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Self-consistent description of metal-insulator phase transition in the two-band model

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A two-band model is proposed for a metal-insulator transition with lattice distortion, with account taken of the intraband and interband Coulomb interaction, as well as of the anisotropy of the Fermi surface. The phase diagram of the system as a function of the degree of band occupation is constructed by solving the system of self-consistency equations for the chemical potential and for the gap. It is shown that two dielectric phases exist, and one or the other is stable, depending on the band occupation. The results are compared with experiments on oxides and sulfides of transition metals.

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1. INTRODUCTION

It is known[1,2] that a narrow-band metal whose electron spectrum satisfies the condition

$$\varepsilon_1(\mathbf{k})-\mu=-\varepsilon_1(\mathbf{k}+\mathbf{Q})+\mu \tag{1}$$

where the wave vector $2\mathbf{Q}$ coincides with the reciprocal-lattice vector, is unstable to doubling of the period of the cell and goes over into the insulator state. At the same time, the band structure of narrow-band transition-metal compounds is characterized by the presence of several bands that intersect in the vicinity of the Fermi level. Therefore more general is a two-band model, in which band 1 satisfies condition (1) while band 2 does not satisfy it. Such a model was proposed in Ref. 3, and it was shown that allowance for the second band greatly broadens the class of possible solutions of the self-consistency equation for the order parameter $\Delta=g(\mathbf{Q})\langle b_{\mathbf{Q}}+b^{+}_{-\mathbf{Q}}\rangle/\sqrt{N}$, where b_q is the annihilation operator of a phonon with wave vector $\mathbf{q}$, and $g(\mathbf{q})$ is the electron-phonon interaction constant. In particular, several nontrivial solutions appear, thus indicating the presence of metastable states.

In Ref. 3, however, no account was taken of the Coulomb interaction. More accurately, account was taken of only that part of this interaction which leads to a renormalization of the interaction constants. In the two-band case there appears also a coupling between the bands on account of the self-consistent occupation numbers, and this changes the self-consistency equation. In addition, it was assumed in Ref. 3, in the course of the solution of the system of self-consistency equations for the chemical potential μ and for the gap Δ, that μ depends little on the temperature T, and $\mu(T=0)$ was substituted in the equation for Δ.

The aim of the present paper is a fully self-consistent description of the metal–insulator transition (MIT) in the two-band model, with account taken of the Coulomb interaction. In addition, we consider the influence of the anisotropy of the Fermi surface, of the pressure, of doping, and of the magnetic field on the MIT.

2. HAMILTONIAN AND GREEN'S FUNCTIONS

We consider a system of electrons and phonons described by a Hamiltonian

$$\mathcal{H}=\mathcal{H}_{el}+\mathcal{H}_{ph}+\mathcal{H}_{el-ph}, \tag{2}$$

where

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$$\mathcal{H}_{el}=\mathcal{H}_0+\mathcal{H}_1,$$

$$\mathcal{H}_0=\sum_{\mathbf{f}\lambda\sigma}(\varepsilon_\lambda-\mu)n_{\mathbf{f}\lambda}{}^{\sigma}+\sum_{\mathbf{fh}\lambda\sigma}b_\lambda(\mathbf{h})\overset{+}{a}_{\mathbf{f}\lambda\sigma}a_{\mathbf{f+h},\lambda\sigma},\quad n_{\mathbf{f}\lambda}{}^{\sigma}=\overset{+}{a}_{\mathbf{f}\lambda\sigma}a_{\mathbf{f}\lambda\sigma},$$

$$\mathcal{H}_1=\frac{1}{2}\sum_{\mathbf{f}\lambda\sigma}\Big\{Un_{\mathbf{f}\lambda}{}^{\sigma}n_{\mathbf{f}\lambda}^{-\sigma}+\sum_{\substack{\lambda'\sigma'\\(\lambda'\neq\lambda)}}(Vn_{\mathbf{f}\lambda}{}^{\sigma}n_{\mathbf{f}\lambda'}^{\sigma'}-J\overset{+}{a}_{\mathbf{f}\lambda\sigma}a_{\mathbf{f}\lambda\sigma'}\overset{+}{a}_{\mathbf{f}\lambda'\sigma'}a_{\mathbf{f}\lambda'\sigma})\Big\}$$

$$+\frac{1}{2}\sum_{\substack{\mathbf{fh}\lambda\lambda'\\ \sigma\sigma'}}K_{\lambda\lambda'}(\mathbf{h})n_{\mathbf{f}\lambda}{}^{\sigma}n_{\mathbf{f+h},\lambda'}^{\sigma'},$$

$$\mathcal{H}_{ph}=\sum_{\mathbf{q}}\omega_{\mathbf{q}}b_{\mathbf{q}}{}^{+}b_{\mathbf{q}},$$

$$\mathcal{H}_{el-ph}=\frac{1}{\sqrt{N}}\sum_{\mathbf{kq}\lambda\sigma}g_\lambda(\mathbf{q})(b_{\mathbf{q}}+b_{-\mathbf{q}}{}^{+})\overset{+}{a}_{\mathbf{k}\lambda\sigma}a_{\mathbf{k-q},\lambda\sigma}.$$

