Metal-dielectric phase transition in matter with localized magnetic moments

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The metal-dielectric transition with spin and charge-density wave formation is considered within the framework of the generalized *s-d* model. A novel mechanism of ordering of the localized spin is described, connected with their exchange magnetization in the inhomogeneous intrinsic field of the band electrons. The amplitude and critical temperature of the spin-density wave are found to be considerably in excess of the parameters of the spin density band wave. Allowance for the spin-phonon interaction leads to coexistence of charge and spin density waves and also to a first-order transition with respect to the temperature.

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1. INTRODUCTION

Usually the metal-dielectric transition (MDT) with doubling of the period and formation of spin density (SDW) and charge density (CDW) waves is considered in a system of band electrons (see, for example, Ref. 1). Such transitions are frequently studied experimentally in the oxides and sulfides of the transition metals, where, along with the band electrons, there are localized electrons which form localized magnetic moments. The theory of a ferromagnetic SDW with account of localized spins has been considered by Vol'kov and Mnatsakanov.[2] The instability of the homogeneous paramagnetic state of a system of localized spins relative to the formation of an antiferromagnetic SDW has been shown previously.[3]

In the present work, we have studied the CDW and the antiferromagnetic SDW and their coexistence in a system with localized magnetic moments. It is shown that the reason for the first-order transition can be not only the corrugation (anisotropy) of the Fermi surface[1,4] for band theories, but also the sufficiently strong spin-phonon interaction, and without account of the latter it is impossible to obtain coexistence of SDW and CDW. Whereas in the band theory, a dielectric state is impossible in the presence of sufficiently strong anisotropy of the Fermi surface, in our theory, a new dielectric phase appears and becomes stable with increase in the anisotropy.

2. SPECTRUM OF QUASIPARTICLES IN AN ANTIFERROMAGNET WITH A DISTORTED LATTICE

We write down the Hamiltonian of the interacting electrons, localized spins, and phonons

$$H=H_0+H_1;$$

$$H_0=H_e^{(0)}+H_S^{(0)}+H_{ph}^{(0)}, \quad H_1=H_{e-e}+H_{e-S}+H_{S-S}+H_{e-ph}+H_{S-ph},$$

$$H_e^{(0)}=\sum_{f\sigma}(\varepsilon-\mu)n_f^\sigma+\sum_{fh\sigma}b(\mathbf{h})a_{f\sigma}^+a_{f+h,\sigma},$$

$$n_f^\sigma=a_{f\sigma}^+a_{f\sigma}, \quad H_S^{(0)}=-H\sum_f S_f^z,$$

$$H_{ph}^{(0)}=\sum_q\omega_q b_q^+b_q, \quad H_{e-e}={}^1/_2U\sum_{f\sigma}n_f^\sigma n_f^{-\sigma},$$

$$H_{e-S}=-J\sum_f S_f\sigma_f, \quad H_{S-S}=-\sum_{fh}I(\mathbf{h})S_fS_{f+h},$$

$$H_{e-ph}=N^{-1/2}\sum_{kq\sigma}g_q(b_q+b_{-q}^+)a_{k\sigma}^+a_{k-q,\sigma},$$

$$H_{S-ph}=N^{-1/2}\sum_{fhq}A_q(\mathbf{h})(b_q+b_{-q}^+)S_fS_{f+h}. \qquad (1)$$

Here $a_{f\sigma}^+$ ($a_{f\sigma}$) are the creation (annihilation) operators of the electron at the lattice point f with spin projection σ, ε is the single-electron energy level in the crystal field; μ is the chemical potential, $b(\mathbf{h})$ is the integral of the jump over the distance $\mathbf{h}=\mathbf{f}'-\mathbf{f}$; S_f and σ_f are the spin operators of the localized and band electrons, respectively, H is the external field in energy units, $b_q^+(b_q)$ are the creation (annihilation) operators of the phonon with wave vector $\mathbf{q}$ and frequency ω_q, $I(\mathbf{h})$ is the effective integral of exchange interaction, the expansion of which in powers of the displacements of the ions leads to the spin-phonon interaction. Physically, the manifestation of this interaction is the magnetostriction. In view of the short-range character of the Heisenberg exchange, we keep only the sum over the z nearest neighbors in H_{S-S} and H_{S-ph}. The Hamiltonian (1) contains both the Hubbard model and the $s-d$ model as special cases.

