

# Effect of a magnetic field on the critical temperature of a structural transition

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The dependence of the structural-transformation temperature  $T_s$  on external magnetic field strength  $H$  is investigated in a system that is unstable with respect to the doubling of the period because of the specific shape of its one-electron spectrum ( $\epsilon(\mathbf{p}) = -\epsilon(\mathbf{p} + \mathbf{Q})$  near the Fermi surface). The contribution of the singlet and triplet electron-hole correlations in the presence of an excess electron concentration is taken into account in the determination of the dependence  $T_s(H)$ . It is found that in a certain concentration range a magnetic field raises the phase-transition temperature and, in particular, can induce a phase transition in a system that, in the absence of a field, is stable at all temperatures. The results obtained in the present paper for a structural transformation are extended to the case of a transition of the system into an antiferromagnetic state for chromium-type substances. It is proposed to use the theory to explain the behavior of  $A-15$ -type compounds in an external magnetic field.

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1. We investigate below the influence of a constant, homogeneous magnetic field  $\mathbf{H}$  on the critical temperature  $T_s$  of a metal-dielectric phase transition if the metal, because of the specific shape of its one-electron spectrum, is unstable with respect to the generation of spin- and charge-density waves. The obtained results are qualitatively valid for quasi-one-dimensional systems.

We shall consider the role of only the spin effects. As has been demonstrated by Abrikosov,<sup>[1]</sup> the orbital effects are important in the ultraquantum case, when the Landau-level spacing is comparable to the Fermi energy  $\epsilon_F$ , and we are interested in values of the field  $\mathbf{H}$  of the order of  $T_s$ . To be sure, the orbital effects in fields  $\mathbf{H}$  of the order of  $T_s$  can turn out to be important because of the phenomenon of magnetic breakdown between electron and hole "pockets." These pockets are formed in the dielectric phase when the various parts of the Fermi surface of the original metallic phase that are responsible for the instability of the metal combine sufficiently badly. A similar situation has been considered by Gordyunin.<sup>[2]</sup> We shall not take this effect into account, assuming that the shape of the Fermi surface of the original metal is such that the pockets are not formed during the phase transition and that the system goes over at once into the dielectric state.

It is well known<sup>[3]</sup> that the metal-dielectric phase transition is, generally speaking, accompanied by the appearance of a two-component order parameter:

$$\hat{\Delta} = \Delta_s + \Delta_t \sigma, \quad (1)$$

where  $\sigma$  is a vector composed of the Pauli matrices. The formation of a singlet parameter  $\Delta_s$  produces a charge-density wave (CDW) and structural distortions, while with a triplet parameter  $\Delta_t$  are connected spin-density waves (SDW) and antiferromagnetic properties. It has previously been shown that the coexistence of SDW and CDW gives rise to ferromagnetism.<sup>[3,4]</sup> In these papers it was found in the computation of the paramagnetic susceptibility of the dielectric phase (the excitonic-in-

ulator phase) that, although during the phase transition in zero magnetic field ( $\mathbf{H} = 0$ ) there first arises only that parameter ( $\Delta_s$  or  $\Delta_t$ ) to which corresponds the larger coupling constant, both components of  $\hat{\Delta}$  coexist already in an arbitrarily weak field  $\mathbf{H}$ . Therefore, in computing the dependence  $T_s(\mathbf{H})$ , it is necessary to simultaneously allow for both types of pairing: singlet and triplet.

2. We shall consider the influence of a magnetic field on a structural-transition temperature, using as an example a metal that is unstable with respect to the doubling of the period. The electronic spectrum of such a metal near the Fermi level possesses the property:  $\epsilon(\mathbf{p}) = -\epsilon(\mathbf{p} + \mathbf{Q})$ , where  $\mathbf{Q}$  is half the reciprocal-lattice vector. This equality is exactly fulfilled with the energy  $\epsilon(\mathbf{p}) = \epsilon_F - \mu$ , where the quantity  $\mu$  characterizes how much the filling of the electronic band differs from half. We shall denote the corresponding "excess" number of electrons by  $N$ . The total Hamiltonian of the system can be written in the form:

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{ee} + \hat{\mathcal{H}}_{ep}. \quad (2)$$

