Inhomogeneous state of excitonic ferromagnet

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(Submitted 15 March 1978)
Zh. Eksp. Teor. Fiz. **75**, 735–747 (August 1978)

Magnetic ordering of band electrons in systems that are unstable to electron-hole pairing is considered. In a doped excitonic dielectric the spatial period of the order parameter is not commensurate with the crystal-lattice period. The phase diagram is plotted and the line of transition from the inhomogeneous (noncommensurate) state of the excitonic dielectric into an inhomogeneous state of an excitonic ferromagnet is determined. In the ferromagnetic phase the system breaks up into domains whose dimensions depend on the impurity concentration. In nonequilibrium systems such as a pumped excitonic dielectric, a magnetic state with long-wave modulation of the order parameter can also set in, but the phase diagram differs substantially from the equilibrium case. The region of inhomogeneous solutions on the phase diagrams is wider than that of homogeneous ones for both equilibrium and nonequilibrium systems.

PACS numbers: 75.60.Ch, 75.30.Kz, 75.30.Hx, 71.35. + z

§1. INTRODUCTION

It is well known that in systems with electron-hole pairing, at a definite ratio of the singlet and triplet coupling constants, a charge-density wave (CDW) can coexist with a spin-density wave (SDW).[1] In a metal–dielectric phase transition, the structure distortions are due to the charge-density wave and the antiferromagnetic properties to the spin-density wave; ferromagnetism sets in when the CDS and SDW coexist. The order parameter is in this case a two-component quantity

$$\hat{\Delta}=\Delta_s+\Delta_t\sigma, \tag{1}$$

where σ is a vector made up of Pauli matrices, while Δ_s and Δ_t are the singlet and triplet order parameters. In the equilibrium case[1] the existence of Δ_s and Δ_t leads to the appearance of spontaneous magnetization, whereas in nonequilibrium systems the simultaneous presence of the singlet and triplet order parameters may, generally speaking, not lead to the appearance of magnetization.[2]

All the investigations of two-band equilibrium systems in which CDW and SDW can coexist[1] were made under the assumption that the order parameters Δ_s and Δ_t are periodic and have either the period of the crystal lattice (if the initial electron spectrum was of the form $\varepsilon_1(\mathbf{p}) = -\varepsilon_2(\mathbf{p})$, or with double this period (if $\varepsilon_1(\mathbf{p}) = -\varepsilon_2(\mathbf{p}+\mathbf{w})$, where $\mathbf{w}$ is half the reciprocal-lattice vector of the crystal). It is known,[3] however, that even in system with one type of pairing (singlet or triplet), in a definite range of temperatures, electron and hole density differences, and interaction constants, the solution energy-wise more favored is the one for an order parameter whose period is not commensurate with the lattice period. If the extrema of the energy bands coincide in momentum space, an additional long-wave modulation with period $\sim(nv_F)^{-1}$ is superimposed on the variation of Δ_s and Δ_t with the period of the crystal structure $(2w)^{-1}$. If the band extrema are separated in momentum space by a vector $\mathbf{w}$, then the period of the system will be doubled, and superimposed on it is also a long-wave modulation with period $\sim(nv_F)^{-1}$, where n is the difference of the concentrations of the electrons and holes in energy units, and v_F is the velocity on the Fermi surface.

The conclusion drawn in Ref. 1 that the dielectric phase (the excitonic-insulator phase) is unstable to a transition into a ferromagnetic phase was based on a calculation of the paramagnetic susceptibility of a commensurate (subsequently also called homogeneous) dielectric phase. It will be shown here that the results of Ref. 1 remain valid in the phase diagram region ($\Delta_{s0}, \Delta_{t0} \gg 2n$), where the influence of the long-wave modulation is small (Δ_{s0} and Δ_{t0} are the singlet and triplet order parameters in the absence of doping). The conclusion that regions where CDW and SDW coexist remains in force also for that part of the phase diagram in which the noncommensurability (inhomogeneity) of the order parameter is substantial and the results of Ref. 1 do not hold.

Besides a doped equilibrium system, we consider here a nonequilibrium system of the pumped excitonic-dielectric type,[4] in which solutions with long-wave modulation can likewise be more favored in the case of one type of pairing than unmodulated ones. Just as in the equilibrium case, the region of existence of noncommensurate (inhomogeneous) solutions for Δ_s and Δ_t turns out to be wider than that for homogeneous ones. For the phase-diagram points $\Delta_{s0}, \Delta_{t0} \gg 5, 5n$) all the results of Ref. 2 remain valid, since the influence of the long-wave modulation in this region is small, but the conclusion that Δ_s and Δ_t coexist extends over a wider region of the diagram than in the homogeneous case.[2]

The problem of magnetic ordering with long-wave modulation, in the case of a single-mode laser regime, is also considered in the present paper. It is mathematically similar to the problem of magnetic ordering in an equilibrium system. It must be recognized, however, that in the laser regime the spatial long-wave modulation of the order parameters is determined not from the condition that the free energy be a minimum, as in the equilibrium system, but by external conditions (e.g., the choice of the resonator parameters). Allowance for this circumstance does not change qualita-

 0038-5646/78/080371-07$02.40

tively the phase diagram, although the very fact of pairing in a state with nonzero frequency can lead in the case of weak damping to instability of the system to a transition into a multimode regime.[5]

§2. MAGNETIC ORDERING WITH NONCOMMENSURATE PERIOD IN A DOPED EXCITONIC DIELECTRIC

Consider an isotropic semimetal having one electron and one hole Fermi surface, both centered at a single point of the Brillouin zone. To investigate the transition of such a system into an inhomogeneous magnetic system we used the Hamiltonian of Ref. 1, in which we retain only the terms that determine the instability of the semimetal to the formation of CDW and SDW. We shall treat the problem hereafter in the high-density approximation ($e^2/\hbar v_F \gg 1$, where e is the electron charge and v_F is its Fermi velocity), so that all the interaction potentials in the Hamiltonian of the problem will be regarded as constants independent of the momentum.

