Diamagnetic anomalies in systems with spontaneous toroidal current

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The behavior of a system with spontaneous current in a homogeneous magnetic field has been studied. The homogeneous magnetic field induces a current order parameter localized in the region of inhomogeneity of the spontaneous order parameter. A scheme for calculating the susceptibility in the vicinity of the transition point is proposed that is based on the establishment of the balance of forces and makes it possible to take into account the dynamic effects in the magnetic field. For magnetics and ferroelectrics, the balance-of-forces scheme is equivalent to the conventional procedure of minimization of the free-energy functional. The magnetic susceptibility of the system is calculated below the point of transition to the current state. The susceptibility is of diamagnetic character, and its magnitude is determined by the square of the current correlation length λ_c. A distinctive feature of the current state is a specific coordinate dependence of the expression for current, ensuring a zero total moment of the current contour. A model in which the diamagnetic susceptibility can assume values close to that of an absolute diamagnetic is described. In conclusion, the behavior of the current state in a magnetic field at $\tilde{T} = 0$ is discussed in terms of a microscopic scheme.

1. INTRODUCTION

In their behavior in a magnetic field, all substances can be divided into two groups: paramagnetics and diamagnetics.[1] The paramagnetics include substances with susceptibility values covering a range of many orders of magnitude. The susceptibility of all known diamagnetics, however, varies over a fairly narrow range.[2] In a class by themselves are superconductors, which are absolute diamagnetics, i.e., substances that completely expel a magnetic field (Meissner effect). Simultaneously with the Meissner effect, superconductors have infinite conductivity. It is natural therefore to consider the possibility of the existence of low-conductivity substances with a high diamagnetism of a nonsuperconducting character.

The present work shows that the current state[3,4] can be used as an example of such a highly diamagnetic state of a collective but not superconducting character. As has now become clear, the current state is more accurately referred to as the toroidal state (TS), since it is related to the ordering of local toroidal moments (Ref. 5).[1)] The position held by the TS in the conventional classification of the states of a solid[1] is determined by the symmetry properties of the solid.

We shall consider an isotropic case in which the macroscopic properties of a solid can be described by means of a vector. Then there exist four vectors which realize irreducible representations of a group formed by the operations of space and time inversion. There are the polar vector **P**, which is symmetric with respect to the time inversion, the polar vector **T**, which changes sign when time is inverted, the axial vector **M**, which has antisymmetry with respect to the time inversion, and the vector **G** symmetric with respect to both the space and time inversion. To each of the vectors one can set in correspondence a specific type of ordering in the solid.[5] Ferroelectric properties correspond to the vector **P**. When the system is described by vector **M**, the ordering is of a magnetic character. The symmetry of vector **G** coincides with that of the moment flux-density vector $d\mathbf{M}/dt$. It can be shown that the appearance of vector **G** against a background of ferroelectric or magnetic ordering corresponds to an orientation-type phase transition, and the transverse susceptibility diverges at the transition point. If, however, the ordering is characterized by vector **T**, the system possesses the magnetoelectric effect,[1,5] and the vector **T** is then the antisymmetric component of the magnetoelectric tensor. Toroidal magnetoelectrics form a subset of the aggregate of magnetic-symmetry classes in which antiferromagnetism is possible. In the toroidal state, however, there is an additional lowering of symmetry relative to antiferromagnetics and is due to a violation of invariance to space inversion. Toroidal magnetoelectrics should also be distinguished from ferromagnetics, where the violation of space and time symmetry takes place independently and is described by the vectors **P** and **M**. Both the spontaneous polarization **P** and the spontaneous magnetization **M** are equal to zero in the toroidal state.

Electric, magnetic, and toroidal moments generate three independent families of electromagnetic multipoles.[5] The description of a system with specified distributions of electron density $\rho(r)$ and current density $j(r)$ in external electric and magnetic fields is not complete unless all three types of multipoles are considered. The vector **G**, in contrast to the other three vectors, is generally not related to any particular type of electromagnetic ordering, but is a particular case of the tensor order parameter describing the field of the displacements in structural and orientational transitions.

Ascher[6] noted that the symmetry of vector **T** coincides with the symmetry of the current-density vector. It would seem that in the toroidal state, the existence of spontaneous currents of density

$$\mathbf{j}(\mathbf{R}) \sim \mathbf{T}(\mathbf{R}) \tag{1}$$

is possible. In the case of an inhomogeneous order parameter $\mathbf{T}(\mathbf{R})$ such that $\langle \mathbf{T}(\mathbf{R}) \rangle = 0$, Bloch's theorem for current (1) is

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fulfilled. However, the existence of current of type (1) is forbidden by the requirement of gauge invariance. Indeed, to the spontaneous current (1) there corresponds a contribution to the energy functional $\delta F = \mathbf{j}\cdot\mathbf{A} \propto -\mathbf{A}\cdot\mathbf{T}(\mathbf{R})$, where $\mathbf{A}$ is the vector potential. Then minimization of the functional with respect to order parameter $\mathbf{T}$ causes the appearance, in the induced order parameter and correspondingly in the energy, of a gauge-noninvariant contribution proportional to the vector potential, and this is impossible. The erroneous conclusion reached in Ref. 6 concerning the possibility of the Meissner effect in TS is actually due to the choice of an incorrect expression for the spontaneous current. The correct gauge-invariant expression for the density of spontaneous current in an inhomogeneous toroidal state, in an approximation linear in $\mathbf{T}(\mathbf{R})$, is of the form[7]

$$\mathbf{j}(\mathbf{R}) = (e/m)\tilde{\gamma}\ \mathrm{rot}\,\mathrm{rot}\,\mathbf{T}(\mathbf{R}), \tag{2}$$

where e is the electron charge, m is the electron mass, and $\tilde{\gamma}$ is a coefficient determined by the details of the microscopic model.

An assessment of the conditions under which the toroidal state is realized requires a microscopic analysis. The microscopic nature of the TS is due to the instability of a system with congruent proportions of the Fermi surface relative to electron-hole pairing.[8] The new state is described by introducing a certain self-consistent potential or order parameter $\Delta(\mathbf{R})$. This potential is the equivalent of crystal potential and it has the following distinguishing features:

(1) possibility of both singlet and triplet spin structure of the potential;

(2) leeway in the phase of the potential, corresponding to different phase shifts of the wave functions of the electrons and holes participating in the pairing.