According to Kopaev and Timerov,[5] as a consequence of the Bose condensation of phonons we have in the dielectric phase $\Delta=2g_Q\langle b_Q\rangle N^{-1/2}\neq 0$ and the electron-phonon interaction reduces to an external field H_Δ. Since the matrix element of the intraband electron-phonon interaction is purely imaginary,[6] the quantity Δ can be complex. In the absence of other order parameters, the phase of Δ is unimportant, because the dielectric gap $E_g=2|\Delta|$ but since we want to consider the coexistence of several forms of the ordering, then the phase of Δ is important. If we write H_Δ not in the momentum representation, as is the usual case, but in the coordinate representation

$$H_\Delta=\Delta\sum_{f\sigma}n_f^\sigma e^{-iQf},$$

then, from the condition that the Hamiltonian for a crystal with a center of inversion is Hermitian, $\Delta^*=\Delta$. It will be shown below that only real combinations of the matrix elements $g_Qg_Q^+$ and $g_QA_Q^+$ enter into the theory.

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Let the mean density of the electrons be n. In a state with a CDW, we distinguish two sublattices:

$$\sum_{\sigma} \langle n^{\sigma}_{A(B)} \rangle = n \pm 2\delta n.$$

We assume that the dielectric state can also be antiferromagnetic:

$$\langle \sigma_{A(B)} \rangle = \pm \langle \sigma \rangle, \quad \langle S_{A(B)} \rangle = \pm \langle S \rangle.$$

The spectrum of the electrons and the filling factors are found from the standard set of equations of Gor'kov[7]:

$$\begin{gathered} E_{k\sigma}{}^{\pm} = \varepsilon - \mu + Un/2 \pm \nu_{k\sigma}, \quad \nu_{k\sigma}{}^2 = b^2(\mathbf{k}) + \Delta_{\sigma}{}^2, \\ b(\mathbf{k}) = \sum_{\mathbf{h}} b(\mathbf{h}) e^{i\mathbf{k}\mathbf{h}}, \quad \Delta_{\sigma} = \Delta + U(\delta n - \eta(\sigma)\langle\sigma\rangle) - {}^1\!/_2 J \eta(\sigma) \langle S \rangle, \\ \eta(\sigma) = +1, \ \sigma = \uparrow, \quad \eta(\sigma) = -1, \ \sigma = \downarrow. \end{gathered} \tag{2}$$

The parameters Δ, $\langle\sigma\rangle$, $\langle S\rangle$, and μ should be found in self-consistent fashion.

3. EQUATIONS OF SELF-CONSISTENCY AND THE CLASSIFICATION OF THE SOLUTIONS

The equation for the chemical potential is

$$n = \frac{1}{N} \sum_{k\sigma} [f(E_{k\sigma}{}^{+}) + f(E_{k\sigma}{}^{-})], \quad f(E) = [e^{E/T} + 1]^{-1}. \tag{3}$$

The amplitude of the CDW is determined by the expression

$$\delta n = \frac{1}{N} \sum_{k\sigma} \frac{\Delta_{\sigma}}{2\nu_{k\sigma}} [f(E_{k\sigma}{}^{+}) - f(E_{k\sigma}{}^{-})], \tag{4}$$

and the amplitude of the band SDW is

$$\langle \sigma \rangle = \frac{1}{N} \sum_{k\sigma} \eta(\sigma) \left[f(E_{k\sigma}{}^{+}) + f(E_{k\sigma}{}^{-}) + \frac{\Delta_{\sigma}}{2\nu_{k\sigma}} (f(E_{k\sigma}{}^{+}) - f(E_{k\sigma}{}^{-})) \right]. \tag{5}$$

In the mean field approximation,

$$\langle S \rangle = SB_S \left\{ \frac{S}{T} \left[H + J\langle\sigma\rangle - \left(I + \frac{A_Q \Delta}{g_Q} \right) z \langle S \rangle \right] \right\}. \tag{6}$$

Here B_S is the Brillouin function for the spin S.