We analyze the system with the aid of the Green's functions

$$G_{ij}^{\alpha\beta}(\mathbf{r}, \mathbf{r}', t, t') = -i\langle T\psi_{i\alpha}(\mathbf{r}, t)\psi_{j\beta}^{+}(\mathbf{r}', t')\rangle, \tag{2}$$

$$F_{ij}^{\alpha\beta}(\mathbf{r}, \mathbf{r}', t, t') = -i\langle T\psi_{i\alpha}(\mathbf{r}, t)\psi_{j\beta}^{+}(\mathbf{r}', t')\rangle, \quad i\neq j. \tag{3}$$

Here i and j are the band indices; α and β are the spin indices; $\psi_{i\alpha}$ and $\psi_{i\alpha}^{+}$ are the electron annihilation and creation operators. For the functions (2) and (3) we can obtain the system of equations

$$\left(i\frac{\partial}{\partial t}+\frac{\nabla_r^2}{2m}+\varepsilon_F\right)G_{11}^{\pm}(\mathbf{r}, \mathbf{r}', t, t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t')+\Delta_{\pm}(\mathbf{r})F_{21}^{\pm}(\mathbf{r}, \mathbf{r}', t, t'),$$
$$\left(i\frac{\partial}{\partial t}-\frac{\nabla_r^2}{2m}-\varepsilon_F\right)F_{21}^{\pm}(\mathbf{r}, \mathbf{r}', t, t') = \Delta_{\pm}^{*}(\mathbf{r})G_{11}^{\pm}(\mathbf{r}, \mathbf{r}', t, t'). \tag{4}$$

The ± index in (4) denotes the spin projection on the z axis in the so-called z-representation,[1] in which the vector Δ_t is directed along the z axis. In accord with (1), in this representation $\hat{\Delta}$ becomes a diagonal matrix with components Δ_+ and Δ_-:

$$\Delta_{\pm}(\mathbf{r}) = \Delta_s(\mathbf{r}) \pm \Delta_t(\mathbf{r}). \tag{5}$$

We investigate the system at a given difference between the electron and hole densities, as was done in Ref. 1 for the homogeneous case. We express the electro-neutrality condition in the form

$$N = \int [G_{11}^{+}(\omega, \mathbf{r}, \mathbf{r}) + G_{11}^{-}(\omega, \mathbf{r}, \mathbf{r}) - G_{22}^{+}(\omega, \mathbf{r}, \mathbf{r}) - G_{22}^{-}(\omega, \mathbf{r}\,\mathbf{r})]\frac{d\omega\, d\mathbf{r}}{4\pi}, \tag{6}$$

where N is the concentration of the doping impurity. We shall need later the difference between the electron and hole densities in energy units, $n = N/4N(0)$, where $N(0)$ is the state density on the Fermi level.

A. Solution when the phase of the order parameter is not fixed

Assume that the Hamiltonian of the system does not contain terms that fix the phase of the order parameter. In this case the self-consistency equations take the form

$$\Delta_s(\mathbf{r}) = \frac{-ig_s}{4\pi}\int [F_{21}^{+}(\omega, \mathbf{r}, \mathbf{r}) + F_{21}^{-}(\omega, \mathbf{r}, \mathbf{r})]\, d\omega,$$
$$\Delta_t(\mathbf{r}) = \frac{-ig_t}{4\pi}\int [F_{21}^{+}(\omega, \mathbf{r}, \mathbf{r}) - F_{21}^{-}(\omega, \mathbf{r}, \mathbf{r})]\, d\omega, \tag{7}$$

where g_s and g_t are the singlet and triplet coupling constants. The simplest solution of the system (7), with allowance for (4), will be sought in the form

$$\Delta_{\pm}(\mathbf{r}) = \Delta_{\pm}\exp(i2\mathbf{q}\mathbf{r}), \tag{8}$$

where $\Delta_{\pm}$ and $\mathbf{q}$ are quantities to be determined. Although the solution (8) is, strictly speaking, valid only if the order-parameter phase is not fixed, it nevertheless makes it possible to answer, at least qualitatively (and even quantitatively, with not too large an error at small $\Delta_{\pm}$) the question of the behavior of the line of the phase-transition into the magnetic state for more realistic models.