Here $a^+_{\mathbf{f}\lambda\sigma}$ is the operator for the creation of an electron in a state described by a Wanier function localized on a site **f** of the lattice in the band $\lambda=1,2$ with spin projection σ; ε_λ are atom-like energy levels, which smear out, as a result of electron hopping with a hopping integral $b_\lambda(\mathbf{h})$ between the nearest neighbors, into narrow tight-binding bands

$$\varepsilon_\lambda(\mathbf{k})=\varepsilon_\lambda+b_\lambda(\mathbf{k}),\quad b_\lambda(\mathbf{k})=\sum_{\mathbf{h}}b_\lambda(\mathbf{h})\exp(i\mathbf{kh}).\tag{3}$$

The $\mathcal{H}_0$ describes two independent bands, and $\mathcal{H}_1$ describes the Coulomb interaction. In view of the tight binding of the electrons we retain in $\mathcal{H}_1$ only the intraatomic and interatomic (with z nearest neighbors) terms. U and V are the matrix elements of the intraatomic Coulomb interaction on one orbital and on different orbitals, and J are the matrix elements of the exchange interaction. $K_{\lambda\lambda'}(\mathbf{h})$ is the matrix element of the interatomic Coulomb interaction.

In the insulator phase, the Bose condensation of the phonons with the wave vector **Q** reduces the electron-phonon interaction to an external field acting on the electrons,[1,2] and we therefore add to $\mathcal{H}_0$

$$\mathcal{H}_\Delta=\sum_{\mathbf{f}\lambda\sigma}\Delta_\lambda\exp(-i\mathbf{Qf})n_{\mathbf{f}\lambda}{}^{\sigma}.$$

The term $\mathcal{H}_\Delta$ singles out the sublattices A and B:

$$\exp(-i\mathbf{Qf})=\begin{cases}+1, & \mathbf{f}=\alpha\in A\\ -1, & \mathbf{f}=\beta\in B\end{cases}.$$

To find the spectrum of the excitations and of the occupation numbers, we introduce two-dimensional anticommutator Green's functions

$$\langle\langle a_{\mathbf{f}\lambda\sigma}(t)|\overset{+}{a}_{\mathbf{f}'\lambda'\sigma'}(0)\rangle\rangle=-i\theta(t)\langle[a_{\mathbf{f}\lambda\sigma}(t)\overset{+}{a}_{\mathbf{f}'\lambda'\sigma'}(0)]_+\rangle,\tag{4}$$

where the angle brackets denote the thermodynamic mean value. For the Fourier transforms of the Green's functions (4) (the vector **k** is defined in half of the initial Brillouin zone)

$$G_{AA}^{(\lambda)}(\mathbf{k},E)=\sum_{\alpha-\alpha'}\exp[-i\mathbf{k}(\alpha-\alpha')]\langle\langle a_{\alpha\lambda\sigma}|\overset{+}{a}_{\alpha'\lambda\sigma}\rangle\rangle_E,$$

$$G_{BA}^{(\lambda)}(\mathbf{k},E)=\sum_{\beta-\alpha'}\exp[-i\mathbf{k}(\beta-\alpha')]\langle\langle a_{\beta\lambda\sigma}|\overset{+}{a}_{\alpha'\lambda\sigma}\rangle\rangle_E$$

we obtain in the mean-field approximation by the standard method

$$G_{AA}^{(1)}=\frac{E-\varepsilon_1{}^B+\Delta+\mu}{D(\mathbf{k},E)},\quad G_{BB}^{(1)}=\frac{E-\varepsilon_1{}^A-\Delta+\mu}{D(\mathbf{k},E)}$$

$$G_{AB}^{(1)}=G_{BA}^{(1)}=\frac{b_1(\mathbf{k})}{D(\mathbf{k},E)},\tag{5}$$

$$D(\mathbf{k},E)=[E-E_1{}^{+}(\mathbf{k})][E-E_1{}^{-}(\mathbf{k})],\quad E_1{}^{\pm}(\mathbf{k})={}^1/{}_2(\varepsilon_1{}^A+\varepsilon_1{}^B)\pm\nu(\mathbf{k})-\mu,$$
$$\nu^2(\mathbf{k})=b_1{}^2(\mathbf{k})+\tilde{\Delta}^2,\quad \tilde{\Delta}=\Delta+{}^1/{}_2(\varepsilon_1{}^A-\varepsilon_1{}^B).$$

Here

$$\varepsilon_1^{A,B}=\varepsilon_1+{}^1/{}_2Un_1^{A,B}+(V-J/2)n_2^{A,B}+z_1K(n_1^{B,A}+n_2^{B,A}),$$
$$n_\lambda{}^{f}=2\langle n_{f\lambda}{}^{\sigma}\rangle.\tag{6}$$

The Green's function (5) and the spectrum of the band 1 differ from the corresponding expressions of Ref. 3 by the substituting $\varepsilon_1^{A,B}\to\varepsilon_1$, and agree with them at $U=V=J=K=0$.

