

FIG. 1.

The conductivity of thin superconducting films in a strong high-frequency field was investigated by Rose and Sherril,<sup>[11]</sup> who found that the dependences of dissipative conductivity on the amplitude is a curve with a maximum. The films investigated by them, however, do not satisfy apparently the condition  $\nu \ll \omega_0$ , so that the theoretical experimental result may not be in agreement in<sup>[11]</sup>.

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<sup>1)</sup>We disregard here the possible multiphoton absorption connected with multiple collisions with the walls, which is pro-

portional to higher powers of  $d$  (see below).

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## Effect of hybridization on the phase transition to the state of an excitonic ferromagnet

O. A. Pankratov

*P. N. Lebedev Physics Institute, USSR Academy of Sciences*  
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A phase transition to the state of an excitonic ferromagnet {B. A. Volkov and Yu. V. Kopaev, Pis'ma Zh. Eksp. Teor. Fiz. 19, 168 (1974) [JETP Lett. 19, 104 (1974)]; Volkov, Kopaev, and A. I. Rusinov, Zh. Eksp. Teor. Fiz. 68, 1899 (1975) [Sov. Phys. JETP 41, 952 (1975)]} is considered within the framework of the electron spectrum model previously proposed for semiconductors of the IV-VI group {Volkov and Kopaev, Zh. Eksp. Teor. Fiz. 64, 2184 (1973) [Sov. Phys. JETP 37, 1103 (1973)]}. It is shown that the transition may be one of either first or second order, depending on the degree of doping and the relation between interelectron interaction constants. Allowance for hybridization does not violate the symmetry between the singlet and triplet pairing, and the phase transition occurs only at finite coupling constants. The model can be used to explain the magnetic properties of some doped narrow-band semiconductors.

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### 1. INTRODUCTION

It is known<sup>[1]</sup> that a system with a single-electron spectrum consisting of two inverted overlapping bands whose extrema lie at one point of the Brillouin zone is unstable to electron-hole pairing that leads to the appearance of a gap in the electron spectrum and to a transition to the state of an excitonic dielectric (ED). Depending on the ratio of the values of the electron-phonon and nucleon interactions, the electron-hole pairing can be realized either in a singlet or in a triplet state. If the constant of the effective interaction that is responsible for the pairing in the singlet state exceeds the corresponding value for the triplet pairing, then the instability leads to the appearance of ED in the singlet state, this being accompanied by the appearance of a charge-density wave and consequently by a structural transformation.<sup>[2]</sup> In the opposite case, the system goes

over into an ED in the triplet state; this produces a spin-density wave and the new phase is antiferromagnetic.

As shown by Volkov and Kopaev,<sup>[4]</sup> for a doped ED, at definite ratios of the interelectron interaction constants, the triplet and singlet pairings can coexist. This lifts the spin degeneracy and leads to the appearance of a spontaneous magnetic moment, inasmuch as at non-zero doping the number of electrons is not equal to the number of holes. This phenomenon is called excitonic ferromagnetism (EF) and has been investigated in detail by Volkov, Kopaev, and Rusinov.<sup>[5]</sup>

The EF model was proposed to explain the magnetic properties of certain narrow-band semiconductors, as well as metals of the iron group. The phase transition into the ED in IV-VI semiconductors (compounds of the

elements of the fourth and sixth groups of the periodic table) was investigated by Volkov and Kopaev.<sup>[6]</sup> Using the data on the structure and electronic spectrum of the IV-VI compounds. Volkov and Kopaev<sup>[6]</sup> have constructed a model Hamiltonian in which account was taken of the interband transitions that exist already in the single-particle part of the Hamiltonian (hybridization of the overlapping bands). It has turned out that in this model the phase transition to the ED is possible only at a sufficiently large coupling constant (compared with the hybridization matrix element). Since the presence of hybridization leads to an energy gap and the electron-hole pairing takes place already in this restructured spectrum, this result is analogous to that obtained by Kozlov and Maksimov,<sup>[7]</sup> who have shown that excitonic instability can develop in semiconductors in which the binding energy of the exciton is larger than the width of the forbidden band.

The presence of hybridization exerts a significant influence also on the electronic properties of transition metals, leading to a modification of the effective inter-electron interactions and of the spectrum of the collective excitations.<sup>[8]</sup> It is therefore of interest to consider the EF model with allowance for interband transitions.

In this paper, within the framework of the model that was proposed in<sup>[6]</sup> for semiconductors of the IV-VI group and includes hybridization, we investigate the phase transition into the state of an excitonic ferromagnet.

## 2. MODEL HAMILTONIAN. EQUATIONS FOR THE ORDER PARAMETERS

1. We write down the complete Hamiltonian in the form

$$H = H_0^e + H_0^{ph} + H_{int}, \quad (1)$$

where  $H_0^e$  is the Hamiltonian of the noninteracting electrons in the periodic field of the lattice,  $H_0^{ph}$  is the Hamiltonian of the free phonons, and  $H_{int}$  describes the Coulomb and electron-phonon interactions. Since the extrema of the conduction band and the valence band of IV-VI semiconductors are located at  $L$  points of the Brillouin zone, we are interested only in electronic states lying near these points, and for  $H_0^e$  we can use the ordinary Hamiltonian of the  $\mathbf{k} \cdot \mathbf{p}$  method, where the basis is made up of the functions  $\psi_{n\mathbf{q}} = \psi_{n\mathbf{k}_0} e^{i\mathbf{q}\mathbf{r}}$  ( $\psi_{n\mathbf{k}_0} = u_{n\mathbf{k}_0} e^{i\mathbf{k}_0\mathbf{r}}$  is the exact solution of the Schrödinger equation in a given periodic potential). The index  $n$  denotes the number of the band, and the vector  $\mathbf{q}$  is measured from the point  $\mathbf{k}_0$  corresponding to the point  $L$  of the Brillouin zone.<sup>[6]</sup>

If  $a_{\alpha}^*(\mathbf{q})$  is the operator for the production of an electron in a state  $\psi_{n\mathbf{q}}$  with spin  $\alpha/2 = \pm \frac{1}{2}$ , then we have for  $H_0^e$ <sup>[6]</sup>

$$H_0^e = \sum_{\mathbf{q}\alpha} [(\epsilon(\mathbf{q}) + \mu) a_{1\alpha}^*(\mathbf{q}) a_{1\alpha}(\mathbf{q}) - (\epsilon(\mathbf{q}) - \mu) a_{2\alpha}^*(\mathbf{q}) a_{2\alpha}(\mathbf{q}) + (V_s(\mathbf{q}) a_{\alpha\alpha}^*(\mathbf{q}) a_{2\alpha}(\mathbf{q}) + \text{c.c.})],$$

where  $\epsilon(\mathbf{q}) = \hbar^2 q^2 / 2m - \epsilon_F$ ,  $m$  is the effective mass,  $\epsilon_F$

is a measure of the band overlap;  $\mu$  is the chemical potential,  $V_s(\mathbf{q}) = \hbar \mathbf{P} \mathbf{q} / m_0$  is the hybridization matrix element,  $m_0$  is the mass of the free electron, and the vector  $\mathbf{P}$  is defined by the relation

$$\mathbf{P} = -i\hbar \int d^3r \psi_{1\mathbf{k}_0}^*(\mathbf{r}) \nabla_r \psi_{2\mathbf{k}_0}(\mathbf{r}).$$

The wave functions  $\psi_{n\mathbf{k}_0}$  are chosen to be pure real, so that the vector  $\mathbf{P}$  is pure imaginary.

