The Semimetal-Dielectric Phase Transition in a Magnetic Field

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A phase transition involving the formation of a dielectric gap in a semimetal located in a quantizing magnetic field is considered. It is shown that the electron gas exhibits properties of both one-dimensional and three-dimensional systems near the phase transition point under consideration.

1. A phase transition in a semimetal with the formation of a dielectric gap in the absence of a magnetic field has been investigated theoretically in some detail (see, for example, the review of Halperin and Rice[1]). The investigation of the analogous transition in the case of a strong magnetic field is appreciably complicated from the theoretical viewpoint, but is more real from the experimental point of view. The phase transition considered by us has already been observed by Brandt and Chudinov.[2]

For a phase transition in a quantizing magnetic field, the effects connected with the one-dimensional dependence of the energy on the momentum are important. These effects were taken into account in the work of Abrikosov.[3] There, however, the electrons and holes were regarded as a one-dimensional gas, i.e., transverse motion of the charged particles in the magnetic field was not taken into account. In the present work, the features of the correlation functions near the phase transition point are investigated with account of this motion. It is shown that the electron gas in a quantizing magnetic field near the phase transition point under study exhibits properties of both one-dimensional and three-dimensional systems.

2. We shall consider a gas of interacting negatively charged electrons e and positively charged holes h, the spectra of which are isotropic in the plane perpendicular to the magnetic field **H**, and are quadratic along **H** with masses respectively equal to m_e and m_h. Our model differs from real semimetals by the equal number of electron and hole bands. However, it allows an equating of the behavior of the electron-hole gas in the magnetic field with three-dimensional[1] and one-dimensional[3] models. The necessary corrections for the case of a different number of bands have been made in Sec. 6.

We shall assume the magnetic field to be sufficiently strong that all the electrons and holes are concentrated in the zeroth Landau band. Since the number of electrons is equal to the number of holes, their Fermi amplitudes are equal. Under these conditions, as has been shown by Abrikosov,[3] significant multiple scattering takes place of the electrons and holes with small total momentum and with transferred momentum of the order of $\pm 2p_0$. Summation of the principal terms of the perturbation theory series leads to a system of "parquet" equations for the two-particle scattering amplitudes.[3] These equations are shown graphically in Figs. 1–4.

The straight lines in these drawings represent the zero Green's functions of the electrons and holes in the zero Landau band:

$$G_{e,h}(\varepsilon_n, p_z) = (i\varepsilon_n - \xi_{e,h}(p_z))^{-1}.$$

The shaded rectangles represent two-particle scattering amplitudes. All the amplitudes (vertices) depend on the logarithms of the external frequencies and the z components of the momenta, measured from the Fermi boundary and, moreover, on the two transverse momenta. The "parquet" equations of Figs. 1–4 are described by the method of Sudakov,[4] i.e., cross sections are obtained with minimal z-momentum of integration. The indices $e^{\pm}$ and $h^{\pm}$ for the internal lines indicate that integration over the z-momenta of the electrons and holes is carried out close to $\pm p_0$.

As has already been pointed out earlier by the author,[5] it is most natural to consider the scattering amplitudes in the representation of the two-dimensional, total transverse momentum of the electrons and holes. We denote the vertices lying on the left sides of the equations of Figs. 1–4 by

$$\frac{2\pi p_0}{m_e}\Gamma_e(\mathbf{k}), \quad \frac{2\pi p_0}{m_h}\Gamma_h(\mathbf{k}), \quad \frac{\pi p_0}{m^*}\Gamma_2(\mathbf{k}), \quad \frac{\pi p_0}{m^*}\Gamma_3(\mathbf{q}),$$

respectively, where **k** is the transverse momentum transferred from e^- to e^+ or from h^- to h^+, and **q** is the total momentum of e^+ and h^- or of e^- and h^+. The dependence of the logarithmic variables is not shown. The transverse momenta are measured in units of $\hbar/\lambda$, where $\lambda = (hc/eH)^{1/2}$ is the magnetic wavelength, i.e., we have used dimensionless variables.