It was found that thanks to the presence of these degrees of freedom in the model, the latter successfully describes the most diverse states of the solid, i.e., orbital[9] and spin[10] ferromagnetism, antiferromagnetism,[11,10] intrinsic and nonintrinsic ferroelectricity,[12] as well as TS.[4] In the model of Ref. 8, the role of vector $\mathbf{T}$ is played by the product $\mathbf{P}_{12}\mathrm{Im}\Delta^s(R)$, where $\mathbf{P}_{12}$ is the interband matrix element of the momentum (hybridization), and $\mathrm{Im}\Delta^s(\mathbf{R})$ is the singlet imaginary component of the potential. To the polarization $\mathbf{P}$ corresponds $\mathbf{P}_{12}\mathrm{Re}\Delta^s(R)$, and to the magnetic moment corresponds $\mathrm{Re}\Delta^t(R)$ or $\mathbf{L}_{12}\mathrm{Im}\Delta^s$, where $\mathbf{L}_{12}$ is the interband matrix element of the angular momentum, and to vector $\mathbf{G}$ corresponds $\mathrm{Im}\Delta^t$ or $\mathbf{L}_{12}\mathrm{Re}\Delta^s(R)$. The main feature of the model is the fact that it admits of asymptotically exact solutions in the weak-interaction limit, when it is possible to indicate system parameters at which one or another of the indicated states will be realized. In another limiting case—that of the model of a semiconductor with a band gap a little smaller than the exciton binding energy[11]—the smallness parameter is the density of the exciton Bose condensate.[13] The interaction in this case is strong but, as before, a multicomponent potential can be introduced. It should therefore be expected that the results obtained with the model involving weak binding and congruent portions of the Fermi surface are not unique and remain qualitatively in force for an intermediate value of the interaction in the presence of partial congruence. As the deviation from congruence increases, there is an increase in the critical value of the interelectron interaction, above which one of the indicated phase transitions or a series of them is possible.

Depending on the ratio of the Coulomb electron-hole interaction constants, either a ferroelectric state ($\mathrm{Re}\Delta^s$) or an antiferromagnetic state ($\mathrm{Re}\Delta^t$) is realized in the limit of an arbitrarily weak interaction. The state with $\mathrm{Im}\Delta^s$, however, can be realized, for example, at a sufficiently high concentration of the charged impurity, to the scattering from which the ferroelectric[14] (antiferromagnetic) state is more sensitive than the toroidal state. Other ways of realizing the toroidal states are also possible.[15] Most favorable to the appearance of $\mathrm{Im}\Delta^s$ are the regions of the domain walls of electron ferroelectrics.[16] Suitable objects are direct-band narrow-gap semiconductors and semimetallic compounds[17] (for which the extrema of the conduction and valence bands coincide in momentum space). The coincidence of the extrema of the bands may itself result from a phase transition, i.e., in the initial phase the congruent regions of the spectrum may be separated in momentum space.

The central problem of TS theory is that of the response of the system to a magnetic field. Let us emphasize that we are dealing with the collective component of the response, caused by interelectron interaction, and not with the one-electron contribution to the response. The latter is primarily determined by the effective masses of electrons and holes, and also by the spin-orbit interaction.[18] The possibility of high diamagnetism of the TS was attributed in Ref. 19 to diamagnetic Larmor precession in a current contour in a magnetic field. However, the consideration of Larmor precession alone when determining the response is justified only in the case of "rigid" wave functions, as is the case in superconductors, and leads to the Meissner effect. In our case, such rigidity is absent, and the change in wave functions corresponds to the paramagnetic contribution and offsets the London term in the response.[20] In Ref. 20, the collective component of the magnetic susceptibility above the transition point to the TS was calculated by minimizing the free-energy functional $\tilde{F}\{\mathbf{T}\}$. In the approximation linear in the magnetic field $\mathbf{B}$

$$\tilde{F}\{\mathbf{T}\} = F\{\mathbf{T}\} - \int d\mathbf{R}\,\frac{e}{m}\,\tilde{\gamma}\mathbf{B}\,\mathrm{rot}\,\mathbf{T}, \tag{3}$$

where $F\{\mathbf{T}\}$ is the usual Landau functional in the absence of a field. In the functional (3) we omitted the term $\chi_f\mathbf{B}^2$ quadratic in the field. The contribution made by order parameter $\mathbf{T}$ to the coefficient χ_f is due to the renormalization to $\mathbf{T}$ of the one-electron spectrum. It was shown in Ref. 20 that above the transition point, the procedure of minimization of the functional is equivalent to summing, in the expression for the current, the ladder diagrams responsible for exciton instability. The susceptibility χ' of the system is determined by the relation $\mathbf{j}_q = \mathbf{q}^2\chi'_q\mathbf{A}_q$, where $\mathbf{A}_q \perp \mathbf{q}$ is different from zero only in the case of an inhomogeneous field ($\chi' \propto q^2, B_q \propto qA_q$) and diverges in paramagnetic fashion at the point of transition to the TS. The order parameter determined from the condition $\delta\tilde{F}/\delta T = 0$ is also induced only by an inhomogeneous field ($T_{\mathrm{in}}\,d \propto qBq$).

The purpose of the present work was to study the response of the system to a homogeneous magnetic field below the point of transition to the TS. Section 2 proposes a scheme for determining the ground state of the system in an external field, free from the necessity of integrating by parts in the minimization of the functional. The scheme is local in character and based on the establishment of the balance of the forces in the system. For ordinary ferromagnetics and ferroelectrics, the scheme of establishment of the balance of forces is equivalent to the procedure of minimization of the functional and gives a Curie-Weiss type law for susceptibility.

The scheme proposed is used in Sec. 3 to describe the RS in a magnetic field near the transition point in various models of order-parameter inhomogeneity: in the model of a single domain wall, in a Fuld-Ferrel-Larkin-Ovchinnikov type model, and in the model of built-in inhomogeneity, when the system is described by Landau's functional with coordinate-dependent coefficients. The induced order parameter proves to be localized in the region with spontaneous current. The susceptibility of the TS is diamagnetic in character, and its magnitude is determined by the new characteristic scale of the theory—the effective radius of current correlations λ_t, so that

$$\chi' = \chi_L (\lambda_T / r_a)^2, \tag{4}$$

where χ_L is the Landau diamagnetic susceptibility, and r_a is a distance of interatomic order of magnitude (usually $\lambda_t \gg r_a$). In a system with built-in inhomogeneity, which may be due to the presence of domain walls, to an inhomogeneous distribution of the impurity, etc., the magnitude of the susceptibility in the vicinity of the point of transition to the TS can reach values close to the susceptibility of an absolute diamagnetic, reaching the value (4) as the temperature is lowered.