To obtain self-consistent equations relative to Δ we use a method proposed in Ref. 5. As a result, we find

$$\Delta = -2g_Q [2g_Q{}^{+} \delta n + A_Q{}^{+} z \langle S \rangle^2] / \omega_Q. \tag{7}$$

Before analyzing the possible solutions, we note that for $n = 1$, i.e., when the initial metallic band is half-filled, it follows from Eq. (3), which is represented in the form

$$n = 1 - \frac{1}{2N} \sum_{k\sigma} \left[\operatorname{th} \frac{\nu_{k\sigma} + \tilde{\varepsilon}}{2T} - \operatorname{th} \frac{\nu_{k\sigma} - \tilde{\varepsilon}}{2T} \right], \tag{8}$$

that $\mu = \varepsilon + U/2$ at all values of the temperature. If we introduce the notation

$$L_{\sigma} = \frac{1}{N} \sum_{k} \frac{\Delta_{\sigma}}{2\nu_{k\sigma}} \operatorname{th} \frac{\nu_{k\sigma}}{2T}, \tag{9}$$

then the set of equations (3)–(7) can be reduced to three equations relative to $\Delta_{\uparrow}$, $\Delta_{\downarrow}$, and $\langle S\rangle$:

$$\begin{aligned} \Delta_{\sigma} = {} & (4|g_Q|^2/\omega_Q - U)(L_{\uparrow} + L_{\downarrow}) + \eta(\sigma) U (L_{\uparrow} - L_{\downarrow}) \\ & - 2z g_Q A_Q{}^{+} \langle S \rangle^2 / \omega_Q - {}^1\!/_2 |J| \eta(\sigma) \langle S \rangle, \end{aligned} \tag{10}$$

$$\begin{aligned} \langle S \rangle = SB_S \Big\{ & -\frac{S}{T} \Big[J(L_{\uparrow} - L_{\downarrow}) + \Big(I + \frac{4 g_Q A_Q{}^{+}}{\omega_Q} (L_{\uparrow} + L_{\downarrow}) \\ & - \frac{2z|A_Q|^2}{\omega_Q} \langle S \rangle^2 \Big) z \langle S \rangle - H \Big] \Big\}; \end{aligned} \tag{11}$$

$$\Delta = \frac{4|g_Q|^2}{\omega_Q} (L_{\uparrow} + L_{\downarrow}) - 2z \frac{g_Q A_Q{}^{+}}{\omega_Q} \langle S \rangle^2, \quad \langle \sigma \rangle = L_{\downarrow} - L_{\uparrow}. \tag{12}$$

If localized spins are absent, then a transition in the limit to the band theory follows from (10) at $\langle S\rangle = 0$. A symmetric solution $\Delta_{\uparrow} = \Delta_{\downarrow}$, $L_{\uparrow} = L_{\downarrow}$ is possible, which corresponds to the CDW and which describes the three dimensional analog of the Peierls transition, as is also an antisymmetric solution $\Delta_{\uparrow} = -\Delta_{\downarrow}$, $L_{\uparrow} = -L_{\downarrow}$ with a SDW that describes a dielectric with antiferromagnetic ordering. The coexistence of the SDW and the CDW within the framework of band theory has been considered in Ref. 8. At $T = 0$, these solutions are described by the formula

$$\begin{gathered} \Delta \equiv \Delta_{00} = 2W e^{-1/\lambda}; \\ \lambda = \lambda_p = (4|g_Q|^2/\omega_Q - U) N(0) \end{gathered}$$

for the symmetric solution, $\lambda = \lambda_s = UN(0)$ for the antisymmetric, $N(0)$ is the density of states at the Fermi level of the initial metallic band of halfwidth $W = |b|z$.