Inasmuch as at the points  $L$  the transitions with participation of acoustic phonons are symmetry-forbidden,<sup>[6]</sup> we take into account in  $H_{int}$  only the interaction with the optical phonons and electron Coulomb interaction of the density-density type. Retaining in the interaction only terms that lead to instability with respect to electron-hole pairing, we have

$$H_{int} = \sum_{\substack{\mathbf{p}_1, \mathbf{p}_2, \mathbf{q} \\ \alpha, \beta}} V(\mathbf{q}) a_{1\alpha}^*(\mathbf{p}_1 - \mathbf{q}) a_{2\beta}^*(\mathbf{p}_2 + \mathbf{q}) a_{2\beta}(\mathbf{p}_2) a_{1\alpha}(\mathbf{p}_1) + \sum_{\mathbf{p}\alpha} [g(\mathbf{p}, \mathbf{q}) a_{1\alpha}^*(\mathbf{p}) a_{2\alpha}(\mathbf{p} + \mathbf{q}) (b_{\mathbf{q}} + b_{-\mathbf{q}}^*) + \text{c.c.}],$$

where  $V(\mathbf{q})$  and  $g(\mathbf{p}, \mathbf{q})$  are the matrix elements of the Coulomb and electron-phonon interactions (they are real quantities at our choice of the phases of the wave functions). Finally, the phonon Hamiltonian is

$$H_0^{ph} = \sum_{\mathbf{q}} \hbar \omega(\mathbf{q}) b_{\mathbf{q}}^* b_{\mathbf{q}},$$

where  $\omega(\mathbf{q})$  is the bare frequency of the optical phonons.

2. We assume that the magnetic moment produced in the system is directed along the  $z$  axis, and introduce in the usual manner the Green's function of the electron<sup>[9,5]</sup>:

$$G_{ij}^{\alpha\alpha}(\mathbf{q}, t) = -i \langle T a_{i\alpha}(\mathbf{q}, t) a_{j\alpha}^*(\mathbf{q}, 0) \rangle.$$

The graphic equation for the Green's functions in the Hartree-Fock approximations are analogous to the equations in<sup>[5]</sup>, but differ in the presence of diagrams corresponding to the hybridization (Fig. 1). The corresponding analytic expressions are

$$G_{11}^{\alpha\alpha}(\mathbf{p}, \omega) = G_{11}^{(0)}(\mathbf{p}, \omega) + G_{11}^{(0)}(\mathbf{p}, \omega) [\Delta_{\pm}^*(\mathbf{p}) + V_s(\mathbf{p})] G_{21}^{\alpha\alpha}(\mathbf{p}, \omega), \quad (2)$$

$$G_{21}^{\alpha\alpha}(\mathbf{p}, \omega) = G_{21}^{(0)}(\mathbf{p}, \omega) [\Delta_{\pm}(\mathbf{p}) + V_s^*(\mathbf{p})] G_{11}^{\alpha\alpha}(\mathbf{p}, \omega).$$

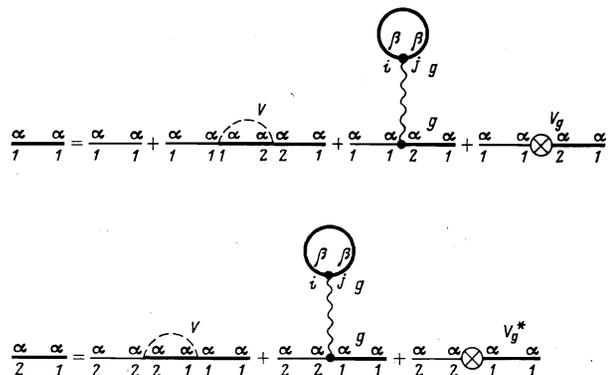


FIG. 1.

Here  $G_{11;22}^{(0)}(\mathbf{p}, \omega) = 1/(\omega \mp \varepsilon(\mathbf{p}) + \mu)$  are the Green's functions of the free electrons in the "non-hybridized" zones,  $\Delta_{\pm} = \Delta_s \pm \Delta_t$ ,  $\Delta_{s(t)}$  are the singlet (triplet) order parameters,<sup>[4,5]</sup> and the upper sign in the symbol  $\Delta_{\pm}$  in (2) corresponds to upward spin ( $\alpha = +1$ ), while the lower sign corresponds to downward spin ( $\alpha = -1$ ). The order parameters  $\Delta_{\pm}$  have the meaning of the spectrum energy gap due to interelectron interaction for upward and downward spin, respectively.

From Fig. 1 we get

$$\Delta_{\pm}(\mathbf{p}) = i \int \frac{d^3\mathbf{q}}{(2\pi)^3} V(\mathbf{p}-\mathbf{q}) G_{21}^{\alpha\alpha}(\mathbf{q}, 0^-) - \frac{4g(\mathbf{p})}{\omega_0} \sum_{\alpha} \int \frac{d^3\mathbf{q}}{(2\pi)^3} g(\mathbf{q}) \text{Im} G_{21}^{\alpha\alpha}(\mathbf{q}, 0^-), \quad (3)$$

where  $g(\mathbf{p}) = g(\mathbf{p}, 0)$  and  $\omega_0 = \omega(0)$ . Solving the system (2) we obtain

$$G_{21}^{\alpha\alpha}(\mathbf{p}, \omega) = \frac{\Delta_{\pm}(\mathbf{p}) + V_{\varepsilon}^*(\mathbf{p})}{2\varepsilon_{\pm}(\mathbf{p})} \left[ \frac{1}{\omega + \mu - \varepsilon_{\pm}(\mathbf{p})} - \frac{1}{\omega + \mu + \varepsilon_{\pm}(\mathbf{p})} \right],$$

$$G_{11}^{\alpha}(\mathbf{p}, \omega) = \frac{1/2(1 + \varepsilon(\mathbf{p})/\varepsilon_{\pm}(\mathbf{p}))}{\omega + \mu - \varepsilon_{\pm}(\mathbf{p})} + \frac{1/2(1 - \varepsilon(\mathbf{p})/\varepsilon_{\pm}(\mathbf{p}))}{\omega + \mu + \varepsilon_{\pm}(\mathbf{p})}, \quad (4)$$

$$G_{22}^{\alpha\alpha}(\mathbf{p}, \omega) = \frac{1/2(1 - \varepsilon(\mathbf{p})/\varepsilon_{\pm}(\mathbf{p}))}{\omega + \mu - \varepsilon_{\pm}(\mathbf{p})} + \frac{1/2(1 + \varepsilon(\mathbf{p})/\varepsilon_{\pm}(\mathbf{p}))}{\omega + \mu + \varepsilon_{\pm}(\mathbf{p})},$$

where  $\varepsilon_{\pm}(\mathbf{p}) = \{\varepsilon^2(\mathbf{p}) + |\Delta_{\pm}(\mathbf{p}) + V_{\varepsilon}^*(\mathbf{p})|^2\}^{1/2}$  is the restructured energy spectrum.

