditions for revealing anomalies in the $\mu(T)$ dependence and hence for elucidating the superconductivity mechanisms.

5. Analytic expressions were obtained for the absolute $(C_S - C_N)$ (44) and relative $(C_S - C_N)/C_N$ (47) jumps of the electron heat capacity at $T = T_c$. The behavior of $(C_S - C_N)$ as a function of the carrier density N_0 does not, generally speaking, duplicate the behavior of $T_c(N_0)$ (see Figs. 1 and 3a) and is determined by the parameters of the theory. Situations are possible in which T_c and $(C_S - C_N)_{T=T_c}$ have maxima at one and the same density N_0 (e.g., curves *3–5*). The character of the dependence of the ratio $(C_S - C_N)/C_N$ at the point $T = T_c$ on N_0 is also determined by the parameters of the theory and depend substantially on the carrier density. This quantity can be either large or small: $(C_S - C_N)/C_N \gtrless 1.43$.

6. At large carrier densities ($\mu \gg T_c$) we have Δ_{12}, $\Delta_{21} \ll \Delta_{11}$, Δ_{22}, so that simpler equations for T_c, Δ_{nm}, $(C_S - C_N)_{T=T_c}$ and $(C_S - C_N)/C_N$ can be obtained by putting $\Delta_{12} = \Delta_{21} = 0$ in (35), (14), (44), and (47). The ensuing results agree with the corresponding equations for phonon[14] and non-phonon[1,18] superconductivity mechanisms.

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