The self-consistency equation (10) in the band limit has the form of the BCS equation and describes a second-order phase transition at the point $T_{c0} = \gamma \Delta_{00}/\pi$. The anisotropy of the Fermi surface, which is connected with jumps to not-nearest neighbors, leads to the appearance of dielectric states that are metastable at $T = 0$ (Ref. 5) and to a first-order transition in the temperature.[4] For the account of this anisotropy, it suffices to redefine

$$L_{\sigma} = \frac{1}{N} \sum_{k} \frac{\Delta_{\sigma}}{2\nu_{k\sigma}} \frac{1}{2} \left[\operatorname{th} \frac{\nu_{k\sigma} + u}{2T} + \operatorname{th} \frac{\nu_{k\sigma} - u}{2T} \right],$$

where $u \ll W$ is the integral of the jump to the not-nearest neighbors.

The second important type of solution corresponds to an antiferromagnetic dielectric with localized spins. If $S \neq 0$, but $A_Q = 0$, then there is an antisymmetric solution $\langle\sigma\rangle \neq 0$, $\langle S\rangle \neq 0$, $\Delta = 0$, determined from the set of two equations

$$\begin{gathered} \Delta_{\downarrow} = 2UL_{\downarrow} + {}^1\!/_2 |J| \langle S \rangle, \\ \langle S \rangle = SB_S \{ S[H + 2JL_{\downarrow} - Iz\langle S \rangle]/T \}. \end{gathered} \tag{13}$$

Under these same conditions, a CDW phase can also exist; the phase realized is the one for which the critical temperature is higher. As we shall see below, account of the localized spins increases T_c for the SDW; therefore, the condition $\lambda_s > \lambda_p$ is sufficient for the existence of the SDW.

Finally, at $S \neq 0$ and $A_Q \neq 0$, the solution of Eqs. (10) and (11) describes a dielectric with antiferromagnetic properties and with distortion of the lattice, i.e., the coexistence of CDW and SDW. The argument of the Brillouin function in (11) at $H = 0$ shows that there are several spin-ordering mechanisms in the considered model:

a) The usual Heisenberg ordering with the exchange integral I, determined both by indirect exchange and by

direct exchange. This spin ordering leads to magnetization of the band electrons due to $s-d$ exchange;

b) Formation of a band SDW can order the localized spins even in the absence of Heisenberg exchange. Here the inverse effect of magnetization of the localized moments in the inhomogeneous molecular field of the band SDW takes place;

c) Formation of a CDW and distortion of the lattice due to spin-phonon interaction (magnetostriction) can lead to ordering of the spins even at $J = I = 0$;

d) A new mechanism of indirect exchange through phonons appears in second order in A_Q.

In the following, we need the thermodynamic potentials of the corresponding phases for the analysis of the solutions that are obtained; therefore, we write out here[9] the expression for the difference in the thermodynamic potentials of the electrons and the non-interacting spins in the effective field

$$h=J\langle\sigma\rangle-(I+A_Q\Delta/g_Q)z\langle S\rangle,$$

in the dielectric and metallic phases

$$\Delta\Omega=\Omega_d-\Omega_M=-2T\sum_\sigma\int_0^W N(\varepsilon)\,d\varepsilon\ln\frac{\mathrm{ch}[(\varepsilon^2+\Delta_B^2)^{1/2}/2T]}{\mathrm{ch}(\varepsilon/2T)}-T\ln\frac{\mathrm{sh}[(S+1/2)h/T]}{\mathrm{sh}(h/2T)}.$$