In Sec. 4, to describe the TS in a magnetic field at $T = 0$, a microscopic calculation scheme was developed for the case of a domain-wall type inhomogeneity. The results obtained are consistent with the results of the phenomenological calculation in Sec. 3.

2. THE BALANCE-OF-FORCES SCHEME

The procedure of minimization of the functional, used in Ref. 20 for calculating the magnetic susceptibility of the TS, describes the reaction of the TS only to an inhomogeneous magnetic field with curl $B \neq 0$. Actually, this procedure is a static one and does not consider the dynamic effects associated with the behavior of the circuit and of the current lines as a whole a magnetic field. Accordingly, the precession in the circuit and the associated diamagnetic component of the response are not considered in the classical sense. From a formal standpoint, the absence of a response to a homogeneous field is due to the integration by parts of the gradient terms during the minimization of the functional. In this approach the surface contribution, which contains information on the response of the system to an external homogeneous field, is discarded. The fact that the interaction of the TS with a homogeneous field is determined precisely by the surface contribution follows directly from the expression for the term expressing the interaction of the current order parameter with the field in the free-energy functional (3). A constant **B** this term is a total derivative and reduces to a surface integral.

This section presents a scheme for determining the ground state of a system described by Landau's functional, based on the establishment of the balance of forces. The scheme permits a local and explicit consideration of the boundary conditions on the surface. The basic idea of the proposed approach is the description of the interaction of the system with the field, not in energy terms, as is usually the case,[1] but in terms of the force characteristics. The switching-on of the field gives rise to an external force. The equilibrium value of the order parameter is determined from the condition of balance of the external and internal forces. The latter result from deformation of the system, i.e., from the appearance of an induced component in the order parameter. Both the external and internal forces stem only from the derivatives with respect to the coordinate of the order parameter. The approach developed is therefore aimed at essentially inhomogeneous systems.

We shall proceed from the expression for free energy density $\mathscr{F}(\mathbf{R})$ in the absence of a field and confine the discussion to the dependence $\mathscr{F}(\mathbf{R})$ only on the first derivatives with respect to the coordinate of the order parameter: $\mathscr{F}(\mathbf{R}) = \mathscr{F}[T(\mathbf{R}), \nabla T(\mathbf{R})]$. Extension to the case of higher derivatives is not difficult. To describe the reaction to an external force, we must exclude from the free energy $\mathscr{F}(\mathbf{R})$ the energy of internal stresses $\mathbf{f}_{\text{int}}$. These stresses are also present in the absence of an external field and are due to the spatial inhomogeneity of free energy density

$$\mathbf{f}_{int}(\mathbf{R}) = \nabla \mathscr{F}(\mathbf{R}). \tag{5}$$

Internal stresses $\mathbf{f}_{\text{int}}$ can be caused by the imposition of specific boundary conditions as well as by the characteristics of collective interactions in the system, as for example in the formation of the inhomogeneous state of superconductors in the internal magnetizing field.[21] An important type of so-called built-in inhomogeneities will be examined in the next section.

In the ground state, the function $\mathscr{F}(\mathbf{R})$ in Eq. (5) minimizes the free-energy functional $F\{T\} = \int \mathscr{F}(\mathbf{R}) d\mathbf{R}$. This means that the free-energy density satisfied the Euler equation

$$\frac{\partial \mathscr{F}}{\partial T} - \frac{\partial}{dx} \frac{\partial \mathscr{F}}{\partial \nabla T} = 0, \tag{6}$$

which is obtained by minimizing the functional $F\{T\}$ (here and below, for the sake of simplicity, we shall consider the dependence of $\mathscr{F}(\mathbf{R})$ on a single coordinate).

Having determined the density of internal stresses $\mathbf{f}_{\text{int}}$ in Eq. (5) by means of the Euler equation (6), we find that in a state of equilibrium

$$U(x) = \text{const}. \tag{7}$$

The function $U(x)$ is related to the free energy density as follows:

$$U = \mathscr{F} - \nabla T (\partial \mathscr{F} / \partial \nabla T). \tag{8}$$

The extension of Eq. (8) to the case of dependence of $\mathscr{F}$ on

$\nabla^2 T$ is as follows:

$$U=\mathcal{F}-\nabla T\frac{\partial \mathcal{F}}{\partial \nabla T}-\nabla^2 T\frac{\partial \mathcal{F}}{\partial \nabla^2 T}+\nabla T\frac{d}{dx}\frac{\partial \mathcal{F}}{\partial \nabla^2 T}. \quad (8')$$

Equality (7) signifies that the free energy density of the system minus the energy of inhomogeneity retains a constant value. Equation (8) resembles formulas that relate various thermodynamic potentials to one another and accomplish the transition from some independent variables to others. The function U, however, is not some thermodynamic potential, for when the external medium specifying the boundary conditions is neglected U does not have a minimum in the state of equilibrium. Equation (7) makes it possible to consider the boundary conditions in local form at any point of the system, since the boundary conditions determine the value of the constant in Eq. (7). When the determination of the constant in Eq. (7) is difficult, for example, for a periodic solution of $T(x)$, use may be made of an alternative form of the equilibrium equation (7)

$$\nabla U(x)=0. \quad (7')$$

The introduction of an external field signifies the appearance in Eq. (7') of a force exerted by the field on the system

$$\nabla U(x)=-f_{ext}. \quad (9)$$

In this case $U(x)$ in Eq. (9), in contrast to Eq. (7'), is a function of an order parameter already dependent on the field. The interaction of the order parameter with the field is described by the right side of Eq. (9). Equation (9) is the fundamental relationship of the balance-of-forces scheme.

The equilibrium state of a system in a field is usually determined from the Euler equation (6), written for the free energy density in a field $\tilde{\mathcal{F}}(x)$. Thus, to describe a system in an external field, there are two possibilities: the Euler equation and the equilibrium equation. We shall discuss the areas of their applicability. Depending on the form of the term for the interaction of the order parameter with the field in the expression for the free energy density in a field $\tilde{\mathcal{F}}(x)$, two cases are possible. We shall discuss the areas of their applicability. Depending on the form of the term for the interaction of the order parameter with the field in the expression for the free energy density in a field $\tilde{\mathcal{F}}(x)$, two cases are possible.

