

permits a satisfactory description of the experimental results, the elastic constants calculated by using the model of the dynamics of the graphite model in the Born-Karman approximation agrees with experiment within the limits of errors, whereas the elastic constants obtained by the analytic-potential method¹⁶ do not agree with the experimental results. The use of the proposed procedure of inelastic scattering of Mössbauer γ radiation for the study of the properties of PG has shown that this method is effective²⁾ when it comes to determining the shear modulus c_{44} and by the same token the quality of the graphite. This method can be used equally well for the separation of the elastic and inelastic components in scattering with high resolution ($\sim 10^{-8}$ eV), both in solids and in liquids or gases that do not contain Mössbauer isotopes.

¹⁾For 14.4-keV radiation, the ratios $\sigma(0)/\mu$ for the reflections (002), (004), (006), and (008) are respectively 1.99, 0.32, 0.1, and 0.06.

²⁾The method of scattering thermal neutrons is not effective for the measurement of elastic moduli $\leq 10^8$ dyn/cm², in view of the small energy resolution, $\sim 10^{-4}$ eV.¹²

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Thermodynamics of electrons in a quantized semimetal film in strong magnetic fields

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A quantized semimetal film in strong transverse magnetic fields H is considered. The thermodynamic characteristics of the system are calculated with allowance for the Coulomb interaction. Transitions to the excitonic phase are predicted for certain relationships between H and the band overlap E_g , and the phase diagram of the system is calculated. Field-induced rearrangements in equilibrium quasi-two-dimensional semiconductors are also studied.

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Quasi-two-dimensional electron systems in strong transverse magnetic fields H are now an object of intensive theoretical and experimental study. The interest in them is stimulated by the complete discreteness of the electron spectrum, which gives rise to their highly unusual properties. The phase transitions in such systems have been studied in a number of papers: the magnetic-field-induced crystallization of electrons in inversion layers (see, e.g., Refs. 1-5), the formation of droplets of a nonequilibrium electron-hole ($e-h$) liquid in quasi-two-dimensional semiconductors in strong fields,⁶ and the transition of an $e-h$ plasma to an excitonic phase in such semiconductors⁷ and in systems with

separated e and h in strong fields.⁸

A special place amongst these "quasi-zero-dimensional" systems is occupied by size-quantized semimetal films⁹ in strong fields H : the properties of such systems have been studied experimentally in a whole series of papers (e.g., Refs. 10 and 11). For a systematic description of the kinetic properties of these systems it is necessary first of all to study the ground state and thermodynamics of the electron Fermi liquid in the films. It is precisely these problems that are considered in the present paper.

We shall confine ourselves to a two-band model of the

semi-metal (in the given case, many-valley effects do not lead to qualitative changes of the results obtained below) and shall consider the case of strong magnetic fields

$$r_H \ll a_{00} \quad (1)$$

and low temperatures

$$T \ll \omega_H \quad (2)$$

Here we have put $\hbar = 1$, $\sigma = 1, 2$ are the band indices, $\omega_{H\sigma} = eH/m_\sigma c$ are the cyclotron frequencies, $r_H = (c/eH)^{1/2}$ is the magnetic length, $a_{00} = 1/m_0 \bar{\epsilon}^2$ are the effective Bohr radii of the electrons in the first and second bands, m_σ are their effective masses, and $\bar{\epsilon}^2 = e^2/\kappa$, where κ is the permittivity of the medium surrounding the film. It turns out that when the conditions (1) and (2) are fulfilled several Landau levels (depending on the relationship between the band overlap E_g and H) are completely filled, while the others are empty [to within small quantities $\sim \exp(-\omega_H/T)$]. As H is changed giant jumps of the electron density occur as a result of the change in the number of completely filled levels. At the upper filled level, in relatively narrow ranges of the parameters, an exciton condensate is formed. Because of the presence of the reservoir of particles the properties of the equilibrium system under consideration differ qualitatively from those of a non-equilibrium two-dimensional $e-h$ system in strong fields,^{6,7} in which the number of electrons and holes is fixed (e.g., by optical pumping).

Below, in Sec. 1, we consider the properties of the system in the ideal-gas approximation. Even in this approximation it is possible to give a qualitative description of certain features of the system: the giant jumps in the density and magnetic susceptibility, and the exponential smallness of the entropy and specific heat. In Sec. 2 the Coulomb interaction is considered. Under the conditions (1) and (2) its contribution to the thermodynamic functions is calculated exactly in the parameter $r_H/a_{00} \ll 1$. The interaction leads to renormalization of the parameters appearing in the formulas obtained in Sec. 1. When the interaction is taken into account the diamagnetic susceptibility is no longer constant between jumps but varies slowly like $H^{-1/2}$. In Sec. 3 second-order transitions to the excitonic phase are predicted. As H is varied the system undergoes a series of such transitions: an exciton condensate is formed at the upper filled Landau level when H and the band overlap E_g have certain relative values. The excitonic phase is analyzed not in the parquet approximation, as in a three-dimensional $e-h$ system in a strong magnetic field,¹² but in the ladder approximation, defined here in terms of a power parameter (and not, as ordinarily, in terms of a logarithmic parameter). A transition is manifested, e.g., in jumps in the magnetic susceptibility: it increases by a factor of $a_0/r_H \gg 1$ relative to the normal case, and changes from diamagnetic to paramagnetic. In Sec. 4 we consider the rearrangements due to the Coulomb interaction in quasi-two-dimensional equilibrium semiconductors ($E_g < 0$) in strong fields H . Above certain values of H it turns out to be favorable for the lowest Landau level to be filled by electrons in the conduction band and by holes

in the valence band. Under the condition (2) these transitions depend only on H and do not depend on T .