We note that the choice of a characteristic transverse momentum is not unique. Thus, for example, the vertex of Fig. 3 can be chosen in the representation of a definite **q**. The momenta **k** and **q** are canonically conjugate quantities and play the role of the momentum and coordinate, respectively, for the pair e^+, e^-. For the pairs e^+, h^- and e^-, h^+, their roles change. $\Gamma_2(\mathbf{q})$ and $\Gamma_2(\mathbf{k})$ are connected with one another by the Fourier transform

$$\Gamma_2(\mathbf{k}) = \int \Gamma_2(\mathbf{q}) e^{i\mathbf{k}\mathbf{q}} \frac{d\mathbf{q}}{2\pi}.$$

A simple method of transition from the representation in Landau functions to the representation of two-dimensional momentum is set forth in [5].

We note that the equations of Figs. 1 and 2 for the vertices Γ_e and Γ_h differ only by the bare integration. Since, in the latter, we shall be interested only in the singular vertex parts which are the same for Γ_e and Γ_h, we then set $\Gamma_e = \Gamma_h$ for simplicity and denote them by Γ_1.

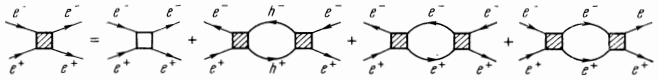

FIG. 1

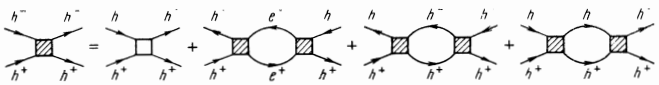

FIG. 2

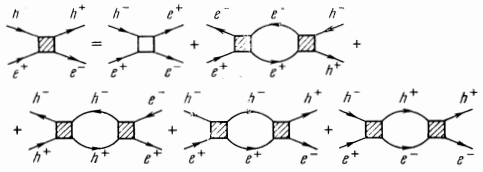

FIG. 3

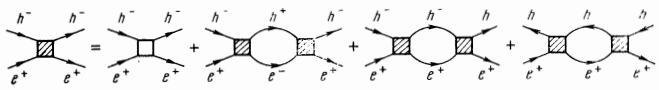

FIG. 4

Evidently, the anisotropic singular solutions for the vertices correspond to excitons with a moment along the field that is not equal to zero, and located in the upper Landau bands. Inasmuch as the fundamental role for the phase transition is played by the low-lying excited states, we can then limit ourselves to the investigation of solutions with zero moment, i.e., we assume that all the vertices depend only on $k = |\mathbf{k}|$ or on $q = |\mathbf{q}|$. Here, in the two-dimensional Fourier transforms, we can immediately carry out integration over the angles, after which they degenerate into the Hankel transformation

$$\int f(q) e^{i\mathbf{k}\mathbf{q}} \frac{d\mathbf{q}}{2\pi} = \int_0^\infty f(q) J_0(kq)\, q\, dq,$$

where $J_0(z)$ is a Bessel function.

In the region in which all the logarithmic variables have the same order, the equations of Figs. 1–4 have the following analytic form:

$$\Gamma_1(k,x) = U(k) + \mu^2 \int_0^x \Gamma_2^2(k,x')\,dx' + \int_0^x \Gamma_1^2(k,x')\,dx' - \int_0^x F_1(k,x')\,dx' \quad (1)$$

$$\Gamma_2(k,x) = W(k) + 2\int_0^x \Gamma_1(k,x')\Gamma_2(k,x')\,dx' - 2\int_0^x F_{23}(k,x')\,dx', \quad (2a)$$

$$\Gamma_2(q,x) = W(q) + 2\int_0^x F_{12}(q,x')\,dx' - 2\int_0^x \Gamma_3(q,x')\Gamma_2(q,x')\,dx' \quad (2b)$$

$$\Gamma_3(q,x) = -V(q) - \int_0^x \Gamma_2^2(q,x')\,dx' - \int_0^x \Gamma_3^2(q,x')\,dx' + \int_0^x F_3(q,x')\,dx', \quad (3)$$

where

$$x = \ln\frac{\varepsilon_0}{\max\{\Omega_n T, v_0|q_z|\}} = \ln\frac{\varepsilon_0}{\max\{\omega_n T, v_0|k_z - 2p_0|\}}$$