Here  $\hat{\mathcal{H}}_0$  is the Hamiltonian of the noninteracting electrons and phonons:

$$\hat{\mathcal{H}}_0 = \sum_{\mathbf{p}, \alpha} \epsilon(\mathbf{p}) a_{\alpha}^+(\mathbf{p}) a_{\alpha}(\mathbf{p}) + \sum_{\mathbf{p}} \hbar \omega(\mathbf{p}) b^+(\mathbf{p}) b(\mathbf{p}), \quad (3)$$

where  $a_{\alpha}(\mathbf{p})$  is the annihilation operator for an electron in a state with spin  $\alpha/2$  ( $\alpha = \pm 1$ ) and quasi momentum  $\mathbf{p}$ , while  $b(\mathbf{p})$  is the phonon-annihilation operator. The Hamiltonian of the Coulomb interelectron interaction has the form:

$$\hat{\mathcal{H}}_{ee} = \sum_{\mathbf{q}} \frac{2\pi e^2}{|\mathbf{q}|^2} \hat{\rho}(\mathbf{q}) \hat{\rho}(-\mathbf{q}), \quad \hat{\rho}(\mathbf{q}) = \sum_{\mathbf{p}, \alpha} a_{\alpha}^+(\mathbf{p} - \mathbf{q}) a_{\alpha}(\mathbf{p}); \quad (4)$$

$\hat{\rho}(\mathbf{q})$  is the operator of the  $\mathbf{q}$ -th Fourier component of the electron density. In (4) we have neglected momentum transfers exceeding  $2Q$ . Finally, let us represent in the vicinity of the momenta  $\pm \mathbf{Q}$  ( $q \ll Q$ ) the operator of interaction of the electrons with the phonon mode that is

unstable at these momenta in the form

$$\hat{\mathcal{H}}_{e,p} = \sum_{\mathbf{q}} \{b^+(\mathbf{Q}-\mathbf{q}) + b(\mathbf{q}-\mathbf{Q})\} \{g\hat{p}(\mathbf{Q}-\mathbf{q}) + g'\hat{p}'(\mathbf{Q}+\mathbf{q})\} + \text{c.c.} \quad (5)$$

In formula (5) we have allowed for umklapp processes. The amplitudes of the normal and umklapp processes are assumed to be equal, since they coincide in the limit as  $\mathbf{q} \rightarrow 0$ . In the single-band approximation the constant  $g$  is purely imaginary, because of the fact that in the monatomic lattice of the metal an ionic displacement caused by a phonon with momentum  $\pm \mathbf{Q}$  creates an anti-symmetric component of the potential. For this choice of phases the Coulomb interaction,  $4\pi e^2/q^2$ , turns out to be real. In all the formulas (3)–(5) the summation over the quasimomenta is performed only over the non-equivalent points of the first Brillouin zone. Therefore, for example, in the formula (5) the complex conjugate terms should be discarded at  $\mathbf{q} = 0$ .

In an external magnetic field, to the Hamiltonian (2) should again be added the Zeeman term  $m\mathbf{H} \cdot \boldsymbol{\sigma}$ , where  $m$  is the Bohr magneton.

3. In accordance with the results of our previous paper,<sup>[4]</sup> let us introduce for the description of the phase transition of a metal into the dielectric state temperature Green functions in the form of matrices in the spin indices ( $\alpha, \beta = \pm 1$ ):

$$\begin{aligned} \hat{G}(\mathbf{p}) &= \{G_{\alpha\beta}(\mathbf{p})\} = \{-\langle T_{\tau} a_{\alpha}(\mathbf{p}, \tau) a_{\beta}^{\dagger}(\mathbf{p}, 0) \rangle\}, \\ \hat{G}(\mathbf{p} \pm \mathbf{Q}, \mathbf{p}) &= \{G_{\alpha\beta}(\mathbf{p} \pm \mathbf{Q}, \mathbf{p})\} = \{-\langle T_{\tau} a_{\alpha}(\mathbf{p} \pm \mathbf{Q}, \tau) a_{\beta}^{\dagger}(\mathbf{p}, 0) \rangle\}. \end{aligned} \quad (6)$$