So far we have made no assumptions concerning the symmetry of the lattice and of the hopping integrals $b_\lambda(\mathbf{h})$, other than the condition (1). This condition can be satisfied in the one-dimensional case only in high-symmetry three-dimensional lattices of the primitive cubic and bcc type. We consider the three dimensional case, and if the symmetry of the integrals $b_\lambda(\mathbf{h})$ coincides with the symmetry of the lattice for both bands, then band 2 should also be described in the decreased Brillouin zone, and its spectrum and Green's functions are obtained from (5) by simply replacing the band indices. More interesting from the point of view of the applicability of the model, however, is the anisotropic case, when the hops in band 1 are along one direction (the z axis), and in band 2 perpendicular in this direction. This anisotropy is connected with the anistropic character of the wave functions of the d electrons. The sublattices A and B are then separated along the z axis, and the hopping across this axis have an intra-sublattice character. Therefore $\Delta_2=0$ and

$$G_{AA,BB}^{(2)}=[E-E_2^{A,B}(\mathbf{k})]^{-1},\quad G_{AB}^{(2)}=G_{BA}^{(2)}=0,$$
$$E_2^{A,B}(\mathbf{k})=\varepsilon_2^{A,B}+b_2(\mathbf{k})-\mu.\tag{7}$$

The expression for $\varepsilon_2^{A,B}$ is obtained from (6) by the band index interchange $1\rightleftharpoons2$.

As shown in Refs. 1 and 2, allowance for deviation of the spectrum in band 1 from the condition (1), for example as a result of hops between the nearest neighbors, leads to anisotropy of the Fermi surface. We shall assume that the spectrum in band 1 is [in place of (3)]

$$\varepsilon_1(\mathbf{k})=\varepsilon_1+b_1(\mathbf{k})-\delta\varepsilon_1(\mathbf{k}).$$

In addition, we wish to consider the influence of a magnetic field on the MIT. To this end it is necessary to take into account the splitting of all the bands in spin. Therefore the spectrum of the electron in the insulator phase is given not by (5) and (7), but by

$$E_1{}^{\pm}(\mathbf{k},\sigma)={}^1/{}_2(\varepsilon_1{}^A+\varepsilon_1{}^B)\pm\nu(\mathbf{k})-\delta\varepsilon_1(\mathbf{k})-\eta(\sigma)\mu_B^{(1)}H-\mu,$$
$$E_2^{A,B}(\mathbf{k},\sigma)=\varepsilon_2^{A,B}+b_2(\mathbf{k})-\eta(\sigma)\mu_B^{(2)}H-\mu,\tag{8}$$
$$\eta(\sigma)=\begin{cases}+1, & \sigma=\uparrow,\\ -1, & \sigma=\downarrow,\end{cases}$$

where $\mu_B^{(\lambda)}$ is the Bohr magneton for the electron in band λ with mass m_λ.

3. SELF-CONSISTENCY EQUATIONS

From the Green's functions (5) and (7) we obtain the occupation numbers:

$$n_1^{A,B}=\frac{1}{N}\sum_{\mathbf{k}\sigma}[f(E_1^+(\mathbf{k},\sigma))+f(E_1^-(\mathbf{k},\sigma))]$$

$$\pm\frac{1}{N}\sum_{\mathbf{k}\sigma}\frac{\tilde\Delta}{\nu(\mathbf{k})}[f(E_1^+(\mathbf{k},\sigma))-f(E_1^-(\mathbf{k},\sigma))],$$

$$n_2^{A,B}=\frac{2}{N}\sum_{\mathbf{k}\sigma}f(E_2^{A,B}(\mathbf{k},\sigma)),\qquad f(E)=(e^{E/T}+1)^{-1}. \tag{9}$$

The self-consistency equation for the chemical potential is of the form

$$\rho=\frac{1}{N}\sum_{\mathbf{k}\sigma}[f(E_1^+(\mathbf{k},\sigma))+f(E_1^-(\mathbf{k},\sigma))+f(E_2^A(\mathbf{k},\sigma))+f(E_2^B(\mathbf{k},\sigma))], \tag{10}$$

where ρ is the number of electrons per cation.

The self-consistency equation for the gap Δ is obtained by the same method as in Refs. 2 and 3, but because of the renormalization of the gap it turns out to be more complicated and we present therefore a new derivation. Averaging the Heisenberg equation of motion

$$i\frac{\partial}{\partial t}b_{\mathrm{Q}}(t)=\omega_{\mathrm{Q}}b_{\mathrm{Q}}+\frac{g_1(\mathrm{Q})}{N^{1/2}}\sum_{\mathbf{k}\sigma}a_{\mathbf{k}1\sigma}^+a_{\mathbf{k}-\mathrm{Q},1\sigma}$$

and taking the Fourier transform with respect to time, we obtain

$$\langle b_{\mathrm{Q}}\rangle_\omega=\frac{\delta(\omega)}{\omega-\omega_{\mathrm{Q}}}\frac{g_1(\mathrm{Q})N^{1/2}}{2}(n_1^A-n_1^B).$$

After taking the inverse Fourier transform and using Eqs. (9) we have

$$\frac{\langle b_{\mathrm{Q}}\rangle}{N^{1/2}}=-\frac{2g_1(\mathrm{Q})}{\omega_{\mathrm{Q}}}\tilde\Delta\Pi_1,\qquad \Pi_1=\frac{1}{N}\sum_{\mathbf{k}\sigma}\frac{f(E_1^+(\mathbf{k},\sigma))-f(E_1^-(\mathbf{k},\sigma))}{2\nu(\mathbf{k})}.$$