1. THERMODYNAMICS OF AN IDEAL QUASI-ZERO-DIMENSIONAL $e-h$ GAS

The Hamiltonian of a free two-dimensional $e-h$ gas in a semimetal film in a magnetic field¹⁾ is

$$\mathcal{H}_0 = \sum_{\sigma=1,2} \int \psi_\sigma^\dagger(\mathbf{r}) \xi_\sigma \psi_\sigma(\mathbf{r}) d^2r, \quad (3)$$

where ψ_σ^\dagger and ψ_σ are the creation and annihilation operators, respectively, for electrons in the first band and holes in the second band; $\xi_\sigma = \pm [\epsilon_\sigma(\mathbf{p} - e\mathbf{A}/c) - \mu]$ (the sign + is for $\sigma=1$, and the sign - for $\sigma=2$); μ is the chemical potential of the electron gas; $\mathbf{A} = (-Hy, 0, 0)$ is the vector potential in the Landau gauge. The dispersion laws of the electrons are

$$\epsilon_1(\mathbf{p}) = p^2/2m_1, \quad \epsilon_2(\mathbf{p}) = E_{g0} - p^2/2m_2$$

(the separation of the extrema of the bands in momentum space is unimportant and has been put equal to zero). The thermodynamic potential Ω_0 for an $e-h$ gas with the Hamiltonian (3) has the form

$$\Omega_0 = -T \ln \text{Sp} \{ \exp(-\mathcal{H}_0/T) \} = -\mathcal{N}_0 T \sum_{k=0}^{\infty} \ln \left\{ \left[1 + \exp\left(\frac{\mu - k\omega_{H1}}{T}\right) \right] \left[1 + \exp\left(\frac{E_g - k\omega_{H2} - \mu}{T}\right) \right] \right\}, \quad (4)$$

where $\mathcal{N}_0 = L_x L_y / 2\pi r_H^2$ is the number of particles in a completely filled Landau level; L_x and L_y are the linear dimensions of the system;

$$E_g = E_g(H) = E_{g0} - \omega_H/2 + \mu^* H$$

is the overlap of the bands in the magnetic field; $\omega_H \equiv \omega_{H1} + \omega_{H2} = eH/mc$, where m is the reduced cyclotron mass; μ^* is the effective Bohr magneton. Inessential constants have been omitted in (4). If $\mu^* \neq e/2mc$, then E_g depends on H . In Secs. 1-3 we investigate the case $E_g(H) > 0$ in the entire range of fields under consideration.²⁾

The chemical potential μ in (4) is determined by the condition that the numbers of electrons and holes are equal: $N_1^e = N_2^h = \mathcal{N}_0$. For equal cyclotron masses $m_1 = m_2$ we find $\mu = E_g/2$ (the case $m_1 \neq m_2$ is discussed below). The number of particles

$$N_1^e = N_2^h = \mathcal{N}_0 \sum_{k=0}^{\infty} \left[\exp\left(\frac{k\omega_H - E_g}{2T}\right) + 1 \right]^{-1} = \mathcal{N}_0 \sum f_k^e(T). \quad (5)$$

It can be seen from (5) that for $T \rightarrow 0$ with the condition

$$n_0 \omega_H < E_g < (n_0 + 1) \omega_H, \quad (6)$$

the levels with $k \leq n_0$ are completely filled and those with $k > n_0$ are vacant. The physical meaning of the condition (6) is clear: those levels which lie in the overlap between the bands are filled. As H is varied, jumps in the number of particles, from $n_0 \mathcal{N}_0$ to $(n_0 + 1) \mathcal{N}_0$, occur at the points $n_0 \omega_H = E_g$. For $T \neq 0$ the jump is spread over an interval

$$|n_0 \omega_H - E_g| / 2T \ll 1, \quad (7)$$

which, under the condition (2), is extremely narrow, so that an exact determination of the number of particles

and the energy inside this interval is of no interest.

The free energy $F_0 = \Omega_0 + \mu(N_1^e - N_2^h)$, so that, substituting into (4) $\mu = E_g/2$, which is obtained from $N_1^e = N_2^h$, we immediately determine F_0 :

$$F_0 = -\mathcal{N}_0 \sum_{k=0}^{n_0} (E_g - k\omega_H) = -\frac{L_x L_y m}{2\pi} (n_0 + 1) \omega_H \left(E_g - \frac{n_0 \omega_H}{2} \right). \quad (8)$$

In this formula (as in all subsequent ones, if there is no stipulation to the contrary) terms that are exponentially small in the temperature are omitted. It is not difficult to convince oneself that F_0 , determined by formula (8), is continuous on the boundaries of the regions (6), so that it can also be applied inside the intervals (7). Since F_0 does not depend on T the entropy and specific heat are equal to zero (to be more precise, they are exponentially small). For $E_g = k\omega_H$, however, the entropy $S = 2\mathcal{N}_0 \ln 2$, i.e., it does not vanish even when $T \rightarrow 0$. But for $E_g - k\omega_H = \delta$, where δ is arbitrarily small, we have

$$\lim_{T \rightarrow 0} S = \lim_{T \rightarrow 0} [2\mathcal{N}_0 \ln(1 + e^{\delta/2T}) - \mathcal{N}_0 \delta/T(1 + e^{\delta/2T})] = 0.$$

We shall determine from (8) the magnetic susceptibility per unit volume:

$$\chi_0 = -\frac{n_0(n_0+1)}{2\pi} \frac{e^2}{mc^2} \frac{1}{d}, \quad (9)$$

where d is the thickness of the film. It is assumed that $d \ll r_H$, a condition that enables us to disregard the upper transverse-quantization levels.⁶ The susceptibility χ_0 is diamagnetic, and, as the number of filled levels is varied, experience jumps, smeared out over the intervals (7), that are larger the greater the number of filled levels. In determining χ_0 we neglected the dependence of E_g on H , assuming the coefficient $e/2mc - \mu^*$ to be small. But in the ultraquantum limit, when only the lowest Landau level ($n_0 = 0$) is filled, it is precisely this dependence which determines χ_0 . In this case the susceptibility is diamagnetic if $e/2mc > \mu^*$, and paramagnetic otherwise.