(1) The interaction of order parameter Δ with field h is described by a term simply proportional to the order parameter, not to its derivatives:

$$\tilde{\mathcal{F}}=\mathcal{F}-h\Delta.$$

This case corresponds to ordinary ferroelectrics and ferromagnetics with interaction terms $\mathbf{P}\cdot\mathbf{E}$ (where $\mathbf{P}$ is the polarization and $\mathbf{E}$ is the electric field) and $\mathbf{M}\cdot\mathbf{B}$, respectively. For a ferromagnetic, the Lorentz force

$$\mathbf{f}_{ext}=[\mathbf{j}\times\mathbf{B}],$$

acting on internal currents $\mathbf{j}=\operatorname{curl}\mathbf{M}$, appears on the right side of Eq. (9). The equilibrium equation in this case reduces to the form

$$\left[\left(\frac{\partial \tilde{\mathcal{F}}}{\partial \mathbf{M}}-\frac{d}{dx}\frac{\partial \tilde{\mathcal{F}}}{\partial \operatorname{rot}\mathbf{M}}\right)\operatorname{rot}\mathbf{M}\right]=0. \quad (10)$$

The first factor in the vector product (10) is the left side of the Euler equation (6), written for the free energy density in an external field $\tilde{\mathcal{F}}$. Hence for a ferromagnetic, the Euler equation and equilibrium Eq. (9) are equivalent. An analogous statement is also easily proven for ferroelectrics. In the case of ferroelectrics, $\mathbf{f}_{ext}$ should be taken to mean the force exerted by the field on the internal charges:

$$\mathbf{f}_{ext}=\mathbf{E}\rho_{int}, \quad \rho_{int}=-\operatorname{div}\mathbf{P}.$$

(2) The interaction of the order parameter with the field is determined by the derivatives of the order parameter with respect to the coordinate. The linear response to a homogeneous field in this case is described by an equilibrium equation: TS (3) is precisely an example of a system with a field dependence of the indicated type. It should be emphasized that in the absence of a field, the structure of the TS (and of any other system) is described by the Euler equation (6), while the quantity U (8) is simply the first integral of the Euler equation. The problem of correct description of the boundary conditions and the associated necessity of switching from the Euler equation to the equilibrium equation arise only when the external field is turned out. Let us note that the equilibrium equation actually represents the results of averaging of Hamilton's equation

$$\partial \hat{H}/\partial \mathbf{r}=-\dot{\hat{\mathbf{p}}} \quad (11)$$

over the ground state of the Hamiltonian $\hat{H}$ of the system (here $\hat{\mathbf{p}}$ is the momentum operator) if the quantum-mechanical analog of the Lorentz equation is used to write the right side of Eq. (11).

We write the equilibrium equation for the TS:

$$\frac{dU}{d\mathbf{R}}=\frac{e}{m}\tilde{\gamma}[\mathbf{B}\operatorname{rot}\operatorname{rot}\mathbf{T}]. \quad (12)$$

If Eq. (12) is written in Fourier components, the left side will be a vector parallel to q. Expanding the vector product for the right side of Eq. (12), we obtain

$$\mathbf{f}_{ext}=(e/m)\tilde{\gamma}\{q^2[\mathbf{B}\times\mathbf{T}]-(\mathbf{qT})[\mathbf{B}\times\mathbf{q}]\}. \quad (13)$$

A term perpendicular to q then appears on the right side of Eq. (12). The apparent contradiction is resolved by the fact that in the approximation considered (with a single anisotropy axis parallel to $\mathbf{T}$), the system will be restructured by an arbitrarily weak field to a state with $\mathbf{q}\perp\mathbf{B}$, and the second term in Eq. (14) will become zero. As indicated in Ref. 16, the condition of free-energy minimum specifies the direction $\mathbf{q}\perp\mathbf{T}$. In the plane normal to $\mathbf{T}$, however, degeneracy along the $\mathbf{q}$ direction takes place. A magnetic field lifts this degeneracy. As the transition point is approached from above in the TS in the presence of a magnetic field, an order parameter is immediately realized such that $\mathbf{q}\perp\mathbf{B}$. The orientation of the current contours becomes perpendicular to the magnetic field, and the Lorentz force turns our automatically to be parallel to q.

On the left side of Eq. (12) is a force arising from the displacement of internal coordinates on δR in the direction of the force, i.e., in the direction of performance of work on the body. A question may arise as to the physical basis of equating this force, which does work, to the Lorentz force, which does none. Indeed, the Lorentz force does no work. However, in a conductor (or, as in our case, in a volume

element) moving under action of the Lorentz force, there is induced an electric field $\mathbf{E}=\mathbf{v}\cdot\mathbf{B}$, where $\mathbf{v}=\delta\mathbf{R}/\delta t$ is the speed of the motion, and this field in a time δt performs work $\delta A=\mathbf{E}\cdot\mathbf{j}\delta t=-[\mathbf{j}\cdot\mathbf{B}]\cdot\delta R$ (see for example Ref. 1). This explains why Eq. (12), which no longer includes time in explicit form, contains the dynamic effects mentioned at the beginning of this section. The system with current will be restructured until the Lorentz force is balanced by the internal stresses due to the spatial changes of the order parameter. Thus the equilibrium equation (12) describes the situations resulting from the dynamic effect, i.e., a restructuring of the current contours—a situation which, as follows from the discussion below and from the analysis given in the introduction, amounts to the appearance of diamagnetic surface current in the system.

3. INDUCED ORDER PARAMETER AND MAGNETIC SUSCEPTIBILITY NEAR THE TEMPERATURE OF TRANSITION TO THE TOROIDAL CURRENT STATE

We shall use the standard definition of magnetic susceptibility

$$\chi'=-\frac{1}{V}\frac{\partial^2\tilde{F}\{T\}}{\partial\mathbf{B}^2}=-\frac{1}{V}\frac{\partial^2\int\tilde{\mathscr{F}}(\mathbf{R})\,d\mathbf{R}}{\partial B^2}. \tag{14}$$

To determine the susceptibility χ' (14), the value of the order parameter found from the equilibrium equation should be substituted in the expression for the free-energy density of a system in a magnetic field.