(Ω_n, q_z, and ω_n, k_z are respectively the total and transferred frequencies and momenta; one can neglect the difference in the Fermi levels ϵ_0 and velocities v_0 of the electrons and holes with logarithmic accuracy), $\mu^2 = (m_e^2 + m_h^2)/4m_e m_h$,

$$F_{ij}(k,x) = \int_0^\infty \Gamma_i(q,x)\Gamma_j(q,x) J_0(kq)\, q\, dq,$$

$$F_i(k,x) = \int_0^\infty \Gamma_i(k_1,x)\Gamma_i(k_2,x) K(k,k_1,k_2)\, k_1 k_2\, dk_1\, dk_2$$

The kernel $K(k, k_1, k_2)$ is derived in [5]. Here we only recall that this kernel describes the interference of the wave functions of the electron-hole pairs with momenta k_1 and k_2 in the intermediate two-electron state.

3. We shall assume that all the bare interactions are small, i.e., $g = e^2/\pi\epsilon v_0 \ll 1$. The Coulomb interaction for small transfers of the z momentum is characterized by the small dimensionless parameter $\kappa^2 = \lambda^2/r^2$, where r is the Debye screening radius. Therefore, the Coulomb nuclei U and V for the transverse momenta k, q $\ll \kappa^{-1}$ depend weakly on them and have the form $g \ln \kappa^{-2} \approx g \ln g^{-1}$. The bare vertices W(k) and W(q) are characterized by large momentum transfers. ($2p_0$ for direct interaction and P_{eh} for exchange, where P_{eh} is the distance between the extrema of the bands.) Consequently, these interactions are short-range, and in accord with [5] have the form

$$W(k) \approx g e^{-k^2/2}, \quad W(q) \approx g e^{-q^2/2}. \quad (4)$$

Thus, we can assume that the terms with the Coulomb logarithms are appreciably larger than terms of type W.

As was shown in [5], the Coulomb terms reduce to expressions of the form $\Gamma_i^2 - F_i$ which enter in Eqs. (1) and (3). Therefore, for not too large x, the change in the vertices Γ_1 and Γ_3 is determined by terms of the order of W^2x and is small in comparison with U and V. Therefore, we can substitute $\Gamma_1 = U$ and $\Gamma_2 = -V$ in Eq. (2a), and remove the function V(q) (which changes slowly for $q \ll \kappa^{-1}$) from under the integral over q. As a result, we obtain

$$\Gamma_2(k,x) = W(k) + 2\int_0^x (U+V)\Gamma_2(k,x)\,dx_1$$

whence

$$\Gamma_2(k,x) = W(k)\exp\left\{2\int_0^x (U+V)\,dx_1\right\},$$

and similarly for $\Gamma_2(q, x)$.

It is easy to see that perturbation theory is violated when Γ_2 becomes of the order of U, i.e., when $g \ln g^{-1}x \ll 1$. It can be expected that the singularities of all the vertex parts lie in this region. Unfortunately, it has not been possible to connect the solutions near the singularities with perturbation theory. Therefore, we shall investigate below the possible types of singularities of the vertex parts without reference to perturbation theory.

4. In this section, we shall assume that the first singularities over x of all the vertices are achieved simultaneously for $x = x_0 \approx g^{-1}$ and for the corresponding transverse momenta equal to zero. It is then easily seen from Eqs. (1)–(3) that these singularities are poles whose residues are easily determined. Therefore, for small positive $\Delta x = x_0 - x$ and small k and q, the vertices have the following form

$$\Gamma_1(k,x) = (2\Delta x + \alpha k^2)^{-1} + f_1(k,x), \quad (5)$$

$$\Gamma_2(k, x) = \pm \mu^{-1}(2\Delta x + \alpha k^2) + f_2(k, x), \quad (6a)$$

$$\Gamma_3(q, x) = -(2\Delta x + \beta q^2) + f_3(q, x), \quad (6b)$$

$$\Gamma_2(q, x) = \pm(2\Delta x + \beta q^2) + g(q, x), \quad (7)$$

where $\alpha, \beta \approx g^{-1}$.