If the cyclotron masses $m_1 \neq m_2$, then, under the condition (6), the chemical potential

$$\mu = [E_g + n_0(\omega_{H1} - \omega_{H2})]/2,$$

i.e., a substantial dependence of μ on H appears. The other formulas are not changed at all.

2. COULOMB INTERACTION IN A NORMAL $e-h$ SYSTEM

In this section we consider a normal semimetal with neglect of the possible $e-h$ pairing. The interaction Hamiltonian is

$$\mathcal{H}_{int} = \frac{1}{2} \sum_{\sigma, \sigma' = 1, 2} \int d^2r d^2r' \psi_{\sigma}^+(\mathbf{r}) \psi_{\sigma'}^+(\mathbf{r}') \frac{\tilde{e}^2 (2\delta_{\sigma\sigma'} - 1)}{|\mathbf{r} - \mathbf{r}'|} \psi_{\sigma}(\mathbf{r}') \psi_{\sigma'}(\mathbf{r})$$

($\delta_{\sigma\sigma'}$ is the Kronecker symbol).

To determine the thermodynamic potential we shall calculate the temperature Green functions¹³ G_{σ} of the electrons of the first band and the holes of the second band. First we shall determine them in the Hartree-Fock approximation; at the end of the section we shall show that under the conditions (1) and (2) the correlation corrections to the thermodynamic functions are

small in the parameter r_H/a_0 . The solutions of the Hartree-Fock equations are found in the same way as in the case of an $e-h$ system with a fixed number of electrons and holes,⁶ and have the form

$$G_{\sigma}(\omega, p_x; y, y') = \sum_{k=0}^{\infty} \chi_{k\sigma} (y) \chi_{k\sigma} (y') g_{k\sigma}(\omega), \quad (10)$$

$$g_{k1}(\omega) = (i\omega - k\omega_{H1} + \varepsilon_{k1} + \mu)^{-1},$$

$$g_{k2}(\omega) = (i\omega + E_g - k\omega_{H2} + \varepsilon_{k2} - \mu)^{-1},$$

where

$$\chi_{k\sigma}(y) = \chi_k(y/r_H - p_x r_H)$$

are oscillator functions with center $y_0 = p_x r_H^2$ and frequency $\omega_{H\sigma}$ (Ref. 14); $\omega = \pi T(2l + 1)$, where l is an integer. The corrections $\varepsilon_{k\sigma}$ to the Landau levels satisfy the equations

$$\varepsilon_{k\sigma} = E_0 \sum_{j=0}^{\infty} I_{kj} f_{j\sigma}(T), \quad (11)$$

where $E_0 = \tilde{e}^2 (\pi/2)^{1/2} / r_H \propto H^{1/2}$, and $f_{k\sigma}$ are the Fermi occupation coefficients of the k th Landau level of band σ :

$$f_{k1}(T) = \{ \exp [(k\omega_{H1} - \varepsilon_k - \mu) / T] + 1 \}^{-1},$$

$$f_{k2}(T) = \{ \exp [(k\omega_{H2} - \varepsilon_k - E_g + \mu) / T] + 1 \}^{-1}. \quad (12)$$

It is possible to calculate the coefficients $I_{kj} = I_{jk}$ in (11) analytically. For $j \geq k$ we have

$$I_{jk} = 2^k \pi^{-k} \int dy dy' dp' dq \chi_k(y-p) \chi_j(y-p') \chi_k(y-p') \chi_j(y'-p')$$

$$\times \exp(iq(y-y'))$$

$$\times (q^2 + (p-p')^2)^{-k} = \frac{(2j-2k-1)!!}{(2j-2k)!!} \left\{ 1 + \sum_{i=1}^j (-1)^i \left[\frac{(2i-1)!!}{(2i)!!} \right]^2 \frac{C_i^k}{C_{j-k+i}^k} \right\}, \quad (13)$$

where for $k=0$ the sum inside the curly brackets must be put equal to zero and for $j=k$ the factor outside the brackets must be taken to be equal to unity.

Confining ourselves to the case of equal masses, when $\omega_{H1} = \omega_{H2} = \omega_H/2$, from the condition $N^e = N^h$ we again find $\mu = E_g/2$. (As in the preceding section, for $m_1 \neq m_2$ the chemical potential will depend on the field in an essential way, and not only as a function of $E_g(H)$; but the other results are not changed.) The occupation numbers of the Landau levels in each band are then equal to

$$f_{k1}(T) = f_{k2}(T) = f_k = \{ \exp [(k\omega_H - 2\varepsilon_k - E_g) / 2T] + 1 \}^{-1}. \quad (12')$$

We denote the renormalized Landau levels by $\mathcal{E}_k = k\omega_H/2 - \varepsilon_k$, where $\varepsilon_k \equiv \varepsilon_{k1} = \varepsilon_{k2}$. From (12') it is clear that under the condition (2) and the condition

$$\mathcal{E}_n < E_g/2 < \mathcal{E}_{n+1}, \quad (14)$$

the levels with $k > n$ are vacant while those with $k < n$ are densely filled. The filling of the n th level occurs in a small ($\sim T$) interval of fields

$$| \mathcal{E}_n - E_g/2 | / T \ll 1. \quad (15)$$

Here and below, n is the label of the highest of the filled levels. When the interaction is taken into account the conditions (14) and (15) replace the conditions (6) and (7). By virtue of the inequality (1), which, as will become clear below, ensures the applicability of the

theory, $\varepsilon_k \approx kE_0 \ll k\omega_H$, so that the change in the spacing between neighboring levels is not large. However, the absolute shift of levels with sufficiently large labels can exceed ω_H . Consequently, the number n of filled levels may not coincide with the n_0 calculated in the ideal-gas approximation: a larger number of levels can now be located in the overlap between the bands.