Since  $V_{\varepsilon}(\mathbf{p})$  is a pure imaginary quantity, with  $V_{\varepsilon}(-\mathbf{p}) = -V_{\varepsilon}(\mathbf{p})$ , the symmetry property of the spectrum  $\varepsilon_{\pm}(-\mathbf{p}) = \varepsilon_{\pm}(\mathbf{p})$ , which follows from the invariance of the Schrödinger equation with respect to the time inversion, is preserved only under the condition that  $\Delta_{\pm}(\mathbf{p})$  be real, and consequently

$$\varepsilon_{\pm}(\mathbf{p}) = \{\varepsilon^2(\mathbf{p}) + |\Delta_{\pm}(\mathbf{p})|^2 + |V_{\varepsilon}(\mathbf{p})|^2\}^{1/2}. \quad (5)$$

Substituting  $G_{21}^{\alpha\alpha}$  from (4) in (3), we obtain a self-consistent system of equations for the order parameters  $\Delta_{\pm}$  (and incidentally we make the usual simplifying assumption, replacing  $V(\mathbf{p})$  and  $g(\mathbf{p})$  by the constants  $\lambda$  and  $g$ , respectively):

$$\Delta_{+} = \left( \lambda + 4 \frac{g^2}{\omega_0} \right) \int \frac{d^3\mathbf{q}}{2(2\pi)^3} \frac{f_{+}(\mathbf{q})}{\varepsilon_{+}(\mathbf{q})} \Delta_{+} + \frac{2g^2}{\omega_0} \int \frac{d^3\mathbf{q}}{(2\pi)^3} \frac{f_{-}(\mathbf{q})}{\varepsilon_{-}(\mathbf{q})} \Delta_{-},$$

$$\Delta_{-} = \left( \lambda + 4 \frac{g^2}{\omega_0} \right) \int \frac{d^3\mathbf{q}}{2(2\pi)^3} \frac{f_{-}(\mathbf{q})}{\varepsilon_{-}(\mathbf{q})} \Delta_{-} + \frac{2g^2}{\omega_0} \int \frac{d^3\mathbf{q}}{(2\pi)^3} \frac{f_{+}(\mathbf{q})}{\varepsilon_{+}(\mathbf{q})} \Delta_{+}, \quad (6)$$

where  $f_{\pm}(\mathbf{q}) = 1 - \theta(\mu - \varepsilon_{\pm}(\mathbf{q}))$  and  $\theta(x)$  is equal to unity or zero respectively if  $x > 0$  and  $x < 0$ . Where necessary, the integrals in (6) are cut off at momenta  $q \approx q_F$  corresponding to  $\varepsilon(q_F) = 0$ . This is equivalent to the assumption that for large momentum transfers  $q > q_F$  the interaction constants vanish. As usual, however, the results of the integration depend little (logarithmically) on  $\varepsilon_F$ .

We introduce the notation  $g_s = \lambda + 8g^2/\omega_0$  and  $g_t = \lambda$ , and then, as can be easily shown from (6),  $g_{s(t)}$  are the constants of the interaction responsible for the pairing in the singlet (triplet) state. A pure singlet (triplet) state of an undoped ED corresponds to

$$\Delta_{+} = \pm \Delta_{-} = \Delta_{s(t)}; \quad \Delta_{s(t)} = 2\varepsilon_F \exp(-1/g_{s(t)}N(0)),$$

where  $N(0) = mq_F/2\pi^2\hbar^2$  is the density of states on the Fermi surface. If we introduce the notation

$$\delta = (\Delta_{s0}/\Delta_{t0})^{1/2}, \quad \gamma = (\Delta_{s0}\Delta_{t0})^{1/2} \text{ and}$$

$$Y(\Delta_{\pm}, \mu) = \frac{1}{N(0)} \int \frac{d^3\mathbf{q}}{2(2\pi)^3} \frac{f_{\pm}(\mathbf{q})}{\varepsilon_{\pm}(\mathbf{q})}, \quad (7)$$

then the system (6) can be represented in the form

$$\Delta_{+} \ln(\gamma/2\varepsilon_F) + \Delta_{-} \ln \delta = -\Delta_{+} Y(\Delta_{+}, \mu), \quad (8)$$

$$\Delta_{-} \ln(\gamma/2\varepsilon_F) + \Delta_{+} \ln \delta = -\Delta_{-} Y(\Delta_{-}, \mu).$$

The form of the function  $Y(\Delta_{\pm}, \mu)$  depends on the ratio of the chemical potential to the minimal or maximal values of the gap (at  $\mathbf{q} \perp \mathbf{P}$  the gap is minimal and equal to  $|\Delta_{\pm}|$ , and at  $\mathbf{q} \parallel \mathbf{P}$  and  $|\mathbf{q}| = q_F$  the gap is maximal and equal to  $[|\Delta_{\pm}|^2 + |V_{\varepsilon}(q_F)|^2]^{1/2}$ ). We write down the hybridization matrix element in the form  $V_{\varepsilon}(\mathbf{q}) = V_{\varepsilon} x$  (where  $V_{\varepsilon} = \hbar|\mathbf{P}|q_F/m_0$ , and  $x$  is the cosine of the angle between the vectors  $\mathbf{P}$  and  $\mathbf{q}$ ), assuming that  $V_{\varepsilon}(\mathbf{q})$  is a slowly-varying function of  $|\mathbf{q}|$  in the vicinity of  $|\mathbf{q}| \sim q_F$ , which makes the main contribution to the integral (7).

We emphasize that the system (8) is fully symmetrical with respect to the singlet and triplet pairings, i. e., it does not change under the substitution  $\Delta_{s0} \rightleftharpoons \Delta_{t0}$ , and  $\Delta_{-} \rightarrow -\Delta_{-}$ , although hybridization induces only a singlet gap and this should seemingly violate this symmetry. However, owing to the dependence of  $V_{\varepsilon}(\mathbf{q})$  on the angle between  $\mathbf{q}$  and  $\mathbf{P}$ , the corresponding increment to  $\Delta_{\pm}$  vanishes upon integration with respect to  $\mathbf{q}$ , a fact taken into account in the derivation of Eqs. (6) and (8).