In the homogeneous case $\mathbf{q}=0$ (Ref. 1) it is possible to find analytically the line of transition into the ferromagnetic state on the $(\Delta_{s0}, \Delta_{t0})$ phase diagram. This line determines the boundary of the region in which nontrivial solutions of the system (7), $\Delta_s \neq 0$ and $\Delta_t \neq 0$, can coexist. In the inhomogeneous case, i.e., at $\mathbf{q}\neq 0$, it is impossible to obtain an analytic solution for the transition line, and we therefore perform a numerical calculation for the case of one order parameter, and then determine on the phase diagram the stability limit of the obtained solution. The information contained in Ref. 3 on the behavior of the system in the case of one order parameter is insufficient for our purposes, since Ref. 3 gives only the function $\Delta(n)$, but not $q(n)$ and $\mu(n)$ (μ is the chemical-potential shift due to doping). The system (7) for the order parameters can be reduced to the form

$$\frac{2\Delta_s}{g_s N(0)} = \Delta_+\left\{\ln\frac{\tilde{\omega}}{\Delta_+} - \frac{\Delta_+}{2Q}[G(r_+^{+}) - G(r_-^{+})]\right\}$$
$$+\Delta_-\left\{\ln\frac{\tilde{\omega}}{|\Delta_-|} - \frac{\Delta_-}{2Q}[G(r_+^{-}) - G(r_-^{-})]\right\}, \tag{9}$$
$$\frac{2\Delta_t}{g_t N(0)} = \Delta_+\left\{\ln\frac{\tilde{\omega}}{\Delta_+} - \frac{\Delta_+}{2Q}[G(r_+^{+}) - G(r_-^{+})]\right\}$$
$$-\Delta_-\left\{\ln\frac{\tilde{\omega}}{|\Delta_-|} - \frac{\Delta_-}{2Q}[G(r_+^{-}) - G(r_-^{-})]\right\};$$
$$r_{\pm}^{+} = (\mu \pm Q)/\Delta_+, \quad r_{\pm}^{-} = (\mu \pm Q)/\Delta_-, \quad Q = v_F q,$$
$$G(r) = \Theta(|r|-1)\operatorname{sign} r\cdot\{|r|\operatorname{Arch}|r| - (r^2-1)^{1/2}\}. \tag{10}$$

The electroneutrality condition (6) reduces to

$$2n = \frac{\Delta_+^2}{4Q}[\gamma(r_+^{+}) - \gamma(r_-^{+})] + \frac{\Delta_-^2}{4Q}[\gamma(r_+^{-}) - \gamma(r_-^{-})], \tag{11}$$

where

$$\gamma(r) = \Theta(|r|-1)\operatorname{sign} r\cdot\{|r|(r^2-1)^{1/2} - \operatorname{Arch}|r|\}. \tag{12}$$

A numerical solution of the system (9)–(12) for the case $\Delta_+ = |\Delta_-| = \Delta$ is shown in Fig. 1 (curves 1, 2, and 3 show $\Delta(n)$, $\mu(n)$, and $Q(n)$, respectively). The value of Q was chosen to minimize the free energy, as was done in Ref. 3.

To find the line of the second-order phase transition from the excitonic-dielectric state into the excitonic ferromagnet state, we expand the system (9)–(12) in powers of Δ_t up to the quadratic terms (we assume that in the initial phase there existed only singlet pairing, and $\Delta_t = 0$; all the results for the case of an initial phase with triplet pairing are obtained by making the substitutions $\Delta_{s0} \rightleftarrows \Delta_{t0}$, $\Delta_s \rightleftarrows \Delta_t$). After cumbersome calculations, we obtain the following equation for the $\Delta_t = 0$ line on the $(\Delta_{s0}, \Delta_{t0})$ diagram.

At $\mu_- > \Delta_s$:

$$\ln\frac{\Delta_{s0}}{\Delta_{t0}} = \frac{\Delta_s^2}{2Q}\{[\mu_- + (\mu_-^2 - \Delta_s^2)^{1/2}]^{-1} - [\mu_+ + (\mu_+^2 - \Delta_s^2)^{1/2}]^{-1}\}. \tag{13}$$

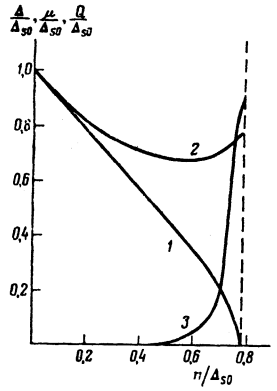

FIG. 1.

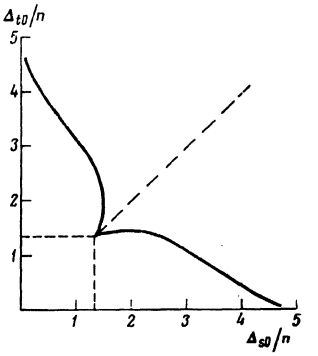

FIG. 2.

At $|\mu_-| > \Delta_s$, $\mu_- < 0$:

$$\ln\frac{\Delta_{s0}}{\Delta_{t0}} = -\frac{\Delta_s^2}{2Q}\{[|\mu_-|+(\mu_-^2-\Delta_s^2)^{1/2}]^{-1}+[\mu_++(\mu_+^2-\Delta_s^2)^{1/2}]^{-1}\}. \quad (14)$$

At $|\mu_-| < \Delta_s$:

$$\ln\frac{\Delta_{s0}}{\Delta_{t0}} = \frac{\Delta_s^2}{2Q}\left\{\frac{\mu_-}{\Delta_s^2}-[\mu_++(\mu_+^2-\Delta_s^2)^{1/2}]^{-1}\right\}. \quad (15)$$

It is seen from Fig. 1 that at $\Delta_{s0} \to 1.324n$ we have $\Delta_s \to 0$, $\mu \to n$, $Q \to 1.2n$, i.e., $\mu_- < 0$, which corresponds to Eq. (14). The coupling-constant region in which the magnetic transition-line lies, as seen from (14) is characterized by the relation $\Delta_{s0} < \Delta_{t0}$. As shown in Ref. 6, for a semimetal with equal electron and hole densities ($n = 0$) this result is unphysical, for a growth of Δ_{t0} in the coexistence region would lead in this case to a physically meaningless decrease of Δ_t. Thus, as $\Delta_s \to 0$ the system (9)–(12) has no magnetic solutions, in contrast to the commensurate case.[1] The reason is that although the absolute magnitude of the gap $|\Delta(\mathbf{r})|$ is a homogeneous and isotropic quantity, the energy spectrum of the system in the inhomogeneous state of the excitonic dielectric is anisotropic:

$$\omega_{1,2} = v_F q \pm (\xi^2+\Delta_s^2)^{1/2}, \quad \xi = p^2/2m - \varepsilon_F. \quad (16)$$