We shall determine the thermodynamic potential Ω from the well known formula (λ is a constant multiplying E_0)

$$\Omega - \Omega_0 = \int_0^{\lambda} \frac{d\lambda}{\lambda} \langle \mathcal{H}_{int}(\lambda) \rangle,$$

i.e., in the Hartree-Fock approximation,

$$\begin{aligned} \Omega - \Omega_0 = & -\frac{T^2 L_x}{(2\pi)^2} \lim_{\tau, \tau' \rightarrow +0} \sum_{\alpha=1,2} \sum_{\omega, \omega'} \int_0^{\lambda} \frac{d\lambda}{\lambda} \int d^2y d^2p dq \\ & \times \left\{ \frac{\lambda \bar{\varepsilon}^2 \exp(iq(y-y'))}{(q^2 + (p_x - p_x')^2)^2} G_{\alpha}(\omega, p_x; y, y'; \lambda) \right. \\ & \left. \times G_{\alpha}(\omega', p_x'; y'; \lambda) \exp(i\omega\tau) \exp(i\omega'\tau') \right\}. \end{aligned} \quad (16)$$

Substituting into this the Hartree-Fock Green functions (10) and $\mu = E_g/2$, we find the free energy F . Carrying out the calculations in (16), we obtain, taking (11) and (13) into account (having replaced $E_0 - \lambda E_0$),

$$F - F_0 = -2E_0 \mathcal{N}_0 \int_0^{\lambda} \frac{d\lambda}{\lambda} \sum_{j,k=0}^{\infty} f_j(\lambda) f_k(\lambda) = -2\mathcal{N}_0 \int_0^{\lambda} \frac{d\lambda}{\lambda} \sum_{k=0}^{\infty} \varepsilon_k(\lambda) f_k(\lambda). \quad (17)$$

It is not possible to perform the integration in (17) in general form. But under the condition (2), outside the narrow intervals (15), the calculation presents no difficulty. From (11) and (12') we have

$$\begin{aligned} \frac{d\varepsilon_k}{d\lambda} &= \frac{\varepsilon_k}{\lambda} + \lambda E_0 \sum_{j=0}^{\infty} I_{jk} \frac{df_j}{d\lambda}, \\ \frac{df_k}{d\lambda} &= -\frac{1}{T} f_k (1 - f_k) \frac{d\varepsilon_k}{d\lambda}. \end{aligned}$$

Since, outside (15), for all values of k either f_k or $1 - f_k$ is exponentially small, we have

$$df_j/d\lambda \propto \exp(-\mathcal{E}_j/T) \ll 1.$$

Therefore,

$$\begin{aligned} F - F_0 &= -2\mathcal{N}_0 \sum_{k=0}^{\infty} \int_0^{\lambda} \left[\exp\left(\frac{k\omega_H - 2\varepsilon - E_g}{2T}\right) + 1 \right]^{-1} d\varepsilon \\ &= -2\mathcal{N}_0 \sum_{k=0}^{\infty} [\varepsilon_k + T \ln(f_k^0/f_k)], \end{aligned} \quad (18)$$

where the f_k are the true occupation numbers (12') and the f_k^0 are the occupation numbers in the absence of the interaction (5). In the region of applicability of the formula (18),

$$T \ln \frac{f_k^0}{f_k} = \begin{cases} -\varepsilon_k, & k > n; \\ +(k\omega_H - E_g), & n \geq k > n_0; \\ 0, & n_0 \geq k. \end{cases}$$

Hence, we finally obtain

$$F = F_0 - 2\mathcal{N}_0 \sum_{k=0}^n \varepsilon_k, \quad \varepsilon_k = E_0 \sum_{j=0}^n I_{kj}. \quad (19)$$

Here \bar{F}_0 is the free energy of the ideal gas with allow-

ance for the fact that the number n of filled levels should be determined not by formula (6) but, when the Coulomb interaction is taken into account, by formula (14).

It follows from (19) that the corrections to the total magnetic moment $\mathbf{M} = -(\partial F/\partial \mathbf{H})$ of the system that arise from the interaction are small in the parameter (1). But the dependence of \mathbf{M} on \mathbf{H} becomes nonlinear, and this leads to a qualitative change in the behavior of the diamagnetic susceptibility. In the intervals between the jumps the susceptibility is not constant but depends on the field H (here, $a_0 \equiv a_{01} + a_{02} = 1/m\bar{\varepsilon}^2$):

$$\chi = \chi_0 \left[1 - \frac{r_H}{a_0} \frac{3}{2} \left(\frac{\pi}{2}\right)^{1/2} \frac{1}{n(n+1)} \sum_{j,k=0}^n I_{jk} \right]. \quad (20)$$

Although the correction terms in (20) are small (all the coefficients $I_{jk} < 1$, so that the sum in (20) is less than n^2), the correction $\Delta\chi \sim H^{-1/2}$ is perfectly observable against the background of the susceptibility χ_0 , which is constant in the regions (14). The dependences of the number of particles and the energy, as can be seen from (12) and (19), undergo only scale changes (Fig. 1) when the interaction is taken into account.

It remains to show that the correlation corrections to (19) are small. The simple polarization operator is calculated in the same way as in Ref. 6, and has the form

$$\Pi(\varepsilon, p) = \sum_{j,k=0}^{\infty} \frac{(f_j - f_k) p^2 \exp(-p^2 r_H^2/2) \Phi_{jk}(p^2)}{e^2 + (\mathcal{E}_j - \mathcal{E}_k)^2}, \quad (21)$$

where $\Phi_{jk}(p^2)$ is a polynomial whose form is unimportant here. Coulomb divergences of the ring diagrams are absent, since $\Pi(p) \sim p^2$ as $p \rightarrow 0$. The correlation corrections, which it is sufficient to calculate in second order of perturbation theory, are found to be small in r_H/a_0 under the condition (1). The question of the cor-