Since $\Gamma_2(k)$ and $\Gamma_2(q)$ are connected with one another by the Hankel transformation, then the pole of one of them corresponds to a slow decrease in the other at high momenta. To be precise, for large k and q,

$$\Gamma_2(k, x) = \beta^{-1} K_0(k\sqrt{2\Delta x \beta^{-1}}), \quad (8a)$$

$$\Gamma_2(q, x) = \alpha^{-1} K_0(q\sqrt{2\Delta x \alpha^{-1}}), \quad (8b)$$

where $K_0(t)$ is the MacDonald function with asymptote $K_0(t) \approx e^{-t}\sqrt{\pi/2t}$. Thus, near the pole x_0, i.e., near the point of the phase transition, all the interactions become long-range of the Coulomb type with the screening parameter

$$\overline{\varkappa}^2 = 2\alpha^{-1}\Delta x \approx g/\Gamma \ll 1.$$

The corrections to the pole terms are easily determined by substituting the latter in the integral over the transverse momenta. As a result, we obtain expressions of the type

$$F_i \approx g^2 \ln^2(\Gamma/g), \quad (9a)$$

$$F_{ij} \approx g\Gamma. \quad (9b)$$

Substituting Eqs. (5)–(7), (9a) and (9b) in Eqs. (1)–(3), we obtain a set of differential equations for the functions f and g. Solving it, we obtain the result that the nonpolar corrections to the vertices are equal to g ln (Γ/g) in order of magnitude.

5. We now consider the region of applicability of Eqs. (1)–(4). In these equations, only the bare interactions of all the "nonparquet" graphs for the vertices are taken into account. As is well known,[6] in the "parquet" equations, to which the problems of purely one-dimensional phase transitions reduce, the contribution of the unconsidered graphs is small only for $\Gamma \ll 1$. However, in our case, the location changes appreciably, thanks to the presence of "fast" integrations over the transverse moment. Thus, for example, in the diagram of Fig. 5, the integrations are carried out over the three transverse momenta, apart from a single logarithmic integration. The contribution of this diagram to $\Gamma_1(k, x)$ for $k = 0$ has the form

$$\int_0^x dx \int_0^\infty dk_1\, dk_2\, dk_3\, dk_4 \Gamma_1(k_1, x)\Gamma_2(k_2, x)\Gamma_3(k_3, x)\Gamma_4(k_4, x) J_0(k_1 k_3) \times J_0(k_2 k_4) J_0(k_3 k_4)$$

and, as is easy to see, does not exceed g^3. Similar situations occur also in the more complicated diagrams.

The contribution of the "nonparquet" diagrams with a large number of singular vertices becomes large only for sufficiently small $\tau = (T - T_c)/T_c$, when the nonlogarithmic integrations over the longitudinal momenta

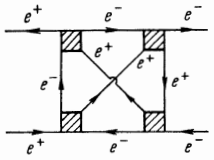

FIG. 5

become significant. In this case, we can rewrite the solutions (5)–(7) as

$$\Gamma(k, k_z) = a[\tau + c(v_0 k_z / T_c)^2 + \alpha k^2]^{-1},$$

where a, c ≈ 1, i.e., they have the form of bare correlation functions of a three-dimensional (anisotropic) system. We further note that all the kernels with which the integrations have been carried out over the transverse momenta are of the order of unity at low momenta. Consequently, in this region, the phase transition has a purely three-dimensional character with the correlation fluctuations corresponding to this dimensionality and the singularities of the thermodynamic quantities. The equations of Figs. 1–4 and their solutions (5)–(7) are valid, in turn, over the entire range of temperatures where the theory of the self-consistent field is applicable.