We write the expression for the free energy density of the system:

$$\mathscr{F}(T)=\alpha|T|^2+\beta|T|^4+\gamma|\nabla T|^2, \tag{15}$$

where $\alpha=a(\tilde{T}-\tilde{T}_c)$ and $\alpha,\beta,\gamma>0$.

Above the temperature of transition to the TS with $\tilde{T}>\tilde{T}_c$, the spontaneous order parameter is equal to zero [$T_0(x)\equiv 0$]. The Lorentz force acting on the induced current appears on the right side of the equilibrium equation (12). It can be shown that for a homogeneous magnetic field, the equilibrium equation with free energy density (15) has no nontrivial solutions when $\tilde{T}>\tilde{T}_c$. For an inhomogeneous field, however, the equilibrium equation gives for the order parameter [and hence, for the susceptibility (14)] a value equal to the result obtained by another method in Ref. 20.

Let us turn to the case $\tilde{T}<\tilde{T}_c$ and consider the situation in which the inhomogeneity of the spontaneous order parameter [and the appearance of spontaneous current (2)] is related to the presence of antisymmetric boundary conditions $T_0(-\infty)=-T_0(\infty)$. The solution of Euler equations which satisfies these boundary conditions is

$$T_0(x)=T_0\,\mathrm{th}\,(x/2^{1/2}\xi_T),\quad \xi_T^2=-\gamma/\alpha,\quad T_0^2=-\alpha/2\beta. \tag{16}$$

The physical meaning of the inhomogeneity of Eqs. (16) is rather obvious. It is a domain wall separating regions of opposite signs of the order parameter. In the state described by the order parameter (16), the spontaneous current (2) and the Lorentz force acting on it (12) are zero at infinity. In the case of a homogeneous magnetic field, this makes it possible immediately to obtain the first integral of the equilibrium equation:

$$\gamma(\nabla T)^2-(e/m)\tilde{\gamma}B\nabla T-\beta(T_0^2-T^2)^2=0. \tag{17}$$

Hence we find the implicitly given expression for the order parameter in a magnetic field:

$$x=2\gamma\int_0^T dT\left\{\tilde{\gamma}\frac{e}{m}B-\left[\frac{e^2}{m^2}\tilde{\gamma}^2B^2+4\beta\gamma(T_0^2-T^2)^2\right]^{1/2}\right\}^{-1/2}. \tag{18}$$

As will be shown presently, the susceptibility is determined by the contribution $T_1(x)$, linear in the field, to the order parameter $T(x)$:

$$T(x)=T_0(x)+T_1(x)+o(B). \tag{19}$$

Since at infinity the order parameter (19) reaches its unperturbed value (16), we have

$$T_1(\pm\infty)=0. \tag{20}$$

From Eq. (18) follows the antisymmetry of the total order parameter $T(x)$ with respect to the coordinate. Hence

$$T_1(x)=-T_1(-x),\quad T_1(0)=0. \tag{21}$$

From Eq. (18) we establish the asymptotics at infinity and at zero:

$$T_1(x\to 0)\sim\frac{e\tilde{\gamma}}{2\gamma m}xB,\quad \max T_1(x\gg\xi_0)\sim\frac{e\tilde{\gamma}}{m(\gamma\alpha)^{1/2}}B. \tag{22}$$

We thus find that even in the linear approximation a homogeneous magnetic field induces an order parameter that is localized in the inhomogeneous region of the spontaneous order parameter (i.e., in the region with spontaneous current) and vanishes at its center. This fact makes it possible to conclude that the susceptibility of the TS is of a diamagnetic character. Let us note that the term of interaction of the order parameter with the field in the functional $\tilde{F}\{\mathbf{T}\}$, having the form $\mathbf{B}$ curl $\mathbf{T}$, becomes zero at the center when the integration involves any solution satisfying the conditions (20) and (21). Therefore, what actually appears in Eq. (14) is $F\{\mathbf{T}\}$, not $\tilde{F}\{\mathbf{T}\}$. Since the minimum of the functional $F\{\mathbf{T}\}$ under the given boundary conditions corresponds to the solution $T_0(x)$ (16), any deviation from $T_0(x)$, for example, depending on the magnetic field (19), leads to an increase in free energy, i.e., the response of the system to the magnetic field is diamagnetic.

To determine the magnitude of the susceptibility, we must separate in $F\{\mathrm{T}\}$ the second-order terms in $T_1(x)$ and first-order terms in $T_2(x)$, where $T_2(x)=0(B^2)$. However, by virtue of the condition of the free energy minimum

$$\delta F/\delta T|_{T=T_0(x)}=0$$

the term containing $T_2(x)$ becomes zero, and the susceptibility is determined exclusively by the contribution to the order parameter linear in the field. We obtain the following estimate for its magnitude from Eqs. (14) and (22):

$$\chi'=cS(m^*/m)^2|\mathbf{P}_{12}|^2\xi_0^2\chi_L. \tag{23}$$

In deriving Eq. (23), we used the expressions for the coefficients of the functional in terms of the microscopic characteristics of the system of Ref. 16 in the model of Ref. 8. In particular, we took account of the fact that $\gamma\sim\xi_0^2$, where ξ_0 is the correlation length of the order parameter. The meaning of the other symbols in Eq. (23) is as follows: c is the

concentration of the domain walls in the sample, m is the mass of the free electron, m^* is the effective mass, $S\sim 1$ is a form factor describing the details of the coordinate dependence of the induced order parameter, and $\chi_L = -e^2k_F/12\pi^2m$ is the Landau diamagnetic susceptibility of the noninteracting electron gas. Assuming $m^* - m$ and omitting an insignificant numerical multiplier, we rewrite Eq. (23) in the form

$$\chi' = \chi_L(\xi_0/r_a)^2|\mathbf{P}_{12}/k_F|^2, \tag{24}$$

where r_a is a characteristic length of the order of atomic size. Thus as follows from Eq. (24), the magnitude of the susceptibility is determined by the square of the correlation length of the order parameter.