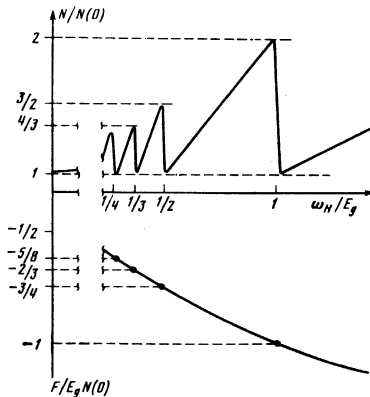


FIG. 1. Dependence of the particle density and energy on the magnetic field. The jumps in the particle density ($N(0)$) is the number of particles when $H = 0$ are depicted in the upper part of the Figure, and the dependence of the free energy on H in the lower part. Both parts of the Figure pertain to an ideal gas. When the interaction is taken into account they are subjected to a simple transformation: the points $1/n$ along the abscissa are replaced by $(1 + 2E_0/E_g)/n$, and the points $-[1/2 + 1/(2n+2)]$ along the ordinate in the lower part of the Figure should be shifted downward by

$$(2E_0/E_g) \sum_{k,j=0}^n I_{kj}.$$

relations at $\varepsilon=0$ ($\varepsilon=2\pi lT$, where l is an integer) and $j=k$, when the expression (21) is not defined, requires a special analysis. It is easy to see that

$$\Pi_{kk}(0, p) \sim \frac{1}{T} f_k(1-f_k),$$

which is exponentially small outside the region (15). Factors of this type also arise in diagrams of higher orders. Consequently, in the considered range of parameters, correlations are certainly unimportant.

Consequently, the Coulomb interaction has been taken into account exactly in the parameter (1) for any values of H outside the intervals (15). But analytic formulas for the latter are simply not needed, since (see Fig. 1) the energy is matched inside these intervals, and the number of particles changes rapidly from $n\mathcal{N}_0$ to $(n+1)\mathcal{N}_0$.

3. TRANSITION TO THE EXCITONIC PHASE

We shall show that, for certain relationships between H and E_g , a quasi-zero-dimensional $e-h$ plasma goes over into an excitonic phase.

We shall consider the second-order vertex diagrams constructed from Green functions of the normal semimetal (Fig. 2). Obviously, only the $e-h$ diagrams in which the Coulomb interaction is attractive are of physical interest. The same frequency factors (irrespective of the band from which the Green functions are taken) correspond to the diagrams of Figs. 2a-c:

$$T \sum_{\omega} g_{k\sigma'}(\omega) g_{l\sigma}(\omega+\varepsilon) = \frac{f_l - f_k}{i\varepsilon + \mathcal{E}_l - \mathcal{E}_k},$$

where ω are the odd frequencies and ε the even frequencies. Integration over the coordinates and momenta gives factors $\sim E_0$ in all diagrams. Consequently, the diagrams a-c for $l \neq k$ are small in the parameter $E_0/\omega_H \sim \gamma_H/a_0$. For $\varepsilon \neq 0$ and $l=k$ they vanish, while for $\varepsilon=0$ and $l=k$ their contribution is

$$\sim (E_0/T) f_l(1-f_l),$$

i.e., small in the considered range of parameters. Corresponding to the diagram of Fig. 2d is the frequency factor

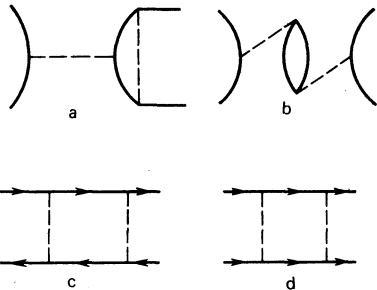


FIG. 2. Second-order vertex diagrams. The solid lines denote Green functions of electrons or holes and the dashed lines denote the Coulomb interaction; the diagrams a)-c) are small, like γ_H/a_0 , outside the region (15) (irrespective of the direction of the arrows, for a) and b); the diagram d) does not have a small factor: ladder diagrams of this type should be taken into account in all orders of perturbation theory.

$$T \sum_{\omega} g_{k1}(-\omega) g_{l2}(\omega+\varepsilon) = (i\varepsilon + \mathcal{E}_l + \mathcal{E}_k - E_g)^{-1} \left[\text{th} \frac{2\mathcal{E}_k - E_g}{4T} + \text{th} \frac{2\mathcal{E}_l - E_g}{4T} \right].$$

For $k=l=n$, where n is the highest filled level, and for $2\mathcal{E}_n - E_g \leq E_0$, this diagram has no small factors. Ladder diagrams of this type, describing the pairing of an electron of the first band and a hole of the second band, must be summed in all orders of perturbation theory. We note that these diagrams are defined here in terms of a power parameter, and not in terms of a logarithmic parameter as in the theory of superconductivity (see Ref. 13) or the theory of an excitonic insulator in the three-dimensional case.¹⁵

To study the rearranged state with allowance for $e-h$ pairing one introduces, as usual, anomalous Green functions. In this section all expressions will be more symmetric if, in the ψ -operators of the second band, we change from the hole representation to the electron representation, which is achieved by the replacements $\psi_2 \rightarrow \bar{\psi}_2$ and $\bar{\psi}_2 \rightarrow \psi_2$ (unimportant constants are omitted). The matrix Green function

$$G_{\sigma\sigma'}(\mathbf{r}, \mathbf{r}'; \tau - \tau') = -\langle T_{\tau} \psi_{\sigma}(\mathbf{r}, \tau) \bar{\psi}_{\sigma'}(\mathbf{r}', \tau') \rangle$$

(where the nondiagonal terms correspond to $e-h$ pairing) satisfies an equation analogous to the Gor'kov-Éliashberg equation in the theory of superconductivity:

$$G_{\sigma\sigma'}(\omega, p_x; y, y') = \delta_{\sigma\sigma'} G_{\sigma}(\omega, p_x; y, y') - \frac{T\bar{e}^2}{2\pi} \sum_{\omega'} \int_{(v \neq \sigma)} dy_1 dy_2 dp_x' dq \times \left\{ \frac{\exp(iq(y_1 - y_2))}{(q^2 + (p_x - p_x')^2)^{3/2}} G_{\sigma}(\omega, p_x; y, y_1) G_{\sigma\sigma'}(\omega', p_x'; y_1, y_2) G_{\sigma\sigma'}(\omega, p_x; y_2, y') \right\}. \quad (22)$$