6. It is seen from Eqs. (1)–(3) that in the case of an arbitrary interaction, a situation can arise in which, for example, only $\Gamma_1(k, x)$ and $\Gamma_2(k, x)$ have polar singularities. Here $\Gamma_2(q, x)$ has a logarithmic singularity and $\Gamma_3(q, x)$ and the corrections f_1 and f_2 are finite. The reverse situation is also possible, where the polar singularities are possessed only by $\Gamma_2(q, x)$ and $\Gamma_3(q, x)$.

Further, the case can occur in which, for example, $\Gamma_1(k, x)$ has a pole and $\Gamma_2(k, x)$ does not. It is easy to see that for this it is necessary that the condition

$$2\int_0^{x_0} F_{23}(k, x_1) \exp\left\{-2\int_0^{x_1} \Gamma_1(k, x_2)\, dx_2\right\} dx_1 = W(k).$$

be satisfied. On the left side of this equality, the integral over x_1 is not sensitive to the existence of singularities in the vertices and, consequently, this condition can be satisfied only randomly for isolated values of k. Thus, these cases do not give information on the behavior of the vertices near the first singularity.

And, finally, we consider the case in which the first singularity lies at $k = k_0 \neq 0$. In this case, polar solutions of the type (5)–(7) are possible, but we must write $(k - k_0)^2$ in the denominators in place of k^2. Such a substitution changes only the form of the corrections. It is easy to obtain the result that all the corrections are equal to $(g\Gamma)^{1/2}$ in order of magnitude.

For real semimetals, where, in contrast with the model considered above, the Fermi momenta of the electrons and holes are not equal (in bismuth, for example, they differ by a factor of three), the vertex Γ_2 is forbidden by the law of conservation of the z component of the momentum. Simultaneously, the equations of Fig. 3 and Eqs. (2a) and (2b) corresponding to it lose their meaning.[1)] The equations of Figs. 1, 2, and 4 and

[1)] The author is grateful to A. A. Abrikosov who called his attention to these circumstances.

Eqs. (1) and (3) corresponding to them remain in force if the terms containing Γ_2 in them are deleted. As a result, the equations for Γ_1 and Γ_3 take the following form:

$$\Gamma_1(k,x) = U(k,x) + \int_0^x \Gamma_1^2(k,x_1)\,dx_1 - \int_0^x F_1(k,x_1)\,dx_1, \qquad (10a)$$

$$\Gamma_3(k,x) = -V(k,x) - \int_0^x \Gamma_3^2(k,x_1)\,dx_1 + \int_0^x F_3(k,x_1)\,dx_1. \qquad (10b)$$

As before, Eqs. (10a) and (10b) have polar solutions which, however, do not now depend on one another. This means that the intraband and interband phase transitions, which correspond to the singularities of the vertices Γ_1 and Γ_2, can occur at different temperatures, depending on the bare interactions U and V.

As was shown in [5], in equations of the type (10a) and (10b), the terms containing the Coulomb logarithms are contracted. Consequently, the temperatures of the transitions are determined only by the short-range parts of the bare interactions.

7. The character of the phase transition is determined by the singularities of the generalized susceptibility of the system. The singularities of the vertex parts considered above show that it is necessary to investigate the susceptibility of the system $\Pi_1(k, \mathbf{x})$, $\Pi_2(k, \mathbf{x})$, and $\Pi(q, \mathbf{x})$ to perturbations of the following types, respectively:

$$\sum_{p_x} e^{ip_x k_y} a_\pm^+(p_x + k_x) a_\mp(k_x), \qquad (11a)$$

$$\sum_{p_x} e^{ip_x k_y} b_\pm^+(p_x + k_x) b_\mp(k_x), \qquad (11b)$$

$$\sum_{p_x} e^{ip_x q_y} a_\pm^+(q_x - p_x) b_\mp^+(p_x), \qquad (11c)$$

where $a_\pm(\mathbf{p_x})$ and $b_\pm(\mathbf{p_x})$ are the annihilation operators of electrons and holes with transverse momenta $\mathbf{p_x}$ and longitudinal momenta near $\pm p_0$. The expressions (11a)–(11c) represent the creation operators of electron-hole pairs with definite transverse momentum k or q. Moreover, we determine the nondiagonal susceptibility $\Pi_3(k, \mathbf{x})$, which represents the amplitude of the transition of the excitation (11a) to the excitation (11b). All these functions are proportional to the corresponding polarization operators and are easily determined by the method of Larkin and Khmel'nitskiĭ.[7] As a result, it is shown that all the generalized susceptibilities have singularities of the form