In the limit of small hybridizations we have $\xi_0 = v_F/\tilde{T}_c$. However, the real values of hybridization in semimetals are large, of the order of the Fermi energy: $|\mathbf{P}_{12}|\sim k_F$. Hybridization results in a decrease of the fraction of the Fermi surface participating in the formation of the order parameter, and hence, in a decrease of the correlation length. In the limit of large hybridizations, it can be shown that

$$\xi_0^2 \sim v_F^2 m/|\mathbf{P}_{12}|k_F\tilde{T}_c. \tag{25}$$

We then obtain for the susceptibility from (24) and (25) in order of magnitude

$$\chi' \approx (|\mathbf{P}_{12}|k_F/m\tilde{T}_c)\chi_L.$$

It should be emphasized that the abnormally high value of diamagnetic susceptibility is not due to the large radius of the current loops, but rather, to the large radius of the electron current correlations. According to the well-known Langevin formula, the diamagnetic susceptibility of an individual electron is proportional to the area of the orbit which it describes. However, the number of orbits per unit area is inversely proportional to the area of the orbits. Therefore, a large orbit radius alone cannot ensure a large value of the susceptibility in terms of a unit volume. When the orbits are mechanically imbedded one into the other, the self-induction effect also supresses the increase in diamagnetism. We introduce into Eq. (24) a new characteristic scale of current correlations $\lambda_T = \xi_0|\mathbf{P}_{12}|/k_F$. We then obtain Eq. (4) for the susceptibility. The mechanism, taking place in the TS, of interelectronic correlations in a magnetic field can be interpreted as a mechanism of effective imbedding of orbits of radius λ_T, whereby the correlations suppress the self-induction effect.

In order to analyze in more detail the dependence of the magnitude of the susceptibility on the parameters of the system, we shall consider a model in which the TS is not localized in the region of the domain wall (16), but occupies right away the entire volume of the sample. The inhomogeneous state in this case is related not to the boundary conditions, but to the change in the sign of the coefficient γ of the gradient term in the functional. The point on the phase diagram at which γ becomes zero and the line of transition to the inhomogeneous state begins is called the Lifshitz point. To determine the minimum of the functional, in the vicinity of the Lifshitz point, the free energy density should be supplemented with a term containing higher derivatives of the order parameter:

$$\mathcal{F}_\tau(R) = \mathcal{F}(\mathbf{R}) + \delta|\nabla^2 T|^2. \tag{26}$$

Here $\mathcal{F}(\mathbf{R})$ is given in Eq. (15), and $\delta > 0$. The corresponding term with higher derivatives

$$\mathbf{j}' = (e/m)\tilde{\delta}\ \mathrm{rot\ rot\ grad}^2\,\mathbf{T}(\mathbf{R}) \tag{26'}$$

should also be added to the expression for current (2) and for the Lorentz force (12).

Like the model (15), the model (26) permits an exact solution for the order parameter, namely, a solution of the form

$$\mathbf{T}_0(\mathbf{R}) = \mathbf{T}_0 \exp(i\mathbf{q}_s\mathbf{R}).$$

Let

$$\gamma = g(\tilde{T} - \tilde{T}_c^q), \quad \text{with} \quad \tilde{T}_c^q > \tilde{T}_c, \quad g > 0.$$

Then at the temperature $\tilde{T}_c^* = \tilde{T}_c + \gamma^2/4\delta a$ a transition takes place to an inhomogeneous state characterized by the wave vector $\mathbf{q}_s$ and the modulus of order parameter $\mathbf{T}_0$

$$q_s^2 = -\gamma/2\delta, \quad T_0^2 = -\alpha^*/2\beta, \quad \alpha^* = a(\tilde{T} - \tilde{T}_c^*). \tag{27}$$

We find from the equilibrium equation that the homogeneous field induces a homogeneous order parameter

$$T_1 = 2i\frac{e}{m}\frac{\tilde{\gamma}}{\gamma}\left(\frac{\beta\delta}{\alpha^*\gamma}\right)^{1/2}([\mathbf{T}_0\times\mathbf{B}]\mathbf{n}_q) \approx \frac{e}{m}\xi_0([\mathbf{P}_{12}\times\mathbf{B}]\mathbf{n}_q). \tag{28}$$

where $\mathbf{n}_q$ is the unit vector of the $\mathbf{q}$ direction.

Substituting the value of the induced order parameter in the formula for the susceptibility, we obtain

$$\chi' = -\left(\frac{e}{m}\right)^2\frac{\tilde{\gamma}^2[\mathbf{T}_0\times\mathbf{q}_s]^2}{2\mathbf{T}_0^2}\left(\frac{\partial^2 U}{\partial \mathbf{T}^2}\right)^{-1}. \tag{29}$$

At the transition point

$$\partial^2 U/\partial T^2 = -\gamma q_s^2 = \gamma^2/2\delta. \tag{30}$$

Expressing q_s^2 in Eq. (29) in terms of the coefficients of the functional (26), we obtain for χ' a formula that is the same as Eq. (24) to within a numerical factor of the order of unity and $c\equiv 1$.

However, analysis of the general equation for the response (29) shows what changes in the initial model can lead to an increase in diamagnetism. In the simplest scheme (27), the order parameter wave vector q_s determines the phase-transition temperature and is uniquely related to the value of the denominator (30) in expression (29). As a result, the singularity of the denominator is substantially suppressed and the correlation radius ζ_0 at $T = 0$ enters into the answer (24). In the general case, such a relationship is not mandatory. Constructed below is a model in which the wave vector of the order parameter can serve as an arbitrarily variable parameter independent of the transition temperature.

We shall consider a system with so-called built-in inhomogeneity. By built-in inhomogeneity is meant a macroscopic modulation of internal microscopic parameters, i.e., interaction constants, forbidden gap width, etc. A built-in inhomogeneity can appear as a result of the technology used to fabricate the sample. The domain walls of ferroelectrics are the most likely examples.[3,16] If the phase transition in such a system is described phenomenologically, the free en-

ergy functional can as before have the form (47). However, all the coefficients now become functions of the coordinates $\alpha = \alpha(\mathbf{R}), \beta = \beta(\mathbf{R})$, etc. We separate in the coefficients the constant and oscillating parts:

$$\alpha(\mathbf{R}) = \alpha_0 + \alpha', \quad \beta(R) = \beta_0 + \beta', \ldots,$$

where

$$\langle \alpha_0 \rangle = \alpha_0, \quad \langle \alpha' \rangle = \langle \beta' \rangle = 0, \quad \langle \ldots \rangle = \frac{1}{V} \int \ldots d\mathbf{R}. \quad (31)$$