The integration of (7) was first carried out with respect to energy, and then with respect to angle, using the assumption  $V_{\varepsilon}/\varepsilon_F \ll 1$ , which is not fundamental but makes it possible to simplify the calculations, and has led to the following expressions:

$$Y(\Delta^2 + V_{\varepsilon}^2 < \mu^2) = \ln \frac{2\varepsilon_F}{\mu + (\mu^2 - \Delta^2 - V_{\varepsilon}^2)^{1/2}} + 1 - \frac{\mu}{V_{\varepsilon}} \arctg \frac{V_{\varepsilon}}{(\mu^2 - \Delta^2 - V_{\varepsilon}^2)^{1/2}} + \frac{\Delta}{V_{\varepsilon}} \arctg \frac{\Delta V_{\varepsilon}}{\mu^2 - \Delta^2 + \mu(\mu^2 - \Delta^2 - V_{\varepsilon}^2)^{1/2}}, \quad (9)$$

$$Y(\Delta^2 < \mu^2 < \Delta^2 + V_{\varepsilon}^2) = \ln \frac{2\varepsilon_F}{(\Delta^2 + V_{\varepsilon}^2)^{1/2}} + 1 - \frac{\pi}{2} \frac{\mu}{V_{\varepsilon}} + \frac{\Delta}{V_{\varepsilon}} \arctg \frac{\Delta}{V_{\varepsilon}}, \quad (10)$$

$$Y(\mu^2 < \Delta^2) = \ln \frac{2\varepsilon_F}{(\Delta^2 + V_{\varepsilon}^2)^{1/2}} + 1 - \frac{\pi}{2} \frac{\Delta}{V_{\varepsilon}} + \frac{\Delta}{V_{\varepsilon}} \arctg \frac{\Delta}{V_{\varepsilon}}. \quad (11)$$

It is seen that expressions (9)–(11) go over continuously into one another with changing  $\mu$ .

The equations for the chemical potential are also different for different intervals of  $\mu$ . If  $n$  is the density of the excess electrons and  $N$  is the density of the electrons of the completely occupied band:

$$n = -i \sum_{\alpha} \int \frac{d\omega d^3\mathbf{q}}{(2\pi)^4} G_{\alpha\alpha}^{\alpha\alpha}(\mathbf{q}, \omega) e^{i\omega\tau} - N,$$

then, using (4), we get

$$n = \int \frac{d^3\mathbf{q}}{(2\pi)^3} [\theta(\mu - \varepsilon_{+}(\mathbf{q})) + \theta(\mu - \varepsilon_{-}(\mathbf{q}))] \equiv n_{+} + n_{-}. \quad (12)$$

It is convenient to introduce the notation  $\tilde{n} = n/4N(0)$

and  $\bar{n}_z = n_z/4N(0)$ ; then integration in (12) yields

$$\bar{n}_z(\Delta_{\pm}^2 + V_g^2 < \mu^2) = \frac{1}{4}(\mu^2 - \Delta_{\pm}^2 - V_g^2)^{3/2} + \frac{\mu^2 - \Delta_{\pm}^2}{4V_g} \operatorname{arctg} \frac{V_g}{(\mu^2 - \Delta_{\pm}^2 - V_g^2)^{1/2}}, \quad (13)$$

$$\bar{n}_z(\Delta_{\pm}^2 < \mu^2 < \Delta_{\pm}^2 + V_g^2) = \pi(\mu^2 - \Delta_{\pm}^2)/8V_g. \quad (14)$$

For an exciton dielectric we have  $\Delta_+^2 = \Delta_-^2 = \Delta^2$  and at  $\mu^2 \leq \Delta^2 + V_g^2$  we obtain

$$\bar{n} = \pi(\mu^2 - \Delta^2)/4V_g. \quad (15)$$

If we put  $4\bar{n}V_g/\pi = \mu_0^2$ , then we get for the ED  $\mu^2 = \mu_0^2 + \Delta^2$ , where  $\mu_0$  has the meaning of the chemical potential at  $\Delta = 0$ , i. e., the chemical potential that would exist in the initial state of the system. We shall henceforth use the dimensionless quantity  $L = \mu_0/V_g$  as a measure of the doping. We confine ourselves mainly to sufficiently "small" doping, i. e., we assume that  $0 < L < 1$ . In practice, interest attaches apparently to just this case, inasmuch, for example,  $\epsilon_F \sim 0.1$  eV and  $V_g/e_F \sim 0.1$  the value  $L = 1$  corresponds to an excess-electron concentration  $n \sim 10^{20}$ , which corresponds to very strong doping.

In view of the indicated symmetry of (8), we can confine ourselves to the case  $\Delta_{s0} < \Delta_{t0}$ . For the considered Hamiltonian (1) this is always the case; it is obvious, however, that the results can be directly generalized also to the case  $\Delta_{s0} < \Delta_{t0}$ .

### 3. GROUND-STATE ENERGY

Let us find the change of the energy of the ground state of the system on going from the initial semimetallic phase to the ED phase. To this end we average the Hamiltonian (1), taking into account the presence of anomalous mean values  $\langle a_{1\alpha}^{\dagger}(\mathbf{q})a_{2\alpha}(\mathbf{q}) \rangle$  and  $\langle b_0 \rangle$ .<sup>[5,6]</sup>

1. On going over to the exciton dielectric we obtain (at  $0 < L < 1$ )

$$\delta E = -\frac{N(0)}{3} \left[ \Delta^2 \left( 1 + \pi \frac{\mu}{V_g} \right) - V_g^2 \ln \left( 1 + \frac{\Delta^2}{V_g^2} \right) - \frac{2\Delta^3}{V_g} \operatorname{arctg} \frac{\Delta}{V_g} - 8\bar{n}(\mu - \mu_0) \right]. \quad (16)$$

If we expand this expression in powers of  $\Delta$ , then it turns out that the coefficient of  $\Delta^2$  vanishes and we obtain

$$\delta E = -\frac{N(0)\Delta^4}{2V_g^2} \left( \frac{\pi}{2} \frac{1}{L} - 1 \right), \quad (17)$$

i. e., the energy gain is proportional to the fourth power of the order parameter. Consequently, in the presence of hybridization, within the framework of the considered Hamiltonian (1), the phase transition to the ED remains a second-order transition.<sup>[10]</sup> (Provided, of course, that the solution  $\Delta$  does not appear jumpwise. It will be proved later on, however, that on going to the ED the order parameter appears in continuous fashion with increasing coupling constant.)

2. The transition to the EF phase is accompanied by

change in the energy of the ground state:

$$\delta E_F = \delta E_+ + \delta E_-,$$

where in analogy with (9)–(11) the form of the expressions for  $\delta E_{\pm}$  depends on the position of the chemical potential.