Let us go over to the Fourier components of these functions at the frequencies  $\omega_n = \pi T(2n \pm 1)$ . Then, using the Hamiltonian (2) with allowance for the external magnetic field  $\mathbf{H}$ , we obtain (just as in<sup>[3,4]</sup>) that in the Hartree–Fock approximation

$$\begin{aligned} [i\omega - \varepsilon(\mathbf{p}) + \mu + m\mathbf{H}\boldsymbol{\sigma}] \hat{G}(\mathbf{p}) + \hat{\Delta}^+ \hat{G}(\mathbf{p} + \mathbf{Q}, \mathbf{p}) &= 1, \\ \hat{\Delta} \hat{G}(\mathbf{p}) + [i\omega - \varepsilon(\mathbf{p} + \mathbf{Q}) + \mu + m\mathbf{H}\boldsymbol{\sigma}] \hat{G}(\mathbf{p} + \mathbf{Q}, \mathbf{p}) &= 0. \end{aligned} \quad (7)$$

Here as the energy reference point, we have chosen the point where  $\varepsilon(\mathbf{p}) = \varepsilon_F - \mu$ . The quantity  $\hat{\Delta}$  in the formulas (7) is determined from the self-consistency conditions:

$$\begin{aligned} \hat{\Delta} &= T \sum_{\mathbf{p}, \alpha} \left\{ \frac{4g'}{\hbar\omega(\mathbf{Q})} \text{Sp}[\text{Re } g \hat{G}(\mathbf{p} + \mathbf{Q}, \mathbf{p})] \right. \\ &\left. - \frac{g_1}{2} \text{Sp} \hat{G}(\mathbf{p} + \mathbf{Q}, \mathbf{p}) + \frac{g_1}{2} \boldsymbol{\sigma} \text{Sp}[\boldsymbol{\sigma} \hat{G}(\mathbf{p} + \mathbf{Q}, \mathbf{p})] \right\}, \end{aligned} \quad (8)$$

where the trace is computed in the spin variables, while  $T$  is the absolute temperature in the energy units. The constant  $g_1$  determines the effective magnitude of the Coulomb interaction (in the high-density approximation  $g_1 \approx 4\pi e^2/Q^2$ ).

The Eqs. (7) have been written with allowance for the equilibrium conditions for the displacements of the lattice atoms. Let us recall that (as has been shown earlier<sup>[3]</sup>) the possibility of a Bose condensation of the phonons will be automatically taken into account in the derivation of the Eqs. (7) for the electronic Green functions if we introduce into these equations the Hartree

diagram containing a loop of the anomalous Green functions  $G(\mathbf{p} \pm \mathbf{Q}, \mathbf{p})$  that is connected with other electronic lines of the  $D_0$  functions of the bare phonon. Therefore, the equilibrium equations for the atomic displacements need not be written out separately. In this case, if necessary, the equilibrium density of the phonon Bose condensate (as well as the displacement of the atoms) is determined by the same loop diagram:

$$\begin{aligned} \langle b_{\mathbf{q}^+ + b_{-\mathbf{q}}} \rangle &= -2D_0(\mathbf{Q})|_{\omega=0} \text{Re} \left\{ T \sum_{\alpha, \mathbf{p}, \mathbf{p}'} g G(\mathbf{p} + \mathbf{Q}, \mathbf{p}) \right\}, \\ D_0(\mathbf{Q}) &= -2\omega(\mathbf{Q}) [\omega^2 + \omega^2(\mathbf{Q})]^{-1}. \end{aligned}$$

It is precisely this formula that is equivalent to the equation for equilibrium of the lattice.

The simultaneous solution of Eqs. (7) and (8) is possible for different choices of the phases of the matrix elements of  $\hat{\Delta}$  (the phases of the elements of the matrix  $\hat{G}(\mathbf{p} + \mathbf{Q}, \mathbf{p})$  coincide with the phases of the elements of the matrix  $\hat{\Delta}$ ). The phases are chosen in the following manner. Since the metal is assumed to be initially unstable against a structural transformation (i.e., the electron–phonon interaction is assumed to be the controlling interaction, as a result of which the frequency of the soft phonon mode vanishes at the phase transition point), the phase of the singlet order parameter  $\Delta_s$  coincides with the phase of  $g$ , since otherwise (for real  $\Delta_s$ ) the contribution of the electron–phonon interaction drops out from Eqs. (8). As to the phase of  $\Delta_t$ , it is chosen on the basis of the results of our previous papers,<sup>[3,4]</sup> where it is shown that in a weak magnetic field  $\mathbf{H}$  the triplet parameter  $\Delta_t$ , directed along  $\mathbf{H}$  and coinciding in phase with  $\Delta_s$ , arises in the excitonic-insulator state with CDW.