On the other hand, in accord with the definitions of Δ and $\tilde\Delta$,

$$\frac{\langle b_{\mathrm{Q}}\rangle}{N^{1/2}}=\frac{1}{2g_1(\mathrm{Q})}\left[\tilde\Delta-\frac{1}{2}(\varepsilon_1^A-\varepsilon_1^B)\right].$$

It follows from (6) that

$$\varepsilon_1^A-\varepsilon_1^B={}^1/_2\tilde U(n_1^A-n_1^B)+{}^1/_2\tilde V(n_2^A-n_2^B),$$

$$\tilde U=U-2z_1K,\quad \tilde V=V-{}^1/_2J-2z_1K.$$

Therefore, using (9) once more, we obtain the self-consistency equations

$$\tilde\Delta[1+(4g_1^2(\mathrm{Q})/\omega_{\mathrm{Q}}-\tilde U)\Pi_1]=\tilde V\Pi_2, \tag{11}$$

where

$$\Pi_2=\frac{1}{2N}\sum_{\mathbf{k}\sigma}[f(E_2^A(\mathbf{k},\sigma))-f(E_2^B(\mathbf{k},\sigma))].$$

Equation (11) contains two effective Coulomb parameters: intraband $\tilde U$, and interband $\tilde V$. The intraband interaction actually only renormalizes the effective coupling constant[1)]

$$g=4g_1^2(\mathrm{Q})/\omega_{\mathrm{Q}}-U+2z_1K,$$

while the interband interaction changes the structure of the equation. We note also that the interaction between the atoms facilitates greatly the condition for the existence of nontrivial solutions of (11) $g>0$, since $\tilde U<U$. In the absence of interband terms we have the usual equation $1+g\Pi_1=0$, which has been considered previously[2,3] and describes MIT of the second kind at $\delta\varepsilon_1=H=0$ at the point $T=T_c$. If the right-hand side of (11) were a constant quantity, then it would play the role of the external field that induces nonzero values of $\tilde\Delta$ in the entire temperature interval, or that lead to a jump of $\tilde\Delta$ at $T\leq T_c$, depending on the sign of $\tilde V$ (a similar equation was investigated in Ref. 5). In our case, the nonzero value of Π_2 is due to the difference between the occupation numbers n_2^A and n_2^B. It is natural to assume that this difference is proportional to the splitting of the level ε_2, and then

$$\Pi_2={}^1/_4(n_2^A-n_2^B)={}^1/_4\alpha(\varepsilon_2^A-\varepsilon_2^B).$$

This is in fact a power-series expansion, since the zeroth term of the series is equal to zero at $\varepsilon_2^A=\varepsilon_2^B$. On the other hand, from Eqs. (6) we have for band 2

$$\varepsilon_2^A-\varepsilon_2^B={}^1/_2\tilde U(n_2^A-n_2^B)+{}^1/_2\tilde V(n_1^A-n_1^B)=2\tilde U\Pi_2+2\tilde V\tilde\Delta\Pi_1,$$

Therefore

$$\Pi_2=\frac{\alpha\tilde V\tilde\Delta}{2-\alpha\tilde U\Pi_1}\Pi_1$$

and the self-consistency equation is written in the form

$$1+\tilde g\Pi_1=0,\quad \tilde g=g+\frac{\alpha\tilde V^2}{2-\alpha\tilde U\Pi_1}, \tag{12}$$

which shows that the interband Coulomb interaction has been reduced to a renormalization of the coupling constant, and that this renormalization does not depend on the sign of $\tilde V$. We present below results of a numerical solution of Eq. (11), which shows that actually the role of the interband term consists in an inessential shift of the transitions temperatures; the phase diagram remains qualitatively unchanged.

We change from summation over the quasimomentum in Eqs. (10) and (11) to integration with respect to energy:

$$\frac{2}{N}\sum_{\mathbf{k}}f_{\lambda=1}(k)=\int_{-W_1}^{W_1}N_1(\varepsilon)d\varepsilon f(\varepsilon),\qquad \frac{1}{N}\sum_{\mathbf{k}}f_{\lambda=2}(k)=\int_{-W_2}^{W_2}N_2(\varepsilon)d\varepsilon f(\varepsilon).$$

The function $\delta\varepsilon_1(k)$ on the Fermi surface is replaced, just as in Ref. 2, by the step function $+u$ in one half of the solid angle of each octant of the Fermi surface and $-u$ in the other. As a result, the system of self-consistency equations takes the form

$$\rho=\sum_\sigma\left\{\frac{1}{2}\int_0^{W_1}N_1(\varepsilon)d\varepsilon[f(E_1^+(u,\sigma))+f(E_1^+(-u,\sigma))\right.$$

$$\left.+f(E_1^-(u,\sigma))+f(E_1^-(-u,\sigma))]+\int_{-W_2}^{W_2}N_2(\varepsilon)d\varepsilon[f(E_2^A(\sigma))+f(E_2^B(\sigma))]\right\}, \tag{13}$$

$$\frac{1}{g}=\sum_\sigma\left\{\frac{1}{4}\int_0^{W_1}N_1(\varepsilon)d\varepsilon\nu^{-1}[f(E_1^-(u,\sigma))+f(E_1^-(-u,\sigma))\right.$$

$$\left.-f(E_1^+(u,\sigma))-f(E_1^+(-u,\sigma))]+\frac{\tilde V}{2g\tilde\Delta}\int_{-W_2}^{W_2}N_2(\varepsilon)d\varepsilon[f(E_2^A(\sigma))-f(E_2^B(\sigma))]\right\}. \tag{14}$$