As a result of this anisotropy, the chemical potential μ at q larger than a certain value lies in the conduction band of the excitonic dielectric for some directions of the momentum $\mathbf{p}$, whereas for other directions it lies either inside the gap or even in the valence band, i.e., a partial redistribution of the electrons among the bands takes place in the system. With increasing Δ_s, the band "overlap" effect decreases and at $\mu \gtrsim Q$, as seen from (15), a line of transition into the magnetic phase appears. On the $(\Delta_{s0}, \Delta_{t0})$ diagram (Fig. 2) this corresponds to $\Delta_{s0} \approx 1.333n$. Finally, with even further increase of Δ_s, the relation $\mu_- > \Delta_s$ begins to be satisfied, $Q \to 0$, and to find the transition line we must use Eq. (13). It is easy to show that as $Q \to 0$ Eq. (13) reduces to

$$\ln\frac{\Delta_{s0}}{\Delta_{t0}} = \Delta_s^2(\mu^2-\Delta_s^2)^{-1/2}[\mu+(\mu^2-\Delta_s^2)^{1/2}]^{-1}. \quad (17)$$

Recognizing that as $Q \to 0$ we have in the case of one type of pairing

$$\mu^2-\Delta_s^2 = n^2, \quad \Delta_s^2 = \Delta_{s0}(\Delta_{s0}-2n), \quad (18)$$

we can obtain for the line of transition into the magnetic phase as $Q \to 0$ the asymptotic expression

$$\Delta_{t0} = \Delta_{s0}\exp(2-\Delta_{s0}/n), \quad (19)$$

which coincides, as it should, with the result of Ref. 1.

We have so far regarded the difference n between the electron and hole densities as specified. Inequality of these densities can be due either to doping or to the presence of some Fermi-surface sections that act as reservoirs of electrons and holes. In the latter case, a fixed n corresponds to a zero capacity of the reservoir. We can consider also another limiting case, a reservoir of infinite capacity, which in our problem corresponds to fixed chemical potential μ. It was shown earlier[1] that in the homogeneous case no ferromagnetic solution is realized at fixed μ, since a more profitable nonmagnetic solution exists. To analyze the system in the presence of long-wave modulation we have used the numerical results of Fulde and Ferrell,[7] who investigated mathematically an analogous problem of the inhomogeneous state of a superconductor in an exchange field. At $1.324\ \mu < \Delta_{s0} < \mu\sqrt{2}$ the magnetic transition lines lies in the region $\Delta_{t0} > \Delta_{s0}$, i.e., the result is unphysical, as already mentioned above. At $\Delta_{s0} > \mu\sqrt{2}$ a first-order phase transition takes place into a homogeneous state with $\Delta_s = \Delta_{s0}$ in which, as already mentioned, no magnetic solution is realized. Thus, at fixed μ there is no region of magnetic solutions on the phase diagram. We emphasize that all the foregoing is valid if the Fermi surfaces have the same shape. On the other hand, if the Fermi surfaces have individual non-coincident sections, then a region of magnetic solutions will apparently be present on the diagram at a finite reservoir capacity.

B. Solution at fixed phase of order parameter

As already mentioned, a solution in the form (8) is incorrect for a doped excitonic dielectric, since the Hamiltonian of the system contains terms that fix the phase of the order parameter. We consider now the case when the order parameters are real (we assume that imaginary order parameters correspond to a state that is energywise less favored, an assumption correct at certain values of the interaction constant[1]). The solution must be sought in the form of a superposition of solutions of the type (8):

$$\Delta_{s,t}(\mathbf{r}) = \Delta_{s,t}\exp(2i\mathbf{qr}) + \Delta_{s,t}^*\exp(-2i\mathbf{qr}). \quad (20)$$

In this case it is impossible to obtain an equation in closed form for the order parameters Δ_s and Δ_t, since

Eq. (20) is, strictly speaking, not an exact solution. At small Δ_s and Δ_t, however, a representation in the form (20) is valid and the problem can be solved by perturbation theory. To this end, we represent the function $F_{21}^{\pm}(\mathbf{r}, \mathbf{r}', t, t')$ in the form

$$F_{21}^{\pm}(\mathbf{r}, \mathbf{r}', t, t') = F_{\mathbf{q}, 21}^{\pm}(\mathbf{r}-\mathbf{r}', t, t')\exp[-i\mathbf{q}(\mathbf{r}+\mathbf{r}')] + F_{-\mathbf{q}, 21}^{\pm}(\mathbf{r}-\mathbf{r}', t, t')\exp[i\mathbf{q}(\mathbf{r}+\mathbf{r}')]. \quad (21)$$