Having chosen the phases of  $\hat{\Delta}$  by the expounded method, we obtain from (8) (for  $\mathbf{H}$  parallel to the  $z$  axis)

$$\Delta_s = \frac{1}{2} g_s T \sum_{\mathbf{p}, \alpha} \text{Sp} \hat{G}(\mathbf{p} + \mathbf{Q}, \mathbf{p}), \quad \Delta_t = \frac{1}{2} g_t T \sum_{\mathbf{p}, \alpha} \text{Sp} [\boldsymbol{\sigma}_z \hat{G}(\mathbf{p} + \mathbf{Q}, \mathbf{p})], \quad (9)$$

where the singlet,  $g_s$ , and the triplet,  $g_t$ , coupling constants are determined by the formulas

$$g_s = 8|g|^2/\hbar\omega(\mathbf{Q}) - g_1, \quad g_t = g_1. \quad (10)$$

The relation between the constants  $g_s$  and  $g_t$  for a real metal can be roughly estimated, using the approximation of nearly free electrons moving in the periodic field of the ions. It is easy to obtain that in this approximation:

$$g = -i \frac{4\pi e^2}{Q} \left( \frac{\hbar n_i}{2\omega(\mathbf{Q})M} \right)^{1/2}, \quad \omega^2(\mathbf{Q}) = \frac{4\pi e^2 n_i}{M}, \quad g_1 \approx \frac{4\pi e^2}{Q^2}.$$

Here  $M$  is the mass of an ion,  $e$  is its charge,  $n_i$  is the ion density, and  $\omega(\mathbf{Q})$  is the plasma frequency of the ions. Substituting these expressions into the formulas (10), we obtain  $g_s \approx 3g_t$ . Notice that if in the formula (5) we exclude the umklapp processes, then we arrive at the “jellium” model, for which  $g_s = g_t$ . Thus, the presence of the lattice, because of the coherence effect in the disposition of the ions, changes the relationship

between the triplet and singlet constants in favor of the latter constant, and the structural phase transition with CDW turns out to be more preferable than the transition with SDW.

Now let us solve Eqs. (7) for  $\hat{G}(\mathbf{p}+\mathbf{Q}, \mathbf{p})$  and substitute the obtained expression into (9). Then, going over, in the usual manner from summation over  $\mathbf{p}$  to integration over the energy  $\varepsilon$  in the vicinity of  $\varepsilon_F$ , we obtain the equations for the determination of the parameters  $\Delta_s$  and  $\Delta_t$ :

$$\begin{aligned} 2\Delta_s \ln(T_{s0}/T) + \Delta_s [I(\Delta_+, \mu_+) + I(\Delta_-, \mu_-)] \\ + \Delta_t [I(\Delta_+, \mu_+) - I(\Delta_-, \mu_-)] = 0, \\ 2\Delta_t \ln(T_{t0}/T) + \Delta_t [I(\Delta_+, \mu_+) + I(\Delta_-, \mu_-)] \\ - \Delta_s [I(\Delta_+, \mu_+) - I(\Delta_-, \mu_-)] = 0. \end{aligned} \quad (11)$$