We shall use two expressions for the state density: the model of a rectangular band for analytic calculations at $T=0$:

$$N_\lambda(\varepsilon)=\begin{cases}N_\lambda(0)=1/2W_\lambda, & |\varepsilon|<W_\lambda\\ 0, & |\varepsilon|>W_\lambda\end{cases}$$

and the model of elliptic bands for the numerical calculations:

$$N_\lambda(\varepsilon)=N_\lambda(0)[1-(\varepsilon/W_\lambda)^2]^{1/2},\quad N_\lambda(0)=2/\pi W_\lambda,$$

at $|\varepsilon|<W_\lambda$ and

$$N_\lambda(\varepsilon)=0 \text{ at } |\varepsilon|>W_\lambda.$$

We note that band 1 is not one-dimensional, and therefore the state density vanishes on the edges of the band. Thus, for example, in the rutile lattice condition (1) is satisfied for $\mathbf{Q}=\pi[a^{-1},0,c^{-1}]$.[6]

4. SOLUTION OF THE SELF-CONSISTENCY EQUATIONS IN LIMITING CASES

In view of the large number of the parameters of the theory, the construction of the complete phase diagram in the parameter space is difficult. In this section we consider some limiting cases in the absence of interband Coulomb interaction, $\tilde{V}=0$.

a) $u=0, H=0$. In this case we obtain the equations of the two-band model, the solutions of which are given in Ref. 3 for $\rho=1$ and in Ref. 7 for $\rho=2$, 3, 4, and 5. An important difference from the single-band model[1,2] is the onset of metastable semimetallic states, at which the Fermi level passes near the top of the band E_1^- and near the bottom of the band E_2.

b) $H=0, W_2<d=\varepsilon_2-\varepsilon_1$. The quantity d is the splitting of the d-level by the crystal field. In this case the bottom of the second band lies above the center of the first, and at $\rho=1$ we have $\mu=\varepsilon_1$ and the model becomes single-band. Equation (14) is then reduced to the corresponding equation of Ref. 2 [here $\lambda=gN_1(0)$]:

$$\frac{1}{\lambda}=\int_0^{W_1}\frac{d\varepsilon}{(\varepsilon^2+\Delta^2)^{1/2}}\frac{1}{2}\left\{\operatorname{th}\frac{(\varepsilon^2+\Delta^2)^{1/2}+u}{2T}+\operatorname{th}\frac{(\varepsilon^2+\Delta^2)^{1/2}-u}{2T}\right\} \tag{15}$$

and as at $T=0$ and $u=0$ the solution

$$\Delta=\Delta_0=2W_1e^{-1/\lambda},\quad \lambda\ll 1.$$

At $\Delta_0/2<u<\Delta_0$ there exists another nontrivial solution of Eq. (15):

$$\Delta=\Delta_1=(\Delta_0(2u-\Delta_0))^{1/2}<\Delta_0;$$

there are no nontrivial solutions at $u>\Delta_0$.[1]

A state is realized with the largest gain in the thermodynamic potential compared with the metallic phase. This gain is[8]

$$\delta\Omega(\Delta,\mu,T)=\Omega_D(\Delta,\mu,T)-\Omega_M(0,\mu,T)=\int_0^\Delta \Delta^2\frac{\partial(1/g)}{\partial\Delta}d\Delta.$$

For the phases Δ_0 and Δ_1 we obtain respectively at $T=0$

$$\delta\Omega(\Delta_0)=-{}^1/_2N_1(0)\Delta_0^2<0,$$

$$\delta\Omega(\Delta_1)=N_1(0)\int_0^{\Delta_1}\frac{\Delta^3d\Delta}{(u^2-\Delta^2)^{1/2}}\frac{1}{u+(u^2-\Delta^2)^{1/2}}>0. \tag{16}$$

Thus, the phase Δ_0 forms the ground state, and Δ_1 is unstable. The same results were obtained in similar problems concerning the antiferromagnetism of chromium[9] and charge density waves in one-dimensional systems.[10] It was also shown in Ref. 9 that at $T=0$ the transition relative to the parameter u can be of either first or second order.

Figure 1 shows the temperature dependence of $\Delta(T)$ obtained by us from (15). A new result compared with $T=0$ is the division of the region $\Delta_2/2<u<\Delta_0$ into two: $\Delta_0/2<u<u_0$ and $u_0<u<\Delta_0$. In the first of them the phase Δ_1 has its own transition temperature $T_1<T_0$, where T_0 is the transition temperature of the phase Δ_0, with a second-order transition at the point T_0. In the second region $T_1=T_0$ and the transition is jumplike, of first order. A critical point exists at $u=u_0$.