Substituting (21) and (20) in (4) and discarding the higher harmonics, we can obtain the following system of equations for the Fourier components of the Green's functions (2) and (3):

$$\begin{aligned}(\omega-\xi)G_{11}^{\pm} &= 1+\Delta_{\pm}F_{\mathbf{q}, 21}^{\pm}(\omega, \mathbf{p}-\mathbf{q})+\Delta_{\pm}^{*}F_{-\mathbf{q}, 21}^{\pm}(\omega, \mathbf{p}+\mathbf{q}),\\ (\omega+\xi-\mathbf{v}_F\mathbf{q})F_{\mathbf{q}, 21}^{\pm}(\omega, \mathbf{p}) &= \Delta_{\pm}^{*}G_{11}^{\pm}(\omega, \mathbf{p}+\mathbf{q}),\\ (\omega+\xi+\mathbf{v}_F\mathbf{q})F_{-\mathbf{q}, 21}^{\pm}(\omega, \mathbf{p}) &= \Delta_{\pm}G_{11}^{\pm}(\omega, \mathbf{p}-\mathbf{q}).\end{aligned} \quad (22)$$

A similar system of equations can be obtained for the functions $G_{22}^{\pm}$ and $F_{12}^{\pm}$.

The system of equations for the order parameter will take the following form:

$$\Delta_s = -\frac{ig_s}{2}[\Delta_+ I_+ + \Delta_- I_-], \quad \Delta_t = -i\frac{g_t}{2}[\Delta_+ I_+ - \Delta_- I_-], \quad (23)$$

where

$$I_{\pm} = \int \frac{d\omega\, d\mathbf{p}}{(2\pi)^4} \frac{\omega+\xi+2\mathbf{v}_F\mathbf{q}}{(\omega-\xi)(\omega+\xi+2\mathbf{v}_F\mathbf{q})(\omega+\xi-2\mathbf{v}_F\mathbf{q})-2|\Delta_{\pm}|^2}. \quad (24)$$

The system (23)–(24) is valid at $|\Delta_{\pm}| \ll v_F q$, for it is precisely in this case that the higher harmonics that are multiples of q can be discarded. Therefore as $q \to 0$, in contrast to (9), the solution (23) will not coincide with the solution in the commensurate case $q = 0$. The representation of the Green's function in the form (21) makes it possible to take into account the change that occurs in the spectrum of the system as a result of the appearance of the order parameter. In fact, at small Δ we expand in the perturbation-theory series not the Green's functions of Eqs. (22), but the mass operator. In the investigated case this is extremely important, since the magnetic state is the result of just the spin splitting of the bands. It can be shown that a formal expansion of the Green's functions in the usual perturbation-theory series leads to impossibility of a ferromagnetic state even in the homogeneous case, but this contradicts the result of Ref. 1.

The determination of the magnetic solutions of the system (23)–(24) is an even more complicated problem than in the case (9). We consider therefore the nonmagnetic solution $\Delta_+ = |\Delta_-| = \Delta_s$. It can be shown that at $v_F q \gg \Delta_s$ we have

$$\Delta_s^2 \approx 1{,}5\Delta_{s0}(\Delta_{s0} - 1.324n). \quad (25)$$

For comparison we note that the solution of the system (9) at $\Delta_+ = |\Delta_-| = \Delta_s$ and $\Delta_s \ll v_F q$ is of the form

$$\Delta_s^2 \approx \Delta_{s0}(\Delta_{s0} - 1.324n). \quad (26)$$

Comparison of solutions (25) and (26) shows that (25) is favored. As to the line of the transition to the magnetic state, at small Δ_s the difference between (25) and (26) is insignificant, and the analysis of Sec. A remains in force.

In contrast to the exponential solution (8), in which the modulus of the order parameter remains a homogeneous and isotropic quantity, when the solution takes the form (20) the modulus of the order parameter varies in space. This means that the distribution of the electron density is also spatially inhomogeneous and the system breaks up into domains. We assume that in the case of doping the positive charge of the ions is uniformly distributed, so that the fluctuations of the electron density disturb the local electroneutrality. The resultant electric fields prevents inhomogeneous distribution of the electrons, so that at a certain value of Δ and at $q_{\min} \ll \Delta/v_F$ the noncommensurate of the system becomes energywise unprofitable. With further increase of Δ (or decrease of n) a phase transition takes place from an inhomogeneous to a homogeneous state. There exists thus a mechanism that limits the domain growth and is due to violation of the local electroneurality of the system. The region of existence of inhomogeneous magnetic solution will be bounded out at lower and higher impurity concentrations.

C. Energy spectrum at a fixed order-parameter phase

The analysis of the spectrum of single-particle excitations in a noncommensurate state of an excitonic dielectric leads, in the case when the order-parameter phase is not fixed, to relation (16). At a fixed phase of (20), when it is impossible to obtain an equation in closed form for the Green's functions and the order parameter, the energy spectrum can be determined by a somewhat different method. We introduce the effective Hamiltonian of the system

$$H = H_0\sigma_z + \Delta(\mathbf{r})\sigma_x, \quad (27)$$

where $H_0 = -\nabla_r^2/2m - \varepsilon_F$; σ_z and σ_x are Pauli matrices. We write the wave function of the system in spinor form:

$$\Psi(\mathbf{r}) = \begin{pmatrix}\Psi_1(\mathbf{r})\\ \Psi_2(\mathbf{r})\end{pmatrix}, \quad (28)$$

where the subscripts 1 and 2 pertain to the conduction and valence bands of the excitonic dielectric, respectively. For the wave function (28) we can write the effective Schrödinger equation

$$(H_0\sigma_z + \Delta(\mathbf{r})\sigma_x)\Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \quad (29)$$

An equation similar to (29) was used in Ref. 5 to investigate the inhomogeneous state of a Peierls dielectric, and in Ref. 9 to find the excitation spectrum of the electrons of a semiconductor in the field of a standing electromagnetic wave.