At  $\mu < \Delta_+$  we have

$$\delta E_+ = -\frac{N(0)}{6} \left[ \Delta_+^2 - V_g^2 \ln \left( 1 + \frac{\Delta_+^2}{V_g^2} \right) + \frac{2\Delta_+^3}{V_g} \operatorname{arctg} \frac{V_g}{\Delta_+} \right]. \quad (18)$$

In the case  $\Delta_+^2 < \mu^2 < \Delta_+^2 + V_g^2$  we have

$$\delta E_+ = -\frac{N(0)}{6} \left\{ (\Delta_+^2 + \Delta_-^2) \left( 1 + \pi \frac{\mu}{V_g} \right) - V_g^2 \left[ \ln \left( 1 + \frac{\Delta_+^2}{V_g^2} \right) + \ln \left( 1 + \frac{\Delta_-^2}{V_g^2} \right) \right] - \frac{2\Delta_+^3}{V_g} \operatorname{arctg} \frac{\Delta_+}{V_g} - \frac{2\Delta_-^3}{V_g} \operatorname{arctg} \frac{\Delta_-}{V_g} - 16\bar{n}(\mu - \mu_0) \right\}. \quad (19)$$

### 4. PARAMAGNETIC SUSCEPTIBILITY OF EXCITONIC INSULATOR

The calculation of the spin susceptibility is analogous to that given in<sup>[5]</sup>. In an external magnetic field  $\mathcal{H}_z$ , the chemical potentials for the electrons with upward and downward spins move apart and are equal to  $\mu_{\pm} = \mu \pm \mu_B \mathcal{H}_z$  ( $\mu_B$  is the Bohr magneton). The magnetic moment is

$$M_z = -i\mu_B \sum_{\mathbf{k}} [G_{11}^{11}(\mathbf{k}, 0^-) - G_{11}^{-1-1}(\mathbf{k}, 0^-)] = \frac{\pi\mu_B N(0)}{2V_g} [(\mu_+^2 - \Delta_+^2) - (\mu_-^2 - \Delta_-^2)].$$

In analogy with Sec. 2, we obtain the self-consistency equations (the case  $\Delta_{\pm}^2 < \mu^2 < \Delta_{\pm}^2 + V_g^2$ ) for an ED in an external magnetic field ( $\Delta_{\pm} = \Delta \pm \Delta_t$ )

$$\Delta_+ \ln \gamma + \Delta_- \ln \delta = \Delta_+ \left[ \frac{1}{2} \ln(\Delta_+^2 + V_g^2) - 1 + \frac{\pi}{2} \frac{\mu_+}{V_g} - \frac{\Delta_+}{V_g} \operatorname{arctg} \frac{\Delta_+}{V_g} \right],$$

$$\Delta_- \ln \gamma + \Delta_+ \ln \delta = \Delta_- \left[ \frac{1}{2} \ln(\Delta_-^2 + V_g^2) - 1 + \frac{\pi}{2} \frac{\mu_-}{V_g} - \frac{\Delta_-}{V_g} \operatorname{arctg} \frac{\Delta_-}{V_g} \right].$$

Solving these equations (jointly with the electroneutrality condition (12)) accurate to terms linear in  $\mathcal{H}_z$  (i. e., in  $\Delta_t$ ), we obtain the magnetic susceptibility

$$\chi = \frac{2\pi\mu_B^2 N(0)}{V_g} \left[ \mu + \frac{\pi\Delta^2}{2V_g} / \left( 2 \ln \delta - \frac{\Delta}{V_g} \operatorname{arctg} \frac{\Delta}{V_g} \right) \right].$$

The first term in this formula corresponds to the susceptibility of the free electrons, while the second is proportional to the triplet gap induced by the external field, and becomes infinite if the condition

$$\Delta_{t0} = \Delta_{t0} \exp(-\Delta/V_g \operatorname{arctg}(\Delta/V_g))$$

is satisfied. Consequently, for constants  $\Delta_{t0}$  larger than this critical value, the ED in the singlet state becomes unstable with respect to triplet pairing, and we find ourselves in the region of coexistence of the singlet and triplet pairings, corresponding to the solution of the system (8)  $\Delta_{\pm} \neq \pm \Delta_{\pm}$  and to the presence of a spontaneous

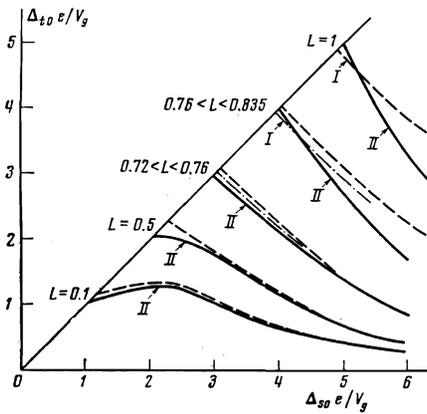


FIG. 2.

magnetic moment. This is the region of the parameters  $\Delta_{s0}$  and  $\Delta_{t0}$  in which excitonic ferromagnetism sets in.

We note, just as in other cases,<sup>[4,5]</sup> the undoped ED turns out to be stable in the entire region of external parameters  $\Delta_{s0}$  and  $\Delta_{t0}$ , inasmuch as in a weak magnetic field  $\mu_B \mathcal{H}_z < |\Delta_x|$  its self-consistency equations do not depend on  $\mathcal{H}_z$  at all. In addition, it is easy to show that, in analogy with the results of<sup>[4]</sup>, in the absence of doping the system (8) has no physically reasonable solutions corresponding to the coexistence of the triplet and singlet pairings.

Let us find the form of the ED instability lines on the  $(\Delta_{s0}, \Delta_{t0})$  plane. The equation for the dimensionless order parameter  $x = \Delta/V_g$  is obtained from the equations of the system (8) by putting in the latter  $\Delta_+ = \Delta_- = \Delta$ . From (8) and (10) we obtain

$$\ln \Delta_{s0} e/V_g = \frac{1}{2} \ln(1+x^2) + \frac{\pi}{2} (L^2+x^2)^{1/2} - x \operatorname{arctg} x; \quad (20)$$

together with the relation that determines the pole  $\chi$ :

$$\ln(\Delta_{s0}/\Delta_{t0}) = x \operatorname{arctg} x, \quad (21)$$

this equation determines parametrically the instability curve of the ED. In Fig. 2, the solid lines correspond to the curves of the instability of the ED in the singlet state at different values of the doping, plotted from (20) and (21).

## 5. INVESTIGATION OF THE SELF-CONSISTENCY EQUATIONS FOR DIFFERENT DEGREES OF DOPING

1. Before we proceed to finding the magnetic solutions, we consider the case of a doped ED. At  $L < 1$  we have for the order parameter Eq. (20), which is easily solved near the limit of the generation of the dielectric phase, i. e., assuming that  $x \ll 1$ :

$$\Delta^2 = \frac{2V_g^2}{\pi/2L-1} \left( \ln \frac{\Delta_{s0} e}{V_g} - \frac{\pi}{2} L \right). \quad (22)$$

It is seen from this expression that the ED exists at a coupling constant

$$\Delta_{s0} > V_g \exp(\pi L/2-1)$$

and  $\Delta$  decreases with increasing doping.