Here

$$I(\Delta, \mu) = \int_0^{\infty} d\varepsilon \{ [n(-E-\mu) - n(E-\mu)] E^{-1} - [n(-\varepsilon) - n(\varepsilon)] \varepsilon^{-1} \}, \quad (12)$$

$$E = (\varepsilon^2 + \Delta^2)^{1/2}, \quad \Delta_{\pm} = \Delta_s \pm \Delta_t, \quad \mu_{\pm} = \mu \pm mH,$$

$$2/g_s N(0) = \ln(2\gamma \varepsilon_F / \pi T_{i0}), \quad i=s, t, \quad \gamma = 1.78 \dots,$$

while  $n(x)$  is the Fermi distribution function and  $N(0)$  is the density of states near the Fermi energy in the metal per spin. The Eqs. (11) should be supplemented by the condition for the conservation of the total number of electrons:

$$\begin{aligned} 2n = N/N(0) = \int_0^{\infty} d\varepsilon [n(E_+ - \mu_+) + n(-E_+ - \mu_+) \\ + n(E_- - \mu_-) + n(-E_- - \mu_-) - 2]. \end{aligned} \quad (13)$$

The Eqs. (11) and (13) completely determine the phase diagram of a system simultaneously having a singlet,  $\Delta_s$ , and triplet,  $\Delta_t$ , dielectric ordering of the electrons in the presence of an external magnetic field.

4. Let us now find the dependence of the critical temperature  $T_s$  of the structural transition on the external magnetic field. For this purpose, it is sufficient to solve the linearized—in  $\Delta_s$  and  $\Delta_t$ —equations (11) and (13) for  $T$ . Then we obtain at once from (13) that  $\mu = n$ , and the Eqs. (11) get transformed into the form

$$\alpha \Delta_s + \kappa \Delta_t = 0, \quad \kappa \Delta_s + (\alpha - \ln \delta^2) \Delta_t = 0; \quad (14)$$

$$\begin{aligned} \alpha = \ln(T_{s0}/T) + (I_+ + I_-)/2; \quad \kappa = (I_+ - I_-)/2, \quad \delta^2 = T_{s0}/T_{i0}, \\ I_{\pm} = I(0, \mu_{\pm}), \quad \mu_{\pm} = n \pm mH. \end{aligned} \quad (15)$$

The compatibility condition for the system (14) determines the basic equation

$$\alpha(\alpha - \ln \delta^2) = \kappa^2 \quad (16)$$

for the determination of the dependence,  $T_s(H)$ , of the phase-transition temperature on the field  $H$ . From the roots of Eq. (16) we should choose that which will appear earlier on the side of the metallic phase. Making this choice, we obtain in place of Eq. (16) that

$$\alpha = \ln \delta - (\ln^2 \delta + \kappa^2)^{1/2}, \quad \ln \delta > 0. \quad (17)$$

Before proceeding with the investigation of Eq. (17),

let us reduce the functions  $I_{\pm}$ , (15), to a form convenient for the subsequent computations. For this purpose, it is necessary to substitute into the integrals  $I(0, \mu)$ , (12), the expression for the Fermi distribution function in the form of the series

$$n(x) = \sum_n (i\omega_n - x)^{-1}$$

and integrate over the energy  $\varepsilon$ . As a result, we find

$$I_{\pm} = \text{Re} \left[ \Psi \left( \frac{1}{2} \right) - \Psi \left( \frac{1}{2} + i \frac{n \pm mH}{2\pi T} \right) \right], \quad (18)$$

$$\Psi(z) = \frac{d \ln \Gamma(z)}{dz} = \lim_{k \rightarrow \infty} [\ln k - z^{-1} - (z+1)^{-1} - \dots - (z+k)^{-1}],$$

where  $\Psi(z)$  is the bigamma function and  $\Gamma(z)$  is the gamma function.

Let us now proceed to the solution of Eq. (17) for  $T_s(H)$  in the following limiting cases: a) weak magnetic field  $H$  or low concentration,  $n$ , of the excess carriers; b) low temperature  $T_s$ ; c) on the diagonal  $mH = n$ ; d) equal coupling constants ( $T_{s0} = T_{t0}$ ).

#### A. Weak field ( $mH \ll 2\pi T_s$ ) or low concentration ( $n \ll 2\pi T_s$ )

It can easily be seen from the formulas (18) that the functions  $I_{\pm}$  do not change under the substitution  $n \pm mH \rightarrow mH \pm n$ . Consequently, according to (17), (15), the structural-phase-transition temperature depends in equal measure on the magnetic field  $H$  and the concentration  $n$ . Therefore, it is sufficient to investigate the case of a weak field  $H$  at fixed  $n$ , the formulas for the low-concentration case being analogous and obtainable with the aid of the substitution  $n \leftrightarrow mH$ .