We are interested in the form of the energy spectrum near the Fermi surface, so that (29) with $|\mathbf{p}| \approx p_F$ can be simplified (p_F is the Fermi momentum). Recognizing furthermore that Δ is given by (20) and choosing the z axis of the system in the direction of the vector $\mathbf{q}$, we easily obtain

$$\begin{aligned}\left(-iv_z\frac{\partial}{\partial z}+\xi\right)\varphi_1 + \varphi_2\Delta\cos 2qz &= E\varphi_1,\\ \left(iv_z\frac{\partial}{\partial z}-\xi\right)\varphi_2 + \varphi_1\Delta\cos 2qz &= E\varphi_2,\end{aligned} \quad (30)$$

where v_z is the projection of v_F on the z axis, $\xi = p^2/2m - \varepsilon_F$, while φ_1 and φ_2 are the slowly varying parts of the wave function

$$\Psi_{1,2} = \exp(i\mathbf{pr})\varphi_{1,2}(\mathbf{r}). \quad (31)$$

A system similar to (30) was solved in Refs. 8 and 9.

We present therefore only the final results of the solution.

At $\Delta \ll v_F q$ the system (30) can be solved by the weak-coupling method. The energy spectrum acquires at $\xi = \pm 2 v_x q$ a gap of magnitude 2Δ. In addition, microgaps with size on the order of $\Delta^2/v_F q$ appear in the spectrum at $\xi = 2 v_x q n (n = 0, \pm 2)$. We note that these results can be obtained also from an analysis of the system (22) for the Green's functions.

At $\Delta \gg v_F q$ Eq. (30) is solved by the tight-binding method for $|\xi| \ll \Delta$. The energy spectrum breaks up into sets of allowed and forbidden minibands. The positions of the midpoints of the allowed bands is given by

$$E_n = (2\Delta q v_x n)^{1/2} (E_n^2 \ll \Delta^2, \quad n = 0, 1, 2 \ldots). \tag{32}$$

The width of the allowed bands is exponentially small at small E_n and is of the order of $(v_x q \Delta)^{1/2} \exp(-\Delta/v_x q)$. With increasing n the width of the allowed bands increases, and the width of the forbidden bands decreases. At $|\xi| \gg \Delta$ the spectrum becomes continuous ($E \approx \xi$).

In accord with the statements made in Sec. B, the case $\Delta \gg v_F q$ can be realized at $q > q_{\min}$ in a bounded region of q. Although the relation $\Delta(\mathbf{r}) = \Delta \cos \mathbf{q} \cdot \mathbf{r}$ is not strictly justified in this case, the general character of the spectrum, i.e., the presence of minibands at $|E| \ll \Delta$, remains nevertheless correct. Dykhne[10] has shown that for any sufficiently slowly varying potential, in the quasiclassical approximation, the results deduced above remain in force, and that at $|E| \ll \Delta$ the width of the allowed bands, as well as the distances between them, do not depend too strongly on the type of the potential.

For real system, the representation of $\Delta(\mathbf{r})$ in the form (20) is, of course, only approximate. The form of $\Delta(\mathbf{r})$ depends essentially on the symmetry of the concrete structure, and the Coulomb interaction that hinders the inhomogeneous distribution of the electrons must be taken into account consistently from the very start of the calculation. It appears that such a problem can be solved only numerically even for the simplest structures.

§3. MAGNETIC ORDERING AND LONG-WAVE MODULATION IN A PUMPED EXCITONIC DIELECTRIC

When an excitonic insulator with gap 2Δ and with a high energy $\hbar\omega_D$ of the Debye phonon is pumped, the distribution function of the excitation can take a quasi-Fermi form.[2] In this case, the state with $q = 0$ is unstable, at sufficiently low temperatures, to long-wave modulation of $\Delta(\mathbf{r})$.[4] The phase of the order parameter $\Delta(\mathbf{r})$ is not fixed in the nonequilibrium system under consideration, and we seek therefore a solution in the form (8).

Assume that an external source excites quasiparticles and quasiholes having a fixed concentration n, and that the positions of the Fermi quasilevels ($+\mu$ for the quasiparticles and $-\mu$ for the quasiholes) are determined from the condition that the excitation density be given. In principle it is also possible to realize another situation, wherein the Fermi quasilevels $\pm\mu$ are fixed by specifying the frequency $\Omega = 2\mu/\hbar$ of the high-power monochromatic source.[2] We shall not consider this case specially, but note that in contrast to an equilibrium with a fixed chemical potential, a nonequilibrium system can have magnetic solutions as well as a saturation of the magnetic state, something not realized in the nonmagnetic state of a pumped excitonic dielectric. We note also that in the case of a pumped system the number of electrons is equal to the number of holes, so that the condition of local electroneutrality is preserved, in contrast to a doped system. Another fundamental difference between the solutuions obtained for pumping and for doping is that even in the presence of two nonzero order parameters Δ_s and Δ_t, no summary magnetic moment is produced by pumping, since the moment of the electrons above the gap is cancelled by the moment of the hole below the gap. In the case of doping, on the other hand, the magnetic moment is due to the presence of excess carriers of like type (electrons or holes).