According to the physical meaning of the problem, α' and β' are smooth funcitons. Let us note that a phenomenological formulation similar to (31) was used in Ref. 22 to describe the pinning of vortices in type II superconductors. The phase transition in such an inhomogeneous system is described in the usual manner by the functional (26) and Eqs. (27), the only difference being that it is necessary to consider right away the inhomogeneity of the order parmeter, even if the transition takes place to the left of the Lifshitz point, i.e., $\gamma(R) > 0$. It is convenient to consider the oscillating parts as small additions:

$$\alpha'/\alpha_0 \ll 1, \quad \beta'/\beta_0 \ll 1, \quad (32)$$

which makes it possible to linearize all the equations. The first of these conditions makes it possible to neglect the local renormalization of the temperature $\tilde{T}_c$ because of α' and to assume the temperature to be constant for the entire system. The discussion in this case will be correct when $|\tilde{T} - \tilde{T}_c| > \max \alpha'/a$, where $\tilde{T}_c$ is determined from the condition $\alpha_0(\tilde{T}_c) = 0$. We isolate a small oscillating part in the order parameter as well:

$$T(\mathbf{R}) = T_0 + T', \quad \langle T' \rangle = 0.$$

The possibility of appearance of the inhomogeneous component of the order parameter to the Lifshitz point, i.e., when $\gamma(\mathbf{R}) > 0$, is due to the presence in the functional of the term $\alpha' T' T_0$ linear in T_0 and T'. By selecting a suitable sign for T_0 or T', one can always achieve an energy gain in excess of the loss due to the gradient term $\gamma|\nabla T|^2$. This is obviously possible in the case of similar spatial dependences of α' and T' ($\langle \alpha' T' \rangle \neq 0$). We isolate them in explicit form

$$\alpha'(\mathbf{R}) = \bar{\alpha} f(\mathbf{R}), \quad T'(\mathbf{R}) = \bar{T} f(\mathbf{R}),$$
$$\bar{\alpha}, \bar{T} = \text{const}, \quad \langle f^2(\mathbf{R}) \rangle = 1.$$

Considering $\bar{\alpha}, \bar{T}, \bar{\beta}$ to be small quantities of the same order, linearizing the functional and minimizing it with respect to T, we obtain for the amplitude of the oscillating part with $\tilde{T} < \tilde{T}_c$ and $\alpha_0 < 0$:

$$\bar{T} = -T_0(\bar{\alpha} + 2T_0^2\bar{\beta})/(-2\alpha_0 + \gamma_0 q'^2), \quad (33)$$

where T_0 is the equilibrium value of the homogeneous component of the order parameter $T_0^2 = -\alpha_0/2\beta$. Thus the inhomogeneous component of the order parameter arises simultaneously with the homogeneous component. The wave vector q' in Eq. (33) is given by the equality

$$\langle (\nabla f(\mathbf{R}))^2 \rangle = q'^2. \quad (34)$$

A condition similar to (32) must be satisfied for the ratio of components T' and T_0:

$$|\bar{T}/T_0| = (\bar{\alpha} + 2T_0^2\bar{\beta})/(-2\alpha_0 + \gamma_0 q'^2) \ll 1.$$

Performing calculations similar to those made in the derivation of Eq. (4), we obtain for susceptibility in the case of built-in inhomogeneity (31)

$$\chi' = \chi_L \left(\frac{\lambda_T}{r_a}\right)^2 \frac{\gamma_0 q'^2}{\alpha_0}. \quad (35)$$

The factor $\gamma_0 q'^2/\alpha_0$, additional in comparison with Eq. (4), can certainly be much greater than unity [while Eqs. (31) are satisfied at the same time]. Let us note that $\gamma_0/\alpha_0 \sim \xi_t^2$, where ξ_t is the correlation length of the order parameter T_0 near T_c. Over this length, a change in T_0 takes place, and hence, in oscillation amplitude $\bar{T}$ when boundary value problems are considered. The oscillation scale q' is of a built-in character, i.e., it is given by the condition of the problem (34). The limitation on the scale q' is $\xi_0^2 q'^2 \ll 1$, where $\xi_0^2 \sim \gamma_0$, and determines the possibility of expanding the free energy functional $F\{T\}$ in powers of q'^2. However, when the limitation on the quantity $|T - T_c| > \max \alpha'/a$ is considered, the inequality $\xi_t^2 q'^2 \gg 1$ is consistent.

It was found above that in the case of a *TS* occupying the entire volume of the sample (27), a homogeneous magnetic field induces a homogeneous order parameter (28) that does not contribute to the local current density. However, differentiating $\tilde{F}\{T_0 + T_1\}$ with respect to **B**, one can readily ascertain that a homogeneous magnetic moment directed opposite to **B** appears in the system. As shown in Sec. 2, the procedure of establishment of the balance of forces, in contrast to the procedure of minimization of the functional, takes into consideration the surface contribution to the response of the system. It is natural therefore to attribute to surface currents the magnetic moment which has appeared in the system.

Let us also note that in the case of the free energy functional with constant coefficients (15) and (26), the magnetic field does not induce an order parameter above the temperature of transition to the *TS*. The susceptibility at the transition point shows up as a jump [see Eq. (24)]. This is not mandatory in a system with built-in inhomogeneity. For built-in inhomogeneity, the equilibrium equation can in some cases also have solutions above the transition point in a specified temperature range. At the same time, the diamagnetic susceptibility will increase as the transition point is approached.

The equations for the induced order parameter and susceptibility of the TS (24) and (35) were derived for the neighborhood of the transition point in the TS. As the temperature is lowered, it is necessary to take into account in the expression for the spontaneous current density terms with higher derivatives with respect to the coordinate of the order parameter. The expressions for the current becomes nonlocal. The dependence of the free energy density on the order parameter also becomes substantially more complex. The problem of studying the *TS* in a magnetic field at $\tilde{T} = 0$ therefore requires one to change from the equilibrium equation to the microscopic scheme of calculation, wherein the order parameter is determined from the equations of motion for the wave functions of the system. In addition, a calculation using the balance-of-forces scheme for the domain-wall-

type inhomogeneity (16) showed that the induced order parameter is localized in a region of space with dimensions of the order of coherence length ξ_t, i.e., the result is at the limit of accuracy of the phenomenological scheme. The details of the spatial behavior of the induced order parameter can also be obtained only in the framework of the microscopic scheme.