The solution for the ED at  $L > 1$  can also be easily obtained, and it is easy to verify that in the case of very strong doping ( $L \gg 1$ ) it goes over into the corresponding expression for the doped ED without hybridization.<sup>[11]</sup> It is obvious that in this limit the region of the energy spectrum which is noticeably distorted by the hybridization remains deep below the Fermi surface, and Eqs. (8) go over into the corresponding equations.<sup>[5]</sup>

2. For the case of nonzero doping, no analytic solution of the system (8) is possible. We start therefore with the simplest particular case  $\Delta_{s0} = \Delta_{t0} = \Delta_0$ , i. e., we seek the solution of (8) for the dimensionless order parameters  $x_{\pm} = \Delta_{\pm}/V_g$  on a diagonal in the  $(\Delta_{s0}, \Delta_{t0})$  plane. The following magnetic solutions are then possible:

- 1)  $x_{\pm} < \mu/V_g$ ,  $x_{+} \neq 0$ ,  $x_{-} = 0$ ;
- 2)  $x_{-} < \mu/V_g < x_{+}$ ,  $x_{+} \neq 0$ ,  $x_{-} = 0$  or  $x_{+} \neq 0$ ,  $x_{-} \neq 0$ .

The solution of the first type satisfies the equation

$$\ln(\Delta_0 e/V_g) = \frac{1}{2} \ln(1+x_{+}^2) + \pi\mu/2V_g - x_{+} \operatorname{arctg} x_{+}, \quad (23)$$

where the chemical potential  $\mu$  is determined at  $x_{+}^2/2 < L^2 < 1 - x_{+}^2/2$  by the relation

$$\mu/V_g = (L^2 + x_{+}^2/2)^{1/2}. \quad (24a)$$

At  $1 - x_{+}^2/2 < L^2$  we obtain from (13) and (14)

$$L^2 + \frac{x_{+}^2}{2} = \frac{\mu^2}{V_g^2} + \frac{1}{\pi} \left[ \left( \frac{\mu^2}{V_g^2} - 1 \right)^{1/2} - \frac{\mu^2}{V_g^2} \operatorname{arctg} \left( \frac{\mu^2}{V_g^2} - 1 \right)^{1/2} \right]. \quad (24b)$$

For the solution of the second type we obtain from (8), (10), and (11) the equations

$$\ln(\Delta_0 e/V_g) = \frac{1}{2} \ln(1+x_{+}^2) + \frac{1}{2} \pi x_{+} - x_{+} \operatorname{arctg} x_{+}, \quad (24c)$$

$$\ln(\Delta_0 e/V_g) = \frac{1}{2} \ln(1+x_{-}^2) + \frac{1}{2} \pi (2L^2+x_{-}^2)^{1/2} - x_{-} \operatorname{arctg} x_{-}. \quad (24d)$$

These equations (i. e., expressions (10) and (11)) are valid at  $L^2 < x_{+}^2/2$  and  $L^2 < \frac{1}{2}$ , respectively.

It is seen from (23) and (24) that the solution  $x_{-} \neq 0$  appears at larger coupling constants than the solution  $x_{+} \neq 0$ ,  $x_{-} < \mu/V_g$ , or  $x_{+} > \mu/V_g$ . Therefore in the region of values of  $\Delta_0$  where a phase transition into the EF takes place we can confine ourselves to the solutions  $x_{+} \neq 0$  and  $x_{-} = 0$ . (The solution  $x_{-} = 0$  corresponds to equality of the singlet and triplet gaps. A similar solution on the diagonal is obtained also in the model of the EF without hybridization.<sup>[5]</sup>)

It follows from (23), (24a), and (24b) that at  $L^2 < \frac{1}{2}$  the order parameter  $x_{+}$  satisfies Eqs. (23) and (24a) for values of  $\Delta_0$  such that  $x_{+} \leq \mu/V_g$  or  $x_{+} \leq L\sqrt{2}$ . At larger coupling constants we have  $x_{+} > \mu/V_g$  and Eq. (24c) is satisfied. At  $L^2 > \frac{1}{2}$  we use Eqs. (23) and (24a) for  $x_{+}^2 \leq 2 - 2L^2$  and Eq. (23), while for  $\mu^2/V_g^2 > x_{+}^2 \geq 2 - 2L^2$  we use Eqs. (23) and (24b), the latter being replaced by (24c) at  $x_{+} \geq \mu/V_g$ .

Equations (23), (24a) can be solved by assuming that  $x_{+} \ll 1$ :

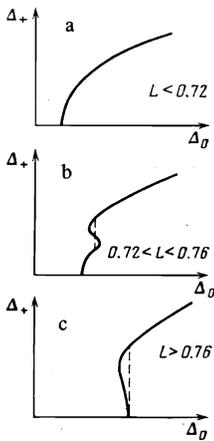


FIG. 3.

$$\Delta_+^2 = \frac{2V_g^2}{\pi/4L-1} \left( \ln \frac{\Delta_0 e}{V_g} - \frac{\pi}{2} L \right). \quad (25)$$

We see therefore directly that  $L = \pi/4$  is a singular point and that the solution of the first type can appear smoothly with increasing  $\Delta_0$  only at  $L < \pi/4$ . The evolution of the solution  $\Delta_+ = \Delta_+(\Delta_0)$  with increasing  $L$  is shown in Fig. 3. (The results of the numerical solution of Eqs. (23) and (24).) It is seen from Fig. 3a that at  $L < 0.72$  the solution  $\Delta_+$  increases monotonically with increasing  $\Delta_0$ . The value of the coupling constant at which a magnetic solution first appeared, as is easily seen from (25) and (22), coincides with the value of  $\Delta_0$  at which the ED appears. On going to the ferromagnetic phase, the gain in energy is given by formula (19):

$$\delta E_F = \delta E_+ \approx - \frac{N(0)\Delta_+^4}{4V_g^2} \left( \frac{\pi}{4L} - 1 \right).$$

The ratio of this quantity to  $\delta E$  for the transition to the ED (17) is equal to

$$\frac{|\delta E_F|}{|\delta E|} = \frac{\pi-2L}{\pi-4L} > 1 \quad (0 < L < 0.72).$$

Consequently, the EF is an energywise more favored phase than ED. We note that since  $\delta E_F$  is proportional to the fourth power of the equilibrium order parameter, the phase transition to the EF state is a second-order transition,<sup>[10]</sup> in contrast to<sup>[5]</sup>, where there was always a first-order transition on the diagonal.

In the case of a doping  $0.72 < L < 0.76$  the solution is shown in Fig. 3b. It is seen from the figure that as  $\Delta_0$  increases we have first a second-order phase transition to an EF, but with further increase of  $\Delta_0$  the gap increases jumpwise. Finally, at  $L > 0.76$ , the solution  $\Delta_+$  immediately appears jumpwise—the transition to the EF becomes of first order (Fig. 3c). With further increase of doping at  $L \approx 0.836$ , the jump of  $\Delta_+$  begins to exceed the chemical potential, and we immediately arrive at a solution of the second type ( $\Delta_+ > \mu$ ,  $\Delta_- = 0$ ). (The solution  $\Delta_- \neq 0$  appears on all the figures in Fig. 3 at larger coupling constants  $\Delta_0$ .)