Here G_{σ} are the Green functions (10) of the normal semimetal (in the electron representation, g_{k2} is given by the expression $g_{k2}(\omega) = (i\omega + \mathcal{E}_k + \mu - E_g)^{-1}$ instead of (10)). It is convenient, as previously, to expand the Green function (22) in the Landau functions χ_{kp_x} :

$$G_{\sigma\sigma'}(\omega, p_x; y, y') = \sum_{k=0}^{\infty} \chi_{kp_x}(y) \chi_{kp_x}(y') g_{\sigma\sigma'}^k(\omega).$$

Substituting this expression into Eq. (22), we find

$$g_{\sigma\sigma'}^k = ((i\omega + \mathcal{E}_k + \mu - E_g) (i\omega - \mathcal{E}_k + \mu) - \Delta_{12}^k \Delta_{21}^k)^{-1} \times \begin{pmatrix} i\omega + \mathcal{E}_k + \mu - E_g & -\Delta_{12}^k \\ -\Delta_{21}^k & i\omega - \mathcal{E}_k + \mu \end{pmatrix}.$$

Here Δ satisfies the self-consistency equations

$$\Delta_{\sigma\sigma'}^k = TE_0 \sum_{j=0}^{\infty} \sum_{\omega} g_{\sigma\sigma'}^j(\omega) I_{jk}.$$

For equal masses, as before, $\mu = E_g/2$. Then for $\Delta_k \equiv \Delta_{12}^k = \Delta_{21}^k$ we obtain the following equations:

$$\Delta_k = E_0 \sum_{j=0}^{\infty} \frac{\Delta_j I_{jk}}{2(\xi_j^2 + \Delta_j^2)^{3/2}} \text{th} \frac{(\xi_j^2 + \Delta_j^2)^{1/2}}{2T}; \quad \xi_j = \mathcal{E}_j - \frac{E_g}{2}. \quad (23)$$

As will become clear below, $\Delta_k \lesssim I_{nk} E_0$, so that for $j \neq n$ all the terms in the right-hand side of (23) are $\sim \Delta_j/\xi_j \leq E_0 I_{n1}^2/\omega_H \lesssim \gamma_H/a_0$. Only the term with $j=n$ does not have this small factor.³⁾ (Of course, this also followed from the analysis of the vertex diagrams, so that, from the outset, in $G_{\sigma\sigma'}$ we could have included the anomalous terms corresponding to $e-h$ pairing at the n th level only.) For $k=n$ we obtain from (23)

$$(\xi_n^2 + \Delta_n^2)^{-1/2} \text{th} [(\xi_n^2 + \Delta_n^2)^{1/2} / 2T] = 2/E_n, \quad E_n = E_0 I_{n0}, \quad (23')$$

while for $k \neq n$ it follows from (23) that $\Delta_k = \Delta_n I_{nk}$. From the condition for Δ to vanish we obtain an equation for the transition temperature T_c :

$$2\xi_n/E_n = \text{th} (\xi_n/2T_c).$$

A solution exists only when

$$2|\xi_n| = |2\mathcal{E}_n - E_n| \leq E_n. \quad (24)$$

The transition temperature reaches its maxima, equal to $E_n/4$, when $\mathcal{E}_n = E_n/2$ (i.e., $\xi_n = 0$). In the ultraquantum limit ($\mathcal{E}_1 > E_n/2$), when only the lowest Landau level $n=0$ is filled, $\mathcal{E}_0 = -\varepsilon_0 = -E_0$, so that $2|\xi_0| = 2E_0 + E_n > E_0$, i.e., the condition (24) cannot be fulfilled. Consequently, rearrangement to the excitonic phase does not occur for $n=0$.

For $n \neq 0$ we find the transition temperature (see Fig. 3)

$$T_{c(n)} = \xi_n / \ln [(E_n + 2\xi_n)/(E_n - 2\xi_n)]. \quad (25)$$

The phase diagram of the system in the coordinates (T, H) is given schematically in Fig. 4. As the field is varied, without going outside the limits of the condition (1), a series of phase transitions to an excitonic condensate occur whenever the condition (24) is fulfilled for the corresponding n and the temperature is low enough ($T < E_n/4$). In fields H for which the condition (24) is not fulfilled, all the levels are either densely filled or vacant. In this case, $e-h$ attraction is compensated in the filled levels by $e-e$ and $h-h$ repulsion. As a level n approaches the boundary of the overlap the energy is lowered whenever the number of particles decreases in such a way that a transition to the excitonic phase becomes possible. Since $E_0 \ll \omega_H$, the width of the regions of existence of the excitonic phase is considerably smaller than the spacings between these regions. It can be shown, however, that the coefficients of all the corrections in r_H/a_0 are numerically small, so that the results obtained can also be valid in fields $r_H \approx a_0$. Then $E_0 \sim \omega_H$, so that the region of existence of the $e-h$ condensate can extend, for the appropriate values of n , over the whole interval between neighboring levels.

We shall consider how the characteristics of the $e-h$ system are changed when exciton pairing is taken into account. The number of particles

$$\begin{aligned} N_i^e = N_i^h &= \frac{TL_z}{2\pi} \lim_{\tau \rightarrow +0} \sum_{\mathbf{p}} \int dy dp_x e^{i\omega\tau} G_{ii}(\omega, p_x; y, y) \\ &= \frac{1}{2} \mathcal{N}_0 \sum_{k=0}^{\infty} \left[1 - (\xi_k^2 + \Delta_k^2)^{-1/2} \text{th} \frac{(\xi_k^2 + \Delta_k^2)^{1/2}}{2T} \right]. \end{aligned} \quad (26)$$

To within $(r_H/a_0)^2$ the expression in square brackets is equal to unity for $k < n$ and zero for $k > n$. Consequently, levels with $k < n$ are completely filled, and those with $k > n$ are vacant, but with power accuracy rather than with exponential accuracy as with neglect of $e-h$ pairing. We find the number of particles in the n th level from (26) and (23') with the condition (24):

$$N_i^e(n) = N_i^h(n) = \frac{1}{2} \mathcal{N}_0 (1 - 2\xi_n/E_n).$$

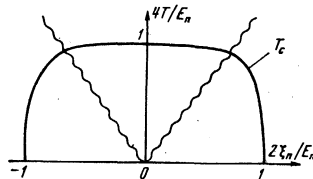


FIG. 3. Dependence of the excitonic-transition temperature T_c on the magnetic field near a level $n \neq 0$. In reduced coordinates the figure is the same for all $n \neq 0$. Above the wavy lines lies the region (15), in which the predictions of the theory have only a qualitative character.