In order to find the change in the phase-transition temperature when a weak magnetic field is switched on, it is necessary to expand the coefficients in Eq. (17) in powers of  $mH/2\pi T_s$  up to the quadratic terms. Using the formulas (15) and (18), we obtain from (17) the equation

$$\begin{aligned} \ln \frac{T_{s0}}{T} + I(0, n) = \ln \delta - \left[ \ln^2 \delta + (\text{Im } \Psi')^2 \right. \\ \left. \times \left( \frac{mH}{2\pi T_s} \right)^2 \right]^{1/2} - \frac{1}{2} \text{Re } \Psi'' \left( \frac{mH}{2\pi T_s} \right)^2, \end{aligned} \quad (19)$$

where  $\Psi^{(n)} = d^n \Psi / dz^n$  at  $z = \frac{1}{2} + in/2\pi T_s$ . The values of  $T_s$  in zero field should be substituted into the right-hand side of this equation. These  $T_s$  values are known from the paper<sup>[5]</sup> by Sarma, who computed the  $H$  dependence of  $T_c$  for a superconductor; a similar equation ((19) for  $H=0$ ) was obtained for the excitonic insulator by Kopaev.<sup>[6]</sup> The plot of the function  $T_s(n)$  for  $H=0$  is shown in Figs. 1, 2, and 3 (the curves in the  $(n, T_s)$  plane). Incidentally, it follows from the symmetry of Eq. (17) under the substitution  $mH \rightarrow n$  that the dependence  $T_s(H)$  for  $n=0$  has a similar shape (the curves in the  $(mH, T_s)$  plane in the figures).

Expanding now the left-hand side of Eq. (19) near the  $T_s$  line for  $H=0$  up to terms linear in  $T_s(H) - T_s(0)$ , we easily find that the change in the structural-transition

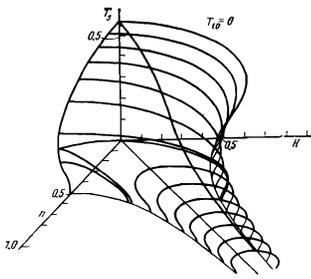


FIG. 1.

temperature in weak magnetic fields  $H$  is proportional to the square of the field (an exception is the  $g_s = g_t$  case):

$$T_s(H) - T_s(0) = \frac{T_{s0}}{2} \left[ 1 + \frac{n}{2\pi T_{s0}} \operatorname{Im} \Psi' \right]^{-1} \left[ \operatorname{Re} \Psi'' + \frac{(\operatorname{Im} \Psi')^2}{\ln \delta} \right] \left( \frac{mH}{2\pi T_{s0}} \right)^2 \quad (20)$$

It follows from this formula that in the region of low concentrations (and high  $T_s$ )  $T_s$  decreases when the field is switched on, i.e., the metallic phase stabilizes. As  $n$  increases, the influence of the magnetic field on  $T_s$  decreases and, at some sufficiently high concentration, the effect changes sign and the metallic phase becomes destabilized when the magnetic field is switched on. The closer the values of the singlet,  $g_s$ , and triplet,  $g_t$ , coupling constants are to each other, the sooner this occurs. We can easily verify all this if we use the expressions (18) for the bigamma function. In fact, in the limit as  $n \rightarrow 0$ , we shall have  $\operatorname{Re} \Psi'' < 0$  and  $\operatorname{Im} \Psi' \rightarrow 0$ , while as  $n$  increases  $\operatorname{Re} \Psi''$  decreases in absolute value, while  $(\operatorname{Im} \Psi')^2$  increases. As has been shown, the derivatives of the bigamma function can easily be expressed in terms of the derivatives of the same order of the function  $T_s(n)$  for  $H = 0$  (see [4]).

### B. Low temperatures ( $2\pi T_s \ll |n \pm mH|$ )

In the low-temperature limit, to determine the region of fields  $H$  and concentrations  $n$  in which the structurally distorted dielectric phase survives, it is convenient to use the asymptotic form of the bigamma function at large values of its argument:  $\Psi(z) \approx \ln z + O(1/z)$ . Then from (15) and (18) we have

$$\alpha \approx \ln \frac{2\pi T_s}{\gamma |n^2 - m^2 H^2|^{1/4}}, \quad \kappa \approx \frac{1}{2} \ln \left| \frac{n - mH}{n + mH} \right|, \quad (21)$$

where  $\gamma$  is defined in (12). Substituting these expressions into the formula (17), we obtain an equation for the phase-transition lines in the  $(mH, n)$  plane (see Figs.