4. TOROIDAL CURRENT STATE IN A MAGNETIC FIELD AT $\tilde{T}=0$

Let us consider a two-band model with band extrema coincident in the momentum space. The Hamiltonian of the model in the Lattinger-Cohn basis is of the form

$$H=\sum_{j,\mathbf{k}}\varepsilon_j(\mathbf{k}+e\mathbf{A}(\mathbf{R}))a_{j\mathbf{k}}^{+}a_{j\mathbf{k}}+\frac{i}{m}\mathbf{P}(\mathbf{k}+e\mathbf{A}(\mathbf{R}))a_{2\mathbf{k}}^{+}a_{1\mathbf{k}}$$
$$+g\sum_{\mathbf{k},\mathbf{q}}a_{1\mathbf{k}}^{+}a_{2\mathbf{k}}^{+}a_{1\mathbf{k}+\mathbf{q}}a_{2\mathbf{k}-\mathbf{q}}+\text{H.c.},\quad j=1,2, \tag{36}$$

where $\mathbf{A}(\mathbf{R})$ is the vector potential of the total magnetic field $\mathbf{B}=\operatorname{curl}\mathbf{A}$; it will be assumed everywhere below that $\operatorname{div}\mathbf{A}(\mathbf{R})=0$. In the Hamiltonian (36) we have averaged over the scale of the unit cell, and separated in explicit form of the interband momentum matrix element (hybridization) $\mathbf{P}=-i\mathbf{P}_{12}=\langle u_1(\mathbf{r})|\nabla|u_2(\mathbf{r})\rangle$, calculated in the Lattinger-Cohn basis; a_{jk}^{+} and a_{jk} are the operators of creation and annihilation of an electron with momentum $\mathbf{k}$ in band j; $\varepsilon_{1,2}(\mathbf{k})$ is the law of dispersion in bands 1 and 2:

$$\varepsilon_1(\mathbf{k})=-\varepsilon_2(\mathbf{k})+\mu \tag{37}$$

(μ is the shift of the Fermi level due to doping). As above, this section will discuss the inhomogeneity along a single coordinate, for example, x. Let us note that the system has a separate direction along P which specifies the direction of the characteristic vector of inhomogeneity in the plane perpendicular to P. We separate the corresponding component in the law of dispersion

$$\varepsilon_1=v_F k+t(\mathbf{k}_\perp), \tag{37'}$$

where k is the quasimomentum reckoned from the Fermi surface in the x direction, and $k_\perp$ is the quasi-momentum of transverse motion.

Use of the Luttinger-Cohn approximation (36) is justified by the fact that in contrast to Peierls' single-band model, in the two-band scheme (37) the Fermi momentum may be assumed to be much smaller than the reciprocal-lattice vector. In the Hamiltonian (36), the electron hole Coulomb interaction potential was replaced by the constant g in the weak-binding approximation ($e^2/v_F\ll 1$). We assume that the constant g includes processes which fix the phase of the order parameter, and the maximum constant g corresponds to the transition to a state with an imaginary order parameter.

The equations for the wave functions of the system are obtained by diagonalizing the Hamiltonian (36) by a canonical transformation which intermixes the wave functions in bands 1 and 2 (at $\mathbf{A}=0$):

$$-t(\mathbf{k}_\perp)\varphi_1-iv_F\nabla_x\varphi_1+i\left(\Delta+\frac{1}{m}\mathbf{P}\mathbf{k}_\perp\right)\varphi_2=(E(k,\mathbf{k}_\perp)+\mu)\varphi_1,$$
$$t(\mathbf{k}_\perp)\varphi_2+iv_F\nabla_x\varphi_2-i\left(\Delta+\frac{1}{m}\mathbf{P}\mathbf{k}_\perp\right)\varphi_1=(E(k,\mathbf{k}_\perp)+\mu)\varphi_2. \tag{38}$$

where $E(k,\mathbf{k}_\perp)$ are the eigenvalues of the Hamiltonian (36) in the $\Delta(x)$ potential. In deriving Eqs. (38), we separated in the basis functions of the transformation the dependence on the x coordinate and on the transverse coordinate $r\varepsilon$:

$$\psi_{1,2\mathbf{k}}(\mathbf{R})=\varphi_{1,2}(x)\exp i(\mathbf{k}_\perp\mathbf{r}_\perp+k_F x).$$

Here k_F is the projection of the Fermi momentum on the x axis.

Introduced into Eq. (38) is a potential (order parameter) $\Delta(x)$ independent of momentum:

$$\Delta(x)=ig\sum_{\mathbf{k}}(u_{\mathbf{k}}v_{\mathbf{k}}^{*}-u_{\mathbf{k}}^{*}v_{\mathbf{k}}), \tag{39}$$

where the wave functions u_k and v_k are given by the relation

$$\varphi_{1,2\mathbf{k}}(x)=\frac{1}{\sqrt{2}}[u_{\mathbf{k}}(x)\pm v_{\mathbf{k}}(x)]\exp[iv_F^{-1}t(\mathbf{k}_\perp)x].$$

In the new notation, Eqs. (38) are

$$-iv_F\nabla u+i\left(\Delta+\frac{1}{m}\mathbf{P}\mathbf{k}_\perp\right)u=(E+\mu)v,$$
$$-iv_F\nabla v-i\left(\Delta+\frac{1}{m}\mathbf{P}\mathbf{k}_\perp\right)v=(E+\mu)u. \tag{40}$$

In contrast to Eqs. (38), by using Eqs. (40) one can express one wave function in terms of the other in local form. The order parameter $\Delta(x)$ and wave functions $u_k(x)$ and $v_k(x)$ are considered smooth functions of the x coordinate.

From Eqs. (39) and (40), one can reconstruct the energy functional of the system at $T=0$:

$$\Phi=\sum_{\mathbf{k}_\perp}\left\{\sum_{E(k)<\mu}\mathscr{E}(k,\mathbf{k}_\perp)+\int dx\frac{1}{m}\mathbf{P}\mathbf{k}_\perp\Delta(x)\right\}$$
$$+\int dx\frac{\Delta^2(x)}{g}. \tag{41}$$

In contrast to Landau's functional, the functional Φ allows exactly for the contribution made to the energy by the bound states in the electronic spectrum.

We shall