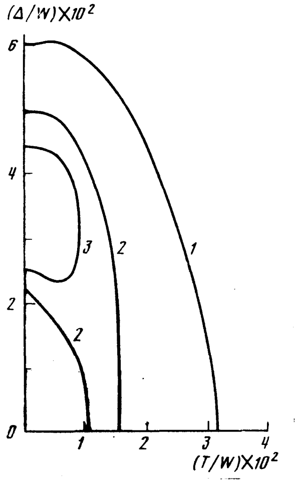

FIG. 1. Temperature dependence of the gap at $d>W_2$ for different values of the interaction constant λ. Here $u=0.03$; curves 1, 2, and 3 correspond to $\lambda^{-1}=3.50$, 3.70, and 3.80. At $\lambda^{-1}>4.11$ there are no nonzero solutions.

5. SOLUTION OF THE SELF-CONSISTENCY EQUATIONS IN THE GENERAL CASE

In this section we are interested in the case $W_2>d$, when the model is essentially two-band. The problem of finding the chemical potential from (13) now becomes complicated, since it is necessary to solve (13) and (14) simultaneoulsy. These equations were solved numerically in the following manner: from each equation we obtained the explicit dependence of $\mu(\Delta)$ at a given value of T and ρ, and then sought the intersection of the two plots $\mu_1(\Delta)$ and $\mu_2(\Delta)$, see Fig. 2. The chemical potential was reckoned from the level ε_1, i.e., $\varepsilon_1=0$. The $\mu_1(\Delta)$ plot obtained from (13) depends little on the temperature, and therefore Fig. 2 shows only one such line. It is seen from Fig. 2 that there exist two solutions for Δ at low temperatures and no solution at all at $T>T_c$. A first-order phase transition connected with the discontinuity of Δ takes place at the point T_c. In

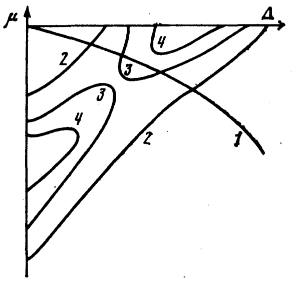

FIG. 2. Scheme for the solution of the system of self-consistency equations for the chemical potential and the gap at $W_2>d$. Curve 1 shows the explicit dependence of $\mu(\Delta)$ for Eq. (13) at $\rho=1$, curves 2, 3, 4 show the same for Eq. (14) at different values of the temperature: $T_2<T_3<T_4$.

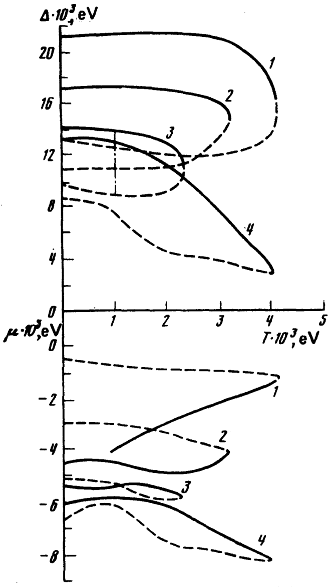

FIG. 3. Temperature dependence of the gap and of the chemical potential at $\lambda^{-1}=3.50$, $W_1=0.5$ eV, $W_2=0.7$ eV, $d=0.69$ eV, $u=0.015$ eV, $V=0$, and $H=0$. Curves 1, 2, 3, and 4 correspond to $\rho=1$, 0.990, 0.982, and 0.980. The solid and dashed lines correspond to the phases Δ_1 and Δ_2, respectively.

addition, with the aid of Fig. 2 it is possible to compare directly the chemical potentials of two phases corresponding to different Δ. At the first-order transition point $\mu(\Delta_1, T_c)=\mu(\Delta_2, T_c)=\mu(0, T_c)$.

Figure 3 shows the temperature dependence of $\Delta(T)$ and $\mu(T)$ obtained in this manner for different values of ρ with the remaining parameters fixed, in the absence of a magnetic field and of interband Coulomb interaction. In the elliptic state density model Δ_0 is of the form

$$\Delta_0=\frac{4}{e}W_1e^{-1/\lambda}.$$

At $\lambda^{-1}=3.50$ and $W_1=0.5$ eV we have $\Delta_0=0.0222$ eV. We note that for all ρ the MIT is of first-order. This is due to the large value of $u, u/\Delta_0 \lesssim 1$. In fact, at $u=0$ a similar soultion of Eqs. (13) and (14) yields an MIT of second order and absence of metastable states in the indicated range of parameters.

At $T=0$ the plane (Δ, μ) breaks up into a number of regions in accordance with the different variants of the location of the Fermi level relative to the four bands $E_\pm(u)$ and $E_\pm(-u)$. A true insulator state, when the E_- bands are filled, and the E_+ bands are empty, and the chemical potential lies in the gap is possible at $\Delta > u-\mu$ ($\mu<0$, see Fig. 3). If $\Delta < u+|\mu|$ (region 1), then the Fermi level crosses the $E_-(u)$ bands, at $\Delta < u-|\mu|$, $u>|\mu|$ (region 2) it does not cross the bands $E_-(u)$, $E_-(-u)$ and $E_+(-u)$, and finally at $u<|\mu|$ and $\Delta<|\mu|-u$ (region 3) it crosses the bands $E_-(u)$ and $E_-(-u)$. Calculation of the thermodynamic potentials shows that the conditions for the stability of the obtained two phases Δ_1 and Δ_2 are determined by the region in which the point (Δ_i, u_i) lands. The phase $\Delta_1=\Delta_0$ is insulating at $\rho=1$ and the energy gain is determined by Eq. (16). The phase Δ_2 lands in this case in region 2 (to compensate for the holes in the E_- bands it is necessary at $\rho=1$ to fill in part the E_+ bands); it is easy to show that for region 2 we have

$$\frac{1}{\lambda}=-\ln\frac{[(u+\mu)^2-\Delta^2]^{1/2}+u+\mu}{2W_1}-\frac{1}{2}\ln\frac{[(u-\mu)^2-\Delta^2]^{1/2}+u-\mu}{\Delta},$$

from which it follows that $\delta\Omega(\Delta_2, \mu_2, 0)>0$, i.e., the Δ_2 phase is unstable.