4. EXCHANGE MAGNETIZATION OF THE LOCALIZED SPINS OF THE BAND WAVE SPIN DENSITY

We consider in more detail case b), which is described by Eqs. (13) at $H = I = 0$. The second of Eqs. (13) at $T = 0$ gives $\langle S\rangle = S\,\mathrm{sign}J$, while for the solution of the first we change from summation over the quasi-momentum to integration over the energy with density of states $N(\varepsilon) = \frac{1}{2}W$ (the rectangular band model). Then

$$L_\sigma=\frac{\Delta_\sigma}{4W}\ln\frac{2W}{|\Delta_\sigma|},\quad |\Delta_\sigma|>u,$$

$$L_\sigma=\frac{\Delta_\sigma}{4W}\ln\frac{2W}{u+(u^2-\Delta_\sigma^2)^{1/2}},\quad |\Delta_\sigma|<u.$$

We denote the larger solution by $\Delta_\downarrow(T = 0) = \Delta_0$ and the smaller by $\Delta_\downarrow(T = 0) = \Delta_1$. They are determined from the equations

$$\frac{\ln 2W}{\Delta_0}=\frac{1-|J|S/2\Delta_0}{\lambda_s},\qquad(14)$$

$$\frac{\ln 2W}{u+(u^2-\Delta_1^2)^{1/2}}=\frac{1-|J|S/2\Delta_1}{\lambda_s}.\qquad(15)$$

At $J = 0$, we then get the results of Kopaev and Timerov[5]:

$$\Delta_0=\Delta_{00},\quad \Delta_1(J=0)\equiv\Delta_{10}=[\Delta_{00}(2u-\Delta_{00})]^{1/2}.$$

Since $\Delta_0 > 0$, it is seen from (14) that the inclusion of the $s-d$ exchange is equivalent to an increase in the Coulomb interaction:

$$\lambda_s\to\lambda_s+|J|S/2\Delta_0\quad\text{at}\quad |J|S\ll 2\Delta_0.$$

As a result, the gap is increased. A graphic solution of Eq. (14) shows that for $u<\Delta_{00}/2$, there is one solution $\Delta_0(J)$; for $\Delta_{00}/2<u<\Delta_0(J)$ there are three solutions $\Delta_0(J)$, $\Delta_1(J)$, $\Delta_2(J)$, if $J<J_1(u)$, and one if $J>J_1(u)$; for $u>\Delta_0(J)$ there is also one solution $\Delta_2(J)$ [Fig. 1(a)]. In this connection, we recall that in the band theory, at $u>\Delta_{00}$, the ordered phase is absent [Fig. 1(b)]. Expansion of the solution (14) in powers of $|J|S/2\Delta_0$ shows that the larger solution increases linearly at small J:

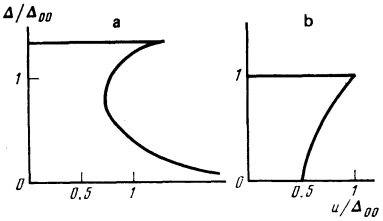

FIG. 1. Dependence of the SDW amplitude on the anisotropy of the Fermi surface at $T = 0$ and $J \neq 0$ (a), $J = 0$ (b).

$$\Delta_0\approx\Delta_{00}(1+|J|S/2\lambda_s\Delta_{00}).\qquad(16)$$

The values of $J_1(u)$ and the solutions $\Delta_{1,2}$ can also be found approximately at small J. Assuming that $|\Delta_1-\Delta_{10}|\ll\Delta_{10}$ we obtain

$$\Delta_{1,2}=[\Delta_{10}^2\pm(\Delta_{10}^4-u^2|J|S(2\Delta_{10}+|J|S/\lambda_s)/\lambda_s)^{1/2}]/(2\Delta_{10}+|J|S/\lambda_s),\qquad(17)$$

whence

$$|J_1|S=\lambda_s\Delta_{10}[(1+(\Delta_{10}/u)^2)^{1/2}-1].$$

As is seen from Fig. 1, the phase transition in the anisotropy parameter of the Fermi surface (it changes as a function of the pressure, of the deviation from stoichiometry, etc.) at $T = 0$ is a first order phase transition from the dielectric state Δ_{00} to the metallic, if $J = 0$, but from the dielectric state Δ_0 to the dielectric state Δ_2 if $J \neq 0$. The magnetic moment in the sublattice at $T = 0$ is

$$M=2\mu_B(\langle\sigma\rangle+S\,\mathrm{sign}(J)).$$

According to Eq. (12), the jump in the gap Δ leads to a jump in the moment.