Following Ref. 2, we write down a system of equations for the order parameters $\Delta_\pm$:

$$\begin{aligned}
\frac{2\Delta_s}{g_s N(0)} &= \Delta_+ \left\{ \ln \frac{\varpi}{\Delta_+} - \frac{\Delta_+}{Q} [G(r_+^+) - G(r_-^+)] \right\} \\
&\quad + \Delta_- \left\{ \ln \frac{\varpi}{|\Delta_-|} - \frac{\Delta_-}{Q} [G(r_+^-) - G(r_-^-)] \right\}, \\
2\frac{\Delta_t}{g_t N(0)} &= \Delta_+ \left\{ \ln \frac{\varpi}{\Delta_+} - \frac{\Delta_+}{Q} [G(r_+^+) - G(r_-^+)] \right\} \\
&\quad - \Delta_- \left\{ \ln \frac{\varpi}{|\Delta_-|} - \frac{\Delta_-}{Q} [G(r_+^-) - G(r_-^-)] \right\}.
\end{aligned} \tag{33}$$

Although the equations for the Green's function and for the order parameters in the case of a pumped excitonic dielectric (33) is outwardly similar to that for a doped excitonic dielectric (9), the solutions (33) and (9) differ substantially. The functions $G(r)$ in (33) are defined as follows:

$$G(r) = \Theta(r-1)[r \cdot \operatorname{Arch}(r) - (r^2-1)^{1/2}], \tag{34}$$

where $r_\pm^\pm$ have the same meaning as in (10). The substantial difference between the functions (34) and (10) is due to the fact that in the case of doping there is a single Fermi level μ of the electrons and holes, whereas in the case of pumping there are respectively two Fermi quasilevels $\pm\mu$ for the electrons and holes.

The condition that the excitation concentration n be specified differs considerably from the condition for the doping problem, that the density difference be given. The cause of this difference is the band "overlap" in the case of sufficiently large $Q > \Delta$. In the case of doping, when the concentration difference of the electrons and holes is specified and is governed only by the impurity concentration, the number of electrons that go from the valence to the conduction band as a result of the "overlap" is equal to the number of produced holes, so that the "overlap" does not influence the form of Eq. (11). In the case of pumping, the total number of electrons in the conduction band is equal to the sum of the number of electrons n injected into the band by the external source and the number of electrons due to the overlap. What is fixed is not the total number of electrons, but only the number injected by the source. Therefore the connection between n, μ, and Δ takes the form

$$2n=\left\{\frac{\Delta_+^2}{4Q}\gamma(r_+^+)-\gamma(r_-^+)-\gamma\left(\frac{Q}{\Delta_+}\right)\right\}+\frac{\Delta_-^2}{4Q}\left\{\gamma(r_+^-)-\gamma(r_-^-)-\gamma\left(\frac{Q}{|\Delta_-|}\right)\right\} \tag{35}$$

where

$$\gamma(r)=\Theta(r-1)\,[r(r^2-1)^{1/2}-\mathrm{Arch}(r)]. \tag{36}$$

In (35), $\gamma(Q/\Delta_\pm)$ is the number of electrons with spin $\pm 1/2$ produced in the conduction band by the overlap.

To construct the phase diagram of a pumped excitonic dielectric we must solve the system (33)–(36) numerically. Besides the second-order phase transition into the state with $\Delta_t \neq 0$ (or $(\Delta_s \neq 0)$, there is also a first-order transition line, on which Δ_s and Δ_t appear jumpwise.[2] We confine ourselves to obtaining the equations for the second-order transition lines. An analysis similar to that of § 2 leads to the following system:

At $\mu_- > \Delta_s$:

$$\ln\frac{\Delta_{s0}}{\Delta_{t0}}=\frac{\Delta_s^2}{Q}\{[\mu_-+(\mu_-^2-\Delta_s^2)^{1/2}]^{-1}-[\mu_++(\mu_+^2-\Delta_s^2)^{1/2}]^{-1}\}. \tag{37}$$

At $\mu_- < \Delta_s$:

$$\ln\frac{\Delta_{s0}}{\Delta_{t0}}=\frac{\Delta_s^2}{Q}\left\{\frac{\mu_-}{\Delta_s^2}-[\mu_++(\mu_+^2-\Delta_s^2)^{1/2}]^{-1}\right\}. \tag{38}$$

In contrast to the corresponding expressions of § 2, the line of transition into the "magnetic" state lies always in the region $\Delta_{s0} > \Delta_{t0}$ (we assume that singlet pairing was realized in the system in the nonmagnetic phase). An analysis of (37) and (38) shows that the second-order transition lines shift towards an increase of the region of existence of "magnetic" solutions with long-wave modulation, compared to the case without modulation. The line of first-order phase transition into the metallic phase also seems to shift towards an increase of the reaction of coexistence of Δ_s and Δ_t compared with the case $q=0$.

§4. LONG-WAVE MODULATION IN THE LASER REGIME

We consider a broadband semiconductor that is stable, under equilibrium conditions, to electron-hole pairing. When pumped by an external source of electrons and holes with frequency $\Omega > E_g$, a quasi-Fermi distribution of the nonequilibrium carriers can be established in the system, and population inversion takes place. If the extrema of the conduction and valence bands of the semiconductor coincide in momentum space, a simultaneous Bose condensation of electron-hole pairs and photons takes place into a state with nonzero frequency, meaning that the system goes over into a lasing regime. Since the doping makes the electron and hole densities unequal, singlet and triplet electron-hole pairings can coexist. The combined magnetic moment is then different from zero, just as in the case of a doped excitonic dielectric, i.e., the resultant state will be ferromagnetic.