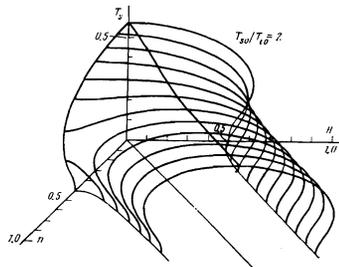


FIG. 2.

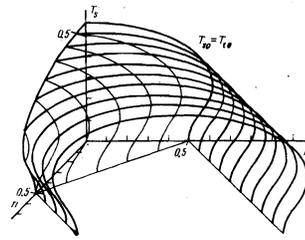


FIG. 3.

1-3) for different relations between the coupling constants  $g_s$  and  $g_t$ . If the triplet coupling constant is equal to zero ( $T_{t0} = 0$ ), then the phase transition lines at the temperature  $T = 0$  form a family of hyperbolas (Fig. 1):

$$|n^2 - m^2 H^2| = \pi^2 T_{s0}^2 / 4\gamma^2. \quad (22)$$

For equal coupling constants ( $\ln \delta = 0$ ), the dielectric-phase boundaries are described by the straight lines (Fig. 3):

$$n = mH \pm \pi T_{s0} / 2\gamma. \quad (23)$$

A simple expression is also obtained for arbitrary values of the constants in the limit of very strong fields and very high concentrations:

$$n = mH \pm \pi T_{s0} / 2\gamma, \quad (24)$$

i.e., in strong magnetic fields the dielectric phase survives at zero temperature in a band of finite width ( $\propto T_{t0}$ ) near the diagonal in the  $(n, mH)$  plane, or, for a given concentration, the phase transition occurs only in a magnetic-field range determined by the formula (24).

### C. Asymptotic value of $T_s(H)$ on the diagonal $n = mH$

In this case, using the asymptotic expansion for the bigamma function in the strong-field limit, we can easily show that

$$T_s = (T_{s0} T_{t0})^{1/2} \quad (25)$$

for  $mH = n \rightarrow \infty$ .

Thus, if both the singlet,  $g_s$ , and triplet,  $g_t$ , coupling constants are greater than zero, then, irrespective of the value of the excess-carrier concentration  $n$ , i.e., for any location of the Fermi level in the metal, the metal will, in a sufficiently strong magnetic field, surely go over into the dielectric state at a finite temperature. This circumstance is not difficult to understand if we take into account the fact that an external magnetic field leads to the separation of the Fermi surfaces of electrons with different spin directions. Therefore, for any value of  $n$  in some magnetic field  $H$  the Fermi level of the electrons in the metal for one of the spin directions will without fail pass through that part of the spectrum where the resonance condition  $\varepsilon(\mathbf{p}) = -\varepsilon(\mathbf{p} + \mathbf{Q})$  is fulfilled.

### D. Equal coupling constants ( $T_{t0} = T_{s0}$ )

With the aid of the formulas (17), (15), and (18), it is easy to verify that for  $T_{t0} = T_{s0}$  the equation for the de-

termination of the phase-transition temperature  $T_s$  in an arbitrary magnetic field coincides with the same equation for  $T_s$  in zero field when  $n$  is replaced by  $n - mH$ , i.e., for equal coupling constants the external magnetic field simply shifts the  $T_s(n)$  curve towards the region of higher concentrations.

In Figs. 1-3 we present the results of numerical computations of the entire  $T_s$  surface as a function of  $n$  and  $mH$  (for different values of  $T_{s0}/T_{t0}$ ), each variable being normalized to  $\pi T_{s0}/\gamma$ . In these figures the space region bounded by the surface and the coordinate planes (including the coordinate origin) belongs to the excitonic-insulator phase and the remaining region belongs to the normal metal.