The quantities $\langle\sigma\rangle$ and $\langle S\rangle$ change with increase in the temperature. The self-consistency equations (13) were solved numerically for different values of u (Fig. 2). The remaining parameters chosen were: $I = A_Q = 0$; $U = 0.8$; $g_Q = 0.1$; $\omega_Q = 0.04$; $J = 0.2$; $z = 6$, $S = 1$. The energy parameters are measured in units of the half-width of the band W. The elliptical density of states $N(\varepsilon) = 2(1-(\varepsilon/W)^2)^{1/2}/\pi W$ was used. It is seen from Fig. 2 that the jumps of the moment and of the gap take place at the same time, while the temperature of the

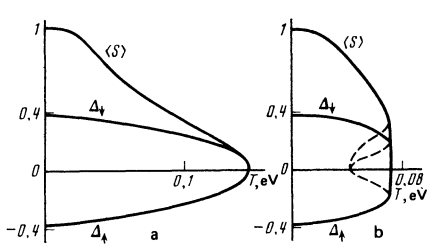

FIG. 2. Temperature dependence of the average spin and gap Δ_0 for $u = 0$ (a), and $u = 0.2$ (b). The dashed lines correspond to the metastable phase.

transition decreases with increase in u. The obtained temperature dependence of $\langle S\rangle$ differs sharply, even at $u = 0$, from the usual magnetization curve for the second order transition. This is connected with the special character of the ordering of the spins, the reason for which here is not the spin-spin interaction, direct or indirect, but the magnetization of the spins by the mean field of the band electrons.

At $u = 0$, when we have a second order transition, we have $\langle\sigma\rangle = \langle S\rangle = 0$ at the point T_c. The quantity T_c is determined by the equation

$$\ln(2\gamma W/\pi T_c) = [\lambda_s + (S+1)J^2/12WT_c]^{-1}, \tag{18}$$

which is similar, as is also (14), to the corresponding BCS equation, but with a renormalized coupling constant, while the renormalization depends on the temperature. A similar result was obtained in Ref. 2 for a ferromagnetic SDW. We note that the renormalization of the coupling constant in Eq. (18) is proportional to J^2 while in (14) it is porportional to J; therefore the increase in T_c/T_{c0} as $J \to 0$ turns out to be less than Δ_0/Δ_{00}. Actually, in this case,

$$T_c = T_{c0}[1 + J^2(S+1)/12\lambda_s^2 WT_{c0}]. \tag{19}$$

If the indirect interaction between the localized spins were absent, and they were magnetized only in the field of the band SDW, then the temperature of the ordering would be T_{c0}. The increase in T_c is connected with the usual indirect interaction in the s–d model, which is proportional to $J^2N(0)$.

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

It is seen from the formulas (12) that account of the spin-phonon interaction makes the construction of a completely antisymmetric solution impossible. Therefore, at small A_Q, the principal effect from the spin-phonon interaction consists in the appearance of a distortion of the lattice and of the CDW, simultaneous with the formation of a SDW. With increase in the interaction constant A_Q the character of the temperature curves of Δ_σ and $\langle S\rangle$ also changes, and the tendency toward a symmetric solution is established, and towards a first-order transition in the parameter A_Q becomes ever stronger even in the absence of anisotropy of the Fermi surface.

The tendency toward a transition from antisymmetric solutions to symmetric as A_Q increases can be seen from the set of equations (10), (11) at $J = 0$ and $A_Q \to 0$. If furthermore, $A_Q = 0$, then we have two uncoupled systems—the band electrons can form an SDW or a CDW with its own critical temperature T_{c0}, while the localized spins are ordered due to the effective exchange I, and their Neel temperature is determined from the usual equation of the mean field

$$\langle S\rangle = SB_S(-IS_z\langle S\rangle/T),$$

which has a nontrivial solution at $I < 0$ (antiferromagnetic character of the exchange). The connection between the band and spin subsystems arises from the spin-phonon interaction.