To describe the laser system we can use Eqs. (9)–(12). In this case μ must be taken to mean the Fermi quasilevel shift due to doping, and ε_F to mean the quantity $(\Omega - E_g)/2$. The transition to such a representation is effected by a known unitary transformation.[11]

The difference between the considered problem and the equilibrium one is that the long-wave modulation, which is characterized by the quantity Q, is determined by external conditions (by the choice of the resonator parameters etc.), and not by minimizing the energy as in the equilibrium case. In addition, the phase of the order parameter is not fixed in the nonequilibrium system, and the solution can be represented in the form (8) for the entire range of variation of the interaction constants and of the concentrations n. We note that representation of the solution in the form (8) corresponds to the regime of a traveling wave in a laser (the standing-wave regime would correspond to a representation in the form (20)).

An analysis similar to that in § 2 leads for small Q $(Q \ll n)$ to the following line of phase transition to the magnetic state:

$$\ln\frac{\Delta_{s0}}{\Delta_{t0}}=\frac{\Delta_{s0}}{n}-2+O\left(\frac{Q^2}{n^2}\right), \tag{39}$$

where $O(Q^2/n^2)$ is a small positive increment. Thus, at $Q \neq 0$ the region of existence of the magnetic solutions expands compared with the case $Q=0$. This result is not valid at excessively small dampings in the system, when the single-mode traveling wave regime turns out to be unstable.[5] This instability is due entirely to the disequilibrium of the system and is the cause of a transition into a multimode lasing regime.

§5. CONCLUSION

Much attention is being paid now to the investigation of the mechanism of ferromagnetic and antiferromagnetic ordering of band electrons. The antiferromagnetism model proposed by Rice[3] has made it possible to explain such an important property of chromium as the noncommensurability of the magnetic period with the lattice period, the transition from the noncommensurate state into a commensurate one in CrMn alloys when the Mn concentration is changed, and finally the appearance of a strain wave in chromium and its alloys. The latter has been interpreted by a number of Japanese authors[12] as magnetostriction due to the onset of higher harmonic component of the CDW against the SDW, the CDW period being double to SDW period. In addition to chromium and its alloys there are two other substances in which the antiferromagnetism is apparently described by the Rice model, viz., the alloys γ-FeMn (Ref. 13), β-Mn (Ref. 14), and possibly NiS (Ref. 15). One cannot exclude, however, the possibility that the long-wave deformation in compounds of this type is due to the mechanism proposed in the present paper. Namely, a CDW appears against the background of an SDW, has the same period, and their beats manifest themselves as a strain wave. In this case there may be no total magnetic moment in the system, long-wave fluctuations of the magnetic moment exist in the simple, and the chemical unit cell of the material in this phase is approximately doubled. The phases of the CDW and SDW are shifted by $\pi/2$ in this case.

In a number of compounds, such as Sc_3In and $ZrZn_3$,

a transition to a ferromagnetic state is observed. These substances are apparently well described by the excitonic-ferromagnet model,[1] so that it is possible to apply to them (of course, only qualitatively), the results obtained above. When the phases of CDW and SDW having the same period coincide, the summary magnetic moment of the sample is not equal to zero and a domain structure is produced. It is of interest to investigate such systems near the temperature of the transition to the ferromagnetic state, as an attempt to observe in them long-wave oscillations of the density and of the magnetic moment. A theoretical calculation with a two-component order parameter and at finite temperatures is a rather laborious task even in the homogeneous case, and will therefore be the subject of a separate paper.

Interest in the investigation of phase transitions in nonequilibrium system is stimulated by the search of means of raising the critical superconducting temperture. We have shown here that under the influence of a pump source the magnetic ordering due to collective effects of coexistence of singlet and triplet electron-hole pairings turns out to be inhomogeneous (modulated), with a period that is determined by the pump intensity. This effect can be observed in experiment by magnetic measurements.

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Translated by J. G. Adashko

Susceptibility and Knight shift in one-dimensional disordered spin systems with isotropic antiferromagnetic interaction

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(Submitted 21 March 1978)
Zh. Eksp. Teor. Fiz. **75**, 748–757 (August 1978)

A one-dimensional model of classical spins with $n = 1,2$, and 3 components (Ising, planar rotator, and Heisenberg models) and with random antiferromagnetic interaction J of the nearest neighbors is considered. In such a system, the average thermodynamic value of the spin at a site is different from zero in a magnetic field. The value of s is random, and its distribution is described by a function $f_s(x)$. An integral equation is obtained for $f_s(x)$ in weak magnetic field, assuming the distribution function $f_J(x)$ to be given. The moments of the distribution of s are calculated as functions of the type of function $f_J(x)$ and of the temperature. Conditions under which the susceptibility of the system χ increases as $T \to 0$ are analyzed. It is shown that if the susceptibility $\chi \to \infty$ as $T \to 0$, then the distribution of s becomes symmetrical as $T \to 0$, and the most probable value $\bar{s}$ of s tends to be zero. The results are used to interpret the experimental data on the temperature dependence of the paramagnetic shift of the NMR in quasi-one-dimensional $Qn(TCNQ)_2$ crystals.

PACS numbers: 75.10.Hk, 76.60.Cq

1. INTRODUCTION

This article is devoted to a theoretical investigation of the properties of one-dimensional spin systems with random exchange interaction. Interest in these systems is due to the experimental investigations of the quasi-one-dimensional TCNQ salts with asymmetric cations[1] and of magnetic polymers such as polymetalphosphines.[2]

The class of magnetic polymers has not yet been investigated in great detail. All that is known is the temperature dependence of the susceptibility of two repre-

0038-5646/78/080377-07$02.40