The filling of the level n occurs, as can be seen from this formula, not in an interval of energies $\sim T$ (as in Fig. 1, where $e-h$ pairing is neglected), but in the interval (24), equal to $2E_n \sim H^{1/2}$.

We shall find the free-energy change in the transition to the excitonic phase (F is the free energy (19) of the normal $e-h$ system):

$$\begin{aligned} F_{exc} - F &= -2E_0 \mathcal{N}_0 \sum_{j,k=0}^{\infty} \int_0^1 \frac{d\lambda}{\lambda} T^2 \sum_{\omega, \lambda} \lambda g_{12}^h(\omega, \lambda) g_{21}^i(\omega', \lambda) I_{jk} \\ &= -2\mathcal{N}_0 \sum_{k=0}^{\infty} \int_0^1 \frac{d\lambda}{\lambda} \frac{\Delta_k^2(\lambda)}{(\xi_k^2 + \Delta_k^2(\lambda))^{1/2}} \text{th} \frac{(\xi_k^2 + \Delta_k^2(\lambda))^{1/2}}{2T} \\ &= 2\mathcal{N}_0 \int_0^{\Delta_n} \frac{d}{d\Delta} \left(\frac{1}{\lambda E_n} \right) \Delta^2 d\Delta. \end{aligned}$$

In the transformations we have used the self-consistency equation (23) and taken into account that the terms with $k \neq n$ give a contribution that is small in r_H/a_0 . The last expression is completely analogous to the corresponding formula in the theory of superconductivity.¹³ But, because of the discreteness of the spectrum (formally, because of the absence of integration over the momentum in Eq. (23)), the final expression that is obtained after substitution of $1/\lambda E_n$ from (23') has an entirely different form:

$$\begin{aligned} F_{exc} - F &= -2\mathcal{N}_0 \left\{ 2T \ln \left[\frac{\text{ch}((\xi_n^2 + \Delta_n^2)^{1/2} / 2T)}{\text{ch}(\xi_n/2T)} \right] \right. \\ &\quad \left. - \frac{\Delta_n^2}{2(\xi_n^2 + \Delta_n^2)^{1/2}} \text{th} \frac{(\xi_n^2 + \Delta_n^2)^{1/2}}{2T} \right\}. \end{aligned} \quad (27)$$

This expression has been obtained formally for all temperatures $T \ll T_c$, but it must be remembered that, like all the formulas obtained here, it is applicable only outside the regions (15). For clarity we give the expansion of the formula (27) near T_c :

$$F_{exc} - F = -\mathcal{N}_0 \Delta_n^4(T) \frac{ET_c - \Delta_n^2(0)}{2E_n^2 \xi_n^2 T_c} = -\mathcal{N}_0 \left(\frac{T - T_c}{T_c} \right)^2 \frac{2\xi_n^2 \Delta_n^4(0)}{E_n^2 T_c [E_n T_c - \Delta_n^2(0)]}. \quad (28)$$

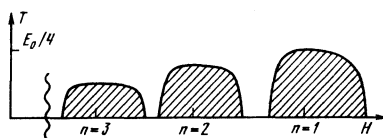


FIG. 4. Phase diagram of the system. The regions of existence of the excitonic phase are shaded; the labels of the levels at which $e-h$ condensation occurs are indicated schematically along the abscissa; for clarity, the Figure is not to scale.

Here $\Delta_n^2(0) = E_n^2/4 - \xi_n^2$ is the value of the "gap" at absolute zero.⁴⁾ The discontinuity of the specific heat at $T = T_c$ is quickly obtained from (28). Outside the region (15) this discontinuity is small. In fact, for $T_c \lesssim \xi_n$ the quantity $|\xi_n - E_n/2| \ll 1$ and $\Delta_n(0) \ll E_n/2$, so that the specific-heat discontinuity

$$(c_{exc} - c)/\mathcal{N}_0 \sim [\Delta_n(0)/E_n]^4 \ln^2[E_n/\Delta_n(0)] \ll 1.$$

Nevertheless, this discontinuity may be perfectly observable against the background of the usual phonon specific heat ($\sim T^3$). Finally, we give the expression for the energy of the system in the excitonic phase at $T \ll \xi_n$:

$$F_{exc} - F = -1/2 \mathcal{N}_0 E_n (1 - 2|\xi_n|/E_n)^2.$$

From this we determine the jump in the magnetic susceptibility at the phase-transition points at low T :

$$\Delta\chi = \frac{1}{2\pi} \frac{e^2}{mc^2} \frac{1}{d} \left(\frac{2}{\pi}\right)^{1/2} \frac{a_0}{r_H} \frac{n^2}{I_{nn}}. \quad (29)$$

Comparing (29) with formula (20) and discarding numerical factors of order unity (taking into account that $I_{nn} \lesssim 1/2$), we find

$$\Delta\chi/\chi \approx a_0/r_H \approx (mE_g/n)^{1/2} a_0 \gg 1.$$

Consequently, the susceptibility increases sharply at the transition to the excitonic phase and changes sign: it changes from diamagnetic to paramagnetic. The behavior of the magnetic susceptibility in the region of existence of the excitonic condensate at the level n is depicted in Fig. 5.

In conclusion we note that the formulas obtained in this section are inapplicable, generally speaking, in the immediate vicinity of T_c . The behavior of a quasi-zero-dimensional system in the fluctuation region requires a separate treatment.