At $T = 0$, Eq. (10) has the form

$$\Delta_\sigma = {}^1/_2\lambda_p \sum_{\sigma_1} \Delta_{\sigma_1} \ln(2W/\Delta_{\sigma_1}) + {}^1/_2\eta(\sigma)\lambda_s \sum_{\sigma_1} \eta(\sigma_1)\Delta_{\sigma_1}\ln(2W/\Delta_{\sigma_1}) - A, \tag{20}$$

$$A = 2zS^2 g_Q A_Q^+/\omega_Q,$$

and Eq. (11) gives $\langle S\rangle = \pm S$ if

$$I + \frac{g_Q A_Q^+}{\omega_Q W}\sum_\sigma \eta(\sigma)\Delta_\sigma \ln\frac{2W}{\Delta_\sigma} - 2zS^2|A_Q|^2/\omega_Q < 0. \tag{21}$$

In the opposite case, $\langle S\rangle = 0$.

Let $\lambda_s > \lambda_p$, so that Eq. (20) has the antisymmetric solution $\Delta_\downarrow = \Delta_{00}$, $\Delta_\uparrow = -\Delta_{00}$. At small A_Q we seek a solution in the form $\Delta_\downarrow = \Delta_{00} - \delta$, $\Delta_\uparrow = -\Delta_{00} - \delta$, $\Delta_{00}/\delta \gg 1$. Linearizing Eq. (20), we easily find

$$\delta = A\lambda_s/(\lambda_s - \lambda_p + \lambda_s\lambda_p).$$

The condition of antiferromagnetic ordering of the localized spins (21) is satisfied not only for $I < 0$ but also for weak ferromagnetic exchange:

$$I < I_1 = 2|A_Q|[zS^2|A_Q| + |g_Q|\delta(1/\lambda_s - 1)/W]/\omega_Q.$$

In the general case, the reasons for the first-order transition can also be the spin-phonon interaction and the anisotropy of the Fermi surface. Moreover, at $u \neq 0$, new solutions appear in the vicinity of T_c, with a smaller gap and with less magnetization of the sublattice. A comparison of the thermodynamic potentials of the two dielectric phases shows that the phase realized is the one with the larger value of $\langle S\rangle$. The SDW and the CDW coexist in this phase, i.e., the localized spins are ordered antiferromagnetically, the band electrons and the spin and charge densities both form double sublattice structures with the same period, and a static distortion of the lattice exists. A change in the effective exchange integral I changes the transition temperature significantly.

6. DISCUSSION OF THE RESULTS

The considered model is applicable to the oxides and sulfides of the transition metals, in which a metal-dielectric transition accompanied by structural and magnetic transformations is observed. Even if there is some doubt about the existence of localized moments in the oxides of vanadium, there are localized spins in the sulfides FeS, CrS and their solid solution $Fe_xC_{1-x}S$. This same model can obviously describe the Verwey transition in magnetite Fe_3O_4. Our theory does not pretend to a description of any specific substance, since the sequence of phase transitions is determined by the particular set of interaction parameters. Nevertheless, we can draw the following general conclusion: in crystals with localized spins the value of the gap and of the critical temperature increase in comparison with purely band systems. Actually, in sulfides the metal-dielectric transition takes place at much higher temperatures ($T_c \sim 10^3$K) than in oxides ($T_c \sim 10^2$K).

The second conclusion is the following: almost all materials of these classes have a clearly expressed first order transition. The spin-phonon interaction contributes to this transition. Moreover, without the

spin-phonon interaction, it is impossible to obtain distortions of the lattice in the antiferromagnetic phase.

In conclusion, we note that the metal-dielectric transition is possible in our mode also in the case of ferromagnetic ordering, on account of the exchange splitting of the narrow conduction band. The theory of such a transition is given in Ref. 10 for a specific case. This case, too, is characterized by high values of the critical temperature.

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