3. In Sec. 4 we have obtained, by calculating the magnetic susceptibility, the stability line of the ED in the singlet state relative to the appearance of a small triplet

order parameter. The EF state produced on going through this line is described by the system of equations

$$\begin{aligned} x_+ \ln \frac{\gamma e}{V_g} + x_- \ln \delta = x_+ \left[ \frac{1}{2} \ln(1+x_+^2) + \frac{\pi}{2} \frac{\mu}{V_g} - x_+ \operatorname{arctg} x_+ \right], \\ x_- \ln \frac{\gamma e}{V_g} + x_+ \ln \delta = x_- \left[ \frac{1}{2} \ln(1+x_-^2) + \frac{\pi}{2} \frac{\mu}{V_g} - x_- \operatorname{arctg} x_- \right]; \end{aligned} \quad (26)$$

$$\mu/V_g = (L^2 + (x_+^2 + x_-^2)/2)^{1/2}.$$

The region of applicability of this system (i. e., of the employed expressions for  $Y(\Delta_+, \mu)$ , (10)) is bounded by the inequality

$$(x_+^2 - x_-^2)/2 < L^2 < 1 - (x_+^2 - x_-^2)/2.$$

Since the triplet gap produced near the phase-transition line is small ( $\nu = \Delta_+/V_g \ll x_+$ ), this inequality reduces to the limitation  $0 < L < 1$ , and consequently the system (26) describes the EF phase near the boundary of the generation in the entire considered doping region. (Of course, that in this range of variation of the coupling constants  $\Delta_{s0}$  and  $\Delta_{t0}$  in which no jumplike solution takes place.) To assess the question of the type of phase transition on the line (20) and (21) we can find a solution of Eqs. (26) accurate to terms of second order in  $\nu$  and to calculate by means of formula (19) the energy gain on going to the EF. It turns out here that the coefficient of  $\nu^2$  in the expansion of  $\delta E_F$  in powers of  $\nu$  vanishes identically, i. e., the energy gain is proportional to the fourth power of the equilibrium order parameter  $\nu$  in accordance with the Landau theory of second-order phase transitions.<sup>[10]</sup> Consequently, the phase transitions into the EF on the line (20), (21) is of second order. However, as seen from an examination of the solutions on the diagonal and from the subsequent analysis of the system (8), at certain values of  $L$  and of the coupling constants the line (20), (21) can be "preceded" by a curve on which the solution takes place jumpwise, and consequently the phase transition to the EF will be of first order.

4. Let us find on the  $(\Delta_{s0}, \Delta_{t0})$  plane the line, passage through which causes the chemical potential to go out of one of the spin subbands, i. e., where a transition from a solution of the type  $\Delta_+ < \mu$  to a solution of the type  $\Delta_- < \mu < \Delta_+$  takes place. This curve was called the strong-ferromagnetism line in<sup>[5]</sup>. The system of equations for the order parameters  $x_{\pm} = \Delta_{\pm}/V_g$  takes in this case the form

$$\begin{aligned} x_+ \ln(\gamma e/V_g) + x_- \ln \delta = x_+ \left[ \frac{1}{2} \ln(1+x_+^2) + \frac{1}{2} \pi x_+ - x_+ \operatorname{arctg} x_+ \right], \\ x_- \ln(\gamma e/V_g) + x_+ \ln \delta = x_- \left[ \frac{1}{2} \ln(1+x_-^2) + \frac{1}{2} \pi (2L^2 + x_-^2)^{1/2} - x_- \operatorname{arctg} x_- \right]; \end{aligned} \quad (27)$$

here  $\mu/V_g = (2L^2 + x_-^2)^{1/2}$ .

Assuming  $x_+ = \mu/V_g$  and  $x_- = x$ , and subtracting and adding Eqs. (27), we obtain

$$\begin{aligned} \ln \frac{\Delta_{s0} e}{V_g} = \frac{1}{(2L^2 + x^2)^{1/2} \pm x} \left[ \frac{1}{2} (2L^2 + x^2)^{1/2} \ln(1+2L^2+x^2) \pm \frac{1}{2} x \ln(1+x^2) \right. \\ \left. + \frac{1}{2} \pi (2L^2 + x^2 \pm x(2L^2 + x^2)^{1/2}) \mp (2L^2 + x^2) \operatorname{arctg} x \right], \end{aligned} \quad (28)$$

where the upper or lower sign in the right-hand side corresponds to  $\Delta_{s0}$  or  $\Delta_{t0}$ , respectively. Equations (28)

specify parametrically the strong-ferromagnetism curve on the  $(\Delta_{s0}, \Delta_{t0})$  plane.

The system (27), however, is valid when  $\mu^2 < V_F^2 + \Delta_-^2$  or  $L^2 < \frac{1}{2}$ . At larger values of the doping it should be replaced by the following system of equations (the case  $\Delta_-^2 + V_F^2 < \mu^2 < \Delta_+^2$ ):

$$x_+ \ln(\gamma e/V_F) + x_- \ln \delta = x_+ [1/2 \ln(1+x_+) + 1/2 \pi x_+ - x_+ \arctg x_+], \quad (29)$$

$$x_- \ln(\gamma e/V_F) + x_+ \ln \delta = x_- \left\{ \ln[(L_1^2 + x_-^2)^{1/2} + (L_1^2 - 1)^{1/2}] + (L_1^2 + x_-^2)^{1/2} \arctg(L_1^2 - 1)^{-1/2} - x_- \arctg \left[ \frac{x_-}{L_1^2 + [(L_1^2 + x_-^2)(2L_1^2 - 1)]^{1/2}} \right] \right\},$$

where the chemical potential is determined by the relation  $\mu^2/V_F^2 = L_1^2 + x_-^2$ , while the quantity  $L_1$  is connected with the doping (which we measure as before in units of  $L$ ) by the equation

$$L^2 = 1/2 L_1^2 + \pi^{-1} [(L_1^2 - 1)^{1/2} - L_1^2 \arctg(L_1^2 - 1)^{1/2}].$$

In analogy with (28), we easily obtain from (29) the specified equations for the strong-ferromagnetism curves at  $L^2 > \frac{1}{2}$ . The strong-ferromagnetism lines for different values of the doping are shown dashed in Fig. 2.

We note first that for sufficiently small doping ( $L < 0.76$ ) the strong and weak ferromagnetism curves come closer together with increasing distance from the diagonal. This means that even though the order parameter increases continuously with increasing coupling constant, as the distance from the diagonal increases it reaches the value  $\mu$  all the more rapidly. If the doping is larger ( $L > 0.76$ ), the strong and weak ferromagnetism lines diverge with increasing distance from the diagonal (just as in<sup>[5]</sup>) and this situation no longer takes place.

The dash-dot line in Fig. 2 shows the line on which the order parameter experiences a jump (Figs. 3b and 3c). It is clear that this line should pass in analogy with the strong-ferromagnetism curve, but to determine it exactly it is necessary to have detailed numerical calculations. It is seen from Fig. 2 that in the case  $L > 0.76$  a part of the ED-EF phase-transition line adjacent to the diagonal corresponds to a first order transition (I) and the remainder to a second order transition (II). At  $L > 0.836$  in the region near the diagonal, the strong-ferromagnetism curve already "overtakes" the weak-ferromagnetism curve.