With decreasing ρ, when holes in the bands E_-, the points (Δ, μ) can land in regions 1 and 3. Thus, for region 1

$$\frac{1}{\lambda}=\ln\frac{2W_1}{\Delta}-\frac{1}{2}\ln\frac{[(u-\mu)^2-\Delta^2]^{1/2}+u-\mu}{\Delta}, \tag{17}$$

$$\delta\Omega(\Delta, \mu, 0)=-{}^1/_2N_1(0)[\Delta^2+(u-\mu)[(u-\mu)^2-\Delta^2]^{1/2}-(u-\mu)^2]<0,$$

i.e., the state of the degenerate p-type semiconductor is more favored in this region than that of the initial metallic state. At the same time, solutions of the metallic type are possible also at $\rho<1$ (region 2), but they are unstable, just as for $\rho=1$, with $\delta\Omega>0$.

Curve 2 on Fig. 3 corresponds to the case when the point (Δ_1, μ_1) lands in region 1 and is stable, while (Δ_2, μ_2) lands in region 2 and is unstable. It is possible however, that the solution (Δ_2, μ_2) lands in the region 1. In fact, it follows from (17) that Δ is obtained in this region as the solution of the equation

$$\Delta^4-2(u-\mu)\Delta_0^2\Delta+\Delta_0^4=0. \tag{18}$$

Equation (18) can have several real solutions, each of which is more favored than the metallic phase. Thus, the condition for the stabilization of the phase Δ_2 is

$$u+\mu=\Delta_2. \tag{19}$$

Physically this condition means that the semimetallic phase Δ_2 is unstable, while the semiconductor phase is stable. Curves 3 of Fig. 3 correspond to this case.

A comparison of the energies of the two semiconductor phases in region 1 can be easily made by using (17). If the chemical potentials of the two phases are the same, $\mu(\Delta_1)=\mu(\Delta_2)$, then

$$\mu(\Delta_1)=\mu(\Delta_2),\text{ то}$$

$$\Omega(\Delta_2, \mu, 0)-\Omega(\Delta_1, \mu, 0)<0$$

at $\Delta_1>\Delta_2$ and

$$\Delta_2^2<[(u-\mu)^2-\Delta_1^2]^{1/2}\times[2(u-\mu)-((u-\mu)^2-\Delta_1^2)^{1/2}], \tag{20}$$

i.e., the phase with the smaller gap is realized. This case corresponds to curve 4 of Fig. 3. Stabilization of the phase Δ_2 means that a triple point exists on the phase diagram of the system in the plane (T, ρ). We note also that allowance for the interband Coulomb interaction with $\tilde{V}=0.05$ eV hardly changes the form of the curves on Fig. 3. The values of ρ corresponding curves 1–4 change only in the fourth decimal place. This agrees with the conclusions of Ref. 2 of a simple and furthermore small renormalization ($\propto\tilde{V}^2$) of the effective coupling constant λ.

The modulation of the Fermi surface, which is responsible for the first-order character of the MIT, leads also to another effect, a possible transition into an incommensurate phase. This question was investigated in detail in a similar model[9] and it was shown that the high-temperature paraphase goes over either directly into a commensurate phase, or else first into an incommensurate phase and then into a commensurate phase, depending on the relation between the parameters u, Δ_2, and W_2/W_1. We shall not pay much attention to this question, however, since later investigations have shown that the fixing of the phase of the displacements in the incommensurate structure upon scattering by impurities and other defects (the pinning effect) makes it unstable compared with the commensurate lattice. Our purpose is to consider the MIT in pure and doped substances such as vanadium oxide, where the incommensurability effects have not been observed; we confine ourselves therefore to transitions of the doubling type.

The phase diagram of the system is shown in Fig. 4. All the lines are first-order transition lines. On the line that separates the normal metallic phase N and the phase Δ_2 the jump of Δ decreases with decreasing ρ, so that one can apparently reach either a second order transition or a first order transition close to second order. This region of ρ, however, was not investigated by us. Figure 4 shows also the phase diagram in a strong magnetic field, from which we see that the lowering the temperature T_0, that corresponds to the triple point proceeds more rapidly than the increase of ρ_0. On the contrary, an increase of W_2 hardly influences T_0, but ρ_0 increases noticeably.

We do not show in Fig. 4 the phase diagrams obtained when varying λ. They are similar in form, and shift to the right at $\lambda^{-1}=3.45$ and to the left at $\lambda^{-1}=3.55$.