$$\Pi_i(k,x) \approx c_i(2\Delta x + \alpha(k-k_0)^2)^{-1},$$

$$\Pi(q,x) \approx c(2\Delta x + \beta(q-q_0)^2)^{-1},$$

where c_i, $c \approx v_0^{-1}$. In the cases considered in Sec. 6, the indicated singularities are possessed by either $\Pi_i(k, \mathbf{x})$ or by $\Pi(q, \mathbf{x})$. For real semimetals, the susceptibility $\Pi_3(k, \mathbf{x})$ loses its meaning.

The singularities of the generalized susceptibility indicate the presence of a phase transition for $T = T_c = \epsilon_0 e^{-\mathbf{x}_0}$. On the basis of the form of these singularities, it can be concluded that the average of the operators (11a) and (11b) in the new phase will differ from zero for $q = q_0$, $q_z = 0$, or for $k = k_0$ and $k_z = \pm 2p_0$. The ground state, as in the one-dimensional model of Abrikosov, is characterized by the presence of a condensate of electron-hole pairs. The spectrum of single-particle excitations has a gap $\Delta(\mathbf{x}) = T_c\varphi(\mathbf{x})$, which, by virtue of the homogeneity of the system, does not depend on $\mathbf{p_x}$. For determination of the function $\varphi(\mathbf{x})$ even with logarithmic accuracy, it is necessary to know the behavior of the vertices far from the singularity, which is impossible within the framework of the present research. We only note that, in contrast with the one-dimensional model of Abrikosov,[3] or the problem of one-dimensional superconductivity,[6] where the function $\varphi(\mathbf{x})$ formally diverges on the Fermi surface, here $\varphi(\mathbf{x})$ tends to a finite limit of the order unity. This is connected with the fact that blocks enter into the equation for the determination of the gap that are irreducible into channels giving the principal polar singularity.

The formation of a condensate of electron-hole pairs is accompanied, in addition to the usual jump in the thermal capacity, by a jump in the magnetic susceptibility χ. The value of the latter is easily estimated from the expression for the contribution to the thermodynamic potential which is identical with the analogous expression in the theory of superconductivity

$$\Delta\Omega \approx -\frac{dn}{d\varepsilon_0}\frac{\Delta^4}{T_c^2},$$

whence

$$\Delta\chi \approx \frac{1}{\hbar^2 v_0 \lambda^2}\left(\frac{dT_c}{dH}\right)^2 \qquad (12)$$

Substituting in (12) the expression for T_c, we obtain the following estimate

$$\Delta\chi \approx \frac{n}{\varepsilon_B}\left(\frac{d\varepsilon_g}{dH}\right)^2,$$

where n is the density of electrons or holes, $\epsilon_B = me^4/\epsilon^2\hbar^2$, ϵ_g the overlap of the electron and hole bands. The value of the jump $\Delta\chi$ is several times greater (in the ratio ϵ_g/ϵ_B) than the phonon susceptibility of the Fermi gas and can therefore be suitable for experimental observation.

In the case in which the condensation takes place in a state with momentum $\mathbf{k}_0$ (or $\mathbf{q}_0$) different from zero, a dipole moment $\mathbf{P} = N\mathbf{P}_0$ should be observed, where N is the electron density in the condensate and $\mathbf{P}_0 = e\lambda^2\mathbf{k}_0$ is the dipole moment of a single exciton. The expression cited by us for $\mathbf{P}_0$ follows from the fact that (see the work of Gor'kov and Dzyaloshinskiĭ[8]) the vector $\lambda^2\mathbf{k}_0$ (or $\lambda^2\mathbf{q}_0$) represents the average distance between the electron and the hole, found in a state with a definite total momentum.

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