5. Let us briefly discuss the results obtained. We have verified that the presence in the system of the triplet instability, together with the singlet instability, changes essentially the behavior of a structurally unstable metal in a magnetic field, although in zero field the possibility of triplet pairing in no way influences  $T_s$ . For the concentration  $n=0$ , i.e., when the dielectric gap arising upon the doubling of the period exactly covers the entire Fermi surface, the presence of a finite triplet coupling constant  $g_t$  also does not influence the value of  $T_s$ , irrespective of the intensity of the magnetic field. This follows directly from the symmetry, noted at the beginning of Sec. 4, of the equations under the substitution  $n \rightleftharpoons mH$ . The role of the triplet instability comes to light as the number,  $n$ , of excess electrons increases. Physically, the influence of the triplet instability manifests itself in the generation in an external magnetic field  $H$  for  $n \neq 0$  in the dielectric phase of SDW (and  $\Delta_t$ ) against a background of CDW (and  $\Delta_s$ ). The values of the dielectric gaps for opposite spin directions then turn out to be equal ( $\Delta_s + \Delta_t$  and  $\Delta_s - \Delta_t$ ). Because of this, there occurs an overflow of part of the excess carriers from one spin subband into the other, and, therefore, the condition for dielectric pairing for electrons with one of the two spin directions slackens and  $T_s$  increases. The degree of independence of the equations for the gaps with different spin directions increases as  $T_{t0}$  approaches  $T_{s0}$  (i.e., as  $g_t$  approaches  $g_s$ ). In the limit when  $g_s = g_t$ , the equations for  $\Delta_s + \Delta_t$  and  $\Delta_s - \Delta_t$  become independent (this can easily be verified by transforming the Eqs. (11)). This clearly facilitates the "overflow" process. Therefore, the greatest effect on the growth of  $T_s$  in a magnetic field appears in the limit as  $T_{t0} \rightarrow T_{s0}$ .

Williamson, Ting, and Fung,<sup>[7]</sup> on placing a  $V_3Si$  sample in a magnetic field, observed a reduction in the structural-transformation temperature that is proportional to the square of the field intensity. In accordance with our theory (formula (20)), such a reduction should be expected if  $n$  is sufficiently small and  $g_s > g_t$ .

One could attempt to explain the results of this experiment on the basis of the phenomenon of magnetic breakdown, whose effect on  $T_s$  has been considered by Gordyunin,<sup>[21]</sup> but, since the electronic spectrum of the A-15-type compounds is assumed to be quasi-one-dimensional, the orbital effects in these materials should be quenched.

All the formulas obtained by us for the structural-transition temperature in a magnetic field remain valid when we make the substitutions  $T_{s0} \rightarrow T_{t0}$  and  $T_s \rightarrow T_t$  ( $T_{t0} > T_{s0}$ ) in them, i.e., in the case of an antiferromagnetic transformation. A triplet gap  $\Delta_t$  and SDW then arise in the system at the Neel temperature  $T_t$ . If now such an antiferromagnet is placed in an external, sufficiently-strong magnetic field, then, first, its Neel temperature will change in accordance with the formulas (20) and (25) (in which the indices  $s$  and  $t$  have been interchanged); second, there will appear in it CDW and a singlet gap  $\Delta_s$ . Consequently, structural distortions (magnetostriction) will appear at moderate  $H$  in the system. In particular, when antiferromagnetic chromium is placed in an external magnetic field, one of its magnetic sublattices is shifted relative to the other in the [111] direction, i.e., the chemical unit cell of bcc chromium should double in a field  $H$ .

Now it is necessary to say a few words about the applicability of the obtained results. On the face of it, it may appear that the effect discussed by us can be correctly analyzed in the weak-coupling model only when the constants  $g_s$  and  $g_t$  are very close to each other, because of the exponential dependences of the temperatures  $T_{s0}$  and  $T_{t0}$  on them. However, because of the square-root dependence of the critical temperature  $T_s$  on  $T_{s0}$  and  $T_{t0}$ , (25), the conditions on the relation between the constants  $g_s$  and  $g_t$  are not so rigid. Thus, if  $T_{t0} \sim 10^{-4} T_{s0}$ , then, according to (25),  $T_s \sim 10^{-2} T_{s0}$ , i.e., the effect is about 1%.

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