4. MAGNETIC-FIELD-INDUCED REARRANGEMENTS IN QUASI-TWO-DIMENSIONAL SEMICONDUCTORS

In this section we consider an equilibrium quasi-two-dimensional semiconductor ($E_g < 0$; see footnote²⁾). As in the three-dimensional case,¹⁶ if the interaction is sufficiently strong the creation of electrons in the conduction band and holes in the valence band may be favored. In the situation under consideration the interaction energy per particle $\sim E_0 \propto H^{1/2}$, so that the field is an external parameter: by increasing it we can induce the phase transition.

All the formulas obtained in Sec. 2 that do not use the explicit form of μ also remain true for $E_g < 0$. The number of quasi-particles in the Landau levels is determined by formula (12). From the electrical-neutrality conditions we find that the Landau levels are populated at low values of T if the inequalities (for $k \neq 0$)

$$\mathcal{E}_k - \mu < 0, \quad \mathcal{E}_k + \mu - E_g < 0.$$

are simultaneously fulfilled. It follows from the first that $\mu > 0$, and from the second (for $E_g < 0$) that $\mu < 0$, i.e., the levels with $k \neq 0$ cannot be filled. For $k=0$ the levels begin to be filled when $-\varepsilon_0 - \mu \leq 0$ and $\mu - E_g - \varepsilon_0 \leq 0$, whence follows the condition

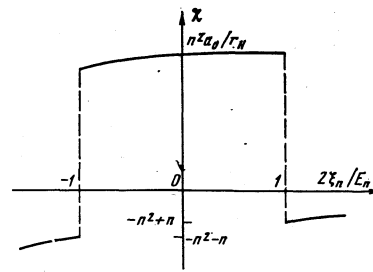


FIG. 5. Behavior of the magnetic susceptibility in the region of the excitonic transition (near the level n): the susceptibility is measured in units of $(\frac{1}{2}\pi d)e^2/mc^2$.

$$2e_0 \geq |E_g|, \quad (30)$$

i.e., the binding energy per $e-h$ pair should exceed the gap. The chemical potential in this case is midway between the bands: $\mu = -|E_g|/2$. As before, we do not consider the region of width T about the point (30).

When

$$(2e_0 - |E_g|)/T \gg 1, \quad (31)$$

dense occupation of the lowest Landau level by electrons in the first band and holes in the second band is favored. With increase of the field the density of electrons and holes increases (together with \mathcal{N}_0) linearly with H . The energy of the new phase is calculated in the same way as in Sec. 2. Under the condition (31) we find

$$F = -\mathcal{N}_0(2E_0 - |E_g|), \quad (32)$$

where we have substituted $\varepsilon_0 = E_0$. The formula (32) is highly visualizable: $2E_0 - E_g$ is the energy gain on creation of an electron-hole pair. The free energy (32) does not depend on T . Only the width of the interval (31) in which the transition to complete occupation occurs is determined by the temperature.

The transition considered is manifested, as in the case of the semimetal, in the behavior of the magnetic susceptibility. At the transition it changes by a jump [extended in the interval (31)] relative to the susceptibility of the electrons in the filled bands. The sign of the jump is determined by the sign of the difference $e/2mc - \mu^*$. The transition is also manifested in the absorption spectra, which, in the ideal case, are line spectra. Before the rearrangement the spectra are determined by transitions of electrons from filled Landau levels of the lower band to empty levels of the upper band. After the rearrangement new series of transitions appear: electrons in the upper band and holes in the lower band undergo transitions from the filled zeroth Landau level to the other (empty) levels.

CONCLUSION

We now discuss the limitations of the model used. Essentially, we have considered the purely two-dimensional case. The effects of the size-quantized transverse motion were not taken into account. But, as in Ref. 6, for a film thickness $d \approx r_H$ allowance for the transverse motion leads to unimportant corrections.

Above, we discussed the rearrangements at Landau levels with a definite spin direction and a fixed quantum number of the transverse motion. Of course, as H is varied, levels with other quantum numbers can also be filled. It is not difficult to take these into account in the framework of the proposed formalism. When this is done the results are not changed qualitatively.

We present some numerical estimates. The calculated effects can be observed (with values of $a_0 \sim 100 \text{ \AA}$, which are usual for semimetals) in fields $H \gtrsim 10^5 \text{ G}$ in films with thickness $d \lesssim 100 \text{ \AA}$ at temperatures $T \lesssim 10 \text{ K}$. By increasing the dielectric permittivity of the support these requirements can be weakened. The singularities of the magnetic susceptibility, including the jumps (with a change of sign in sufficiently strong fields) in transitions to the excitonic phase, can be observed experimentally. Numerically, the value of χ can be very considerable: its ratio (in the normal phase) to the susceptibility of the three-dimensional semimetal is n^2/dp_F (p_F is the Fermi momentum of the three-dimensional semimetal). Although very large n are not achieved in fields satisfying the condition (1), this ratio can be rather large. Optical observations of the changes in the absorption and scattering spectra at the rearrangements are also possible.

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- ¹Since the spin degeneracy is lifted, throughout the paper we consider electrons and holes with a single, well defined direction of the angular momenta, e.g., along the field H .
- ²We do not consider here the trivial semiconductor \Rightarrow semimetal rearrangements associated with the possible change of sign of $E_g(H)$ on variation of H .
- ³The series in the right-hand side of (23) is, of course, convergent: for fixed k and $j \rightarrow \infty$ the factor $I_{jk} \sim j^{-1/2}$, so that for $j \gg k$ a general term of the series is $\sim (E_0/\omega_H) I_{jk}^2/|j-k|$

$\sim (E_0/\omega_H)j^{-2}$. As a result of the summation a numerically small coefficient of r_H/a_0 is obtained.

⁴It is worth mentioning that in the given system the transition temperature $T_{c(n)}$ is not proportional to $\Delta_n(0)$. The dependence of $T_{c(n)}$ on $\Delta_n(0)$ is easily obtained from (24) by substituting $2\xi_n/E_n = (1 - 4\Delta_n^2(0)/E_n^2)^{1/2}$.

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