Since the theory describes a first-order transition, the critical fluctuations near the transition point do not play any role and the mean-field approximation, in which all the results were obtained, is valid in the entire temperature interval.

6. DISCUSSION OF RESULTS

Our model is applicable to narrow-band substances in which an MIT accompanied by a structural transition with doubling of the period and not accompanied by magnetic transformations is possible. These include both oxides and sulfides of transition metals. All these compounds have uniaxial symmetry, band 1 ensures hopping along the z axis. Therefore the use of the single-band model will lead to an incorrect description of the metallic phase—to anisotropy of the metallic properties. At the same time the conductivity and the paramagnetic susceptibility are in fact almost isotropic.[11] In these substances the MIT is as a rule of first-order, but the two-band model[3], which does not take into account the anisotropy of the Fermi surface due to violation of condition (1), describes an MIT of second order. Only allowance for this anisotropy in the two-band model, i.e., a synthesis of the two models of Ref. 2 and 3, which was carried out in the present paper, has made it possible to describe qualitatively correctly both the properties of the metallic phase and the jump of the gap, and consequently also the conductibility at the transition point.

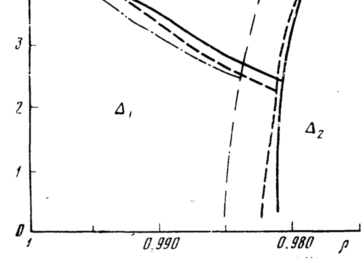

FIG. 4. Phase diagram of the system at the parameter values indicated in Fig. 3, but with $V=0.05$ eV—solid line; the same but in a magnetic field $\mu_B H=0.001$ eV ($H\sim 100$ kOe)—dashed line; $H=0$, $W_2=0.705$ eV, and the remaining values the same—dash-dot line.

Our conclusion that the phase Δ_2 becomes stabilized with decreasing ρ agrees with the experimental data[12-15] on $V_{1-x}Me_x^{3+}O_2$, where Me = Al, Ga, Cr, Fe. In this system there exist two phases with distorted lattice: M_1 and M_2, and the phase diagram has a triple point. Our treatment of these compounds is based on the rigid band model, since the only parameter that is changed by doping is assumed to be the occupation of the band ρ. Since each impurity ion produces a V^{5+} ion for compensation, it follows that $\rho=1-2x$, if the impurity is of the substitutional type. Favoring the applicability of the rigid band model is the result of Ref. 15, according to which the form of the phase diagram is identical when the doping is by either a transition or a nontransition metal, and also of Ref. 16, where the holes produced by the trivalent impurities were compensated by the extra electrons of Mo^{4+}. As a result, ρ increased and in the experiment the phase $M2$ (Δ_2 in our notation), which is stable in the absence of Mo, is replaced upon doping by the phase $M1$ (Δ_1).

Thus, the rigid-band model describes qualitatively correctly the situation in $V_{1-x}Me_xO_2$, but a more correct description of the phase diagram should include, for example, allowance for the scattering of the electrons by a random impurity potential, the changes of the parameters of the band structure by doping, etc. It is therefore meaningless to investigate Eqs. (13) and (14) at large deviations of ρ from unity. In addition, the symmetry of the phases $M1$ and $M2$ is actually more complicated. This is due to the presence of two cations per VO_2 cell. In a simplified model, the phases Δ_1 and Δ_2 have identical symmetry of the displacement of the cations along the z axis, and differ only in the value of the order parameter Δ. For the same reason, the theory does not include an intermediate T phase between $M1$ and $M2$.

The anisotropic character of the band structure of substances of the VO_2 type makes it possible to alter the parameters of one band while changing little the parameters of the other, by applying different uniaxial pressures. Thus, for example, pressure in the plane perpendicular to the c axis should lead primarily to an increase of the width of the second band W_2. Figure 4 shows that with increasing W_2 the triple point shifts to the left, therefore at high pressure it is possible to attain $\rho_0 \geqslant 1$, and as a result the phase $M2$ (Δ_2) which is metastable in VO_2 under normal conditions, becomes stabilized under pressure. This phenomenon is known from experiment.[17]

We have also considered the question of the influence of a strong magnetic field on the MIT. As follows from Fig. 4, at $\rho = 1$ the shift of T_c in a field $H \sim 100$ kOe is practically zero, but the value of T_0 corresponding to the triple point shifts noticably downward. The reason for the difference in the behavior of T_c and T_0 is apparently the following: if the MIT were of second order, then near T_c there would exist a temperature interval in which $\Delta(T) \lesssim \mu_B H$, and it is in this interval where the influence of the field on the MIT manifests itself, as a result of which the shift of T_c in the second-order transition is $\delta T_c \sim \mu_B H$ (see, e.g., Ref. 18). In a first-order transition the jump Δ in the region of the transition is much larger than $\mu_B H$, and therefore there is practically no influence of the field on T_c. At the same time, in the $\Delta_1 \to \Delta_2$ transition the jump of the gap is much smaller (see Fig. 3), and at the triple point it is completely absent. Therefore $\delta T_0 \sim \mu_B H$ appears here for the same reason as for the second-order transition. That the magnetic field has no influence on T_c in V_2O_3 was demonstrated experimentally in Ref. 19, while the displacement of the triple point with changing field, to our knowledge, was not investigated.

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