## 6. DISCUSSION

In the EF mode that does not take hybridization into account<sup>[4,5]</sup> the transition to the ferromagnetic state is possible at arbitrarily weak interelectron interaction and is a second-order phase transition in the entire range of variation of the singlet  $\Delta_{s0}$  and triplet  $\Delta_{t0}$  coupling constants. An exception is only the case  $\Delta_{s0} = \Delta_{t0}$ , when the transition to the EF is of first order.

Allowance for the hybridization makes the phase transition to the EF possible only at coupling constants comparable with the hybridization matrix element  $V_F$ , in analogy with the well known results.<sup>[6,7]</sup> In addition, it

turns out that the order of the transition is determined by the value of the doping and by the ratio of the singlet and triplet coupling constants. In the case of sufficiently small doping ( $L < 0.76$ ), the transition to the EF is of second order in the entire range of variation of  $\Delta_{s0}$  and  $\Delta_{t0}$ , including also on the diagonal ( $\Delta_{s0} = \Delta_{t0}$ ). In the doping interval  $0.72 < L < 0.76$  in the region of  $\Delta_{s0}$  and  $\Delta_{t0}$  adjacent to the diagonal, there are jumps of the order parameter in the EF phase with increasing coupling constant. At larger doping ( $L > 0.76$ ) there is produced near the diagonal an entire region of  $\Delta_{s0}$  and  $\Delta_{t0}$  in which the phase transition to the EF is of first order.

Although an interaction of the type  $(\hbar/m_0)\mathbf{P} \cdot \mathbf{q} a_{1\alpha}^*(\mathbf{q}) a_{2\alpha}(\mathbf{q})$ , corresponding to hybridization, induces anomalous mean values of only the singlet type  $\langle a_{1\alpha}^* a_{2\alpha} \rangle$ , yet owing to the angular dependence of the matrix elements it does not violate the symmetry of the singlet and triplet pairings and it does not lead to their coexistence in a system without doping. Thus, all the lines of Fig. 2 can be continued symmetrically relative to the diagonal. Analogously,<sup>[4,5]</sup> the ferromagnetic state appears only in a system with doping and, just as in<sup>[4,5]</sup>, the order parameter (magnetization) decreases with further increase of doping and vanishes at a certain value of  $L$ . Now, however, the contribution of the doping to the suppression of the excitonic instability is proportional not to  $\mu_0/\Delta_0$  ( $\mu_0$  is the chemical potential in the initial semimetallic phase and  $\Delta_0$  is the coupling constant), but to  $\mu_0/V_F$ .

An interpretation of the experiments with narrow-band semiconductors,<sup>[12]</sup> in which a similar behavior of the magnetization was observed, and also of other investigations of magnetic properties of semiconductors,<sup>[13]</sup> was presented in<sup>[4,5]</sup>. It is obvious that the arguments advanced there remain valid also for the considered model of the EF with allowance for hybridization, which is in qualitative agreement with these experiments. For a quantitative comparison of the theory with the experimental results for semiconductors of the  $A_4B_6$  group, however, it is necessary to take into account the spin-orbit interaction, which is quite large in these semiconductors.

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# Susceptibility of inhomogeneous quasi-one-dimensional Fermi systems with repulsion

K. B. Efetov

L. D. Landau Theoretical Physics Institute, USSR Academy of Sciences

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Quasi-one-dimensional Fermi systems with repulsion are considered. The effect of impurities is studied in those cases in which these structures are one-dimensional antiferromagnets. It is found that the impurities lead to a logarithmic or fractional-power increase in the susceptibility at low temperatures. The power in the temperature dependence of the susceptibility does not depend on the impurities and is determined by the interaction between the electrons. It is shown that phase transitions that do not alter the one-dimensional character of the spin interactions or impede this increase in the susceptibility are possible.

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## 1. INTRODUCTION

At the present time there is no doubt that many of the highly conducting quasi-one-dimensional complexes of TCNQ are metals at high temperatures. The question of the state of these substances at low temperatures is, however, more complicated. One of the possible states is the antiferromagnetic state which can arise if the conduction electrons form a Fermi system with repulsion. Such systems have been studied previously in a particular case in the Hubbard model.<sup>[1-3]</sup> At low temperatures the magnetic susceptibility remains finite and the specific heat depends linearly on the temperature. In this work it is shown that the defects that can be present in the system strongly affect the magnetic properties and make possible a logarithmic or power increase of the susceptibility as the temperature is lowered. The temperature dependence of the specific heat remains linear.

The interaction of electrons from different strands does not alter the behavior of the susceptibility at low temperatures, even though it can lead to a phase transition at finite temperatures. Hopping from strand to strand can have a substantial influence.

## 2. INFLUENCE OF INHOMOGENEITIES ON THE SPIN CORRELATION FUNCTIONS

We shall consider a system of parallel conducting strands. We assume that the probability of electron hops from strand to strand is small. We also assume that the interaction of electrons from different strands is small. There are reasons to believe that even strong

interaction of electrons from different strands, which can lead to a phase transition, has little effect on the spin correlation functions. However, we shall speak of this later. In this section we assume the strands to be isolated. We write the Hamiltonian of one strand in the form

$$\hat{H} = - \sum_{i,j} T_{ij}^{\alpha,\alpha'} a_{i\alpha}^+ a_{j\alpha'} + \frac{1}{2} \sum_{i,j,\alpha,\alpha'} V_{ij} a_{i\alpha}^+ a_{j\alpha'}^+ a_{j\alpha} a_{i\alpha} - \mu \sum_{i,\alpha} a_{i\alpha}^+ a_{i\alpha} - H \sum_i S_i, \quad (1)$$

where  $a_{i\alpha}^+$  ( $a_{i\alpha}$ ) are the creation (annihilation) operators for electrons with spin  $\alpha$  at site  $i$ ,  $T_{ij}^{\alpha,\alpha'}$  are the overlap integrals,  $\mu$  is the chemical potential, and

$$S = \sum_{\alpha,\beta} \sigma_{\alpha\beta} a_{\alpha}^+ a_{\beta}, \quad (2)$$

where  $\sigma$  is the vector whose components are the Pauli matrices.

The impurities lead to the result that the quantities  $T_{ij}$  and  $V_{ij}$  do not depend only on the difference  $i-j$ , and also to the fact that the transition amplitude  $T_{ij}^{\alpha,\alpha'}$  is a matrix.

We shall assume that the parameters of the Hamiltonian (1) are such that in the absence of impurities the system is a one-dimensional antiferromagnet. Such a case occurs in, e.g., the Hubbard model with a half-filled band.<sup>[1]</sup> The model considered by Ovchinnikov,<sup>[4]</sup> with a quarter-filled band and sufficiently strong non-local repulsion, also describes a one-dimensional antiferromagnet. In the absence of impurities the susceptibility of such systems remains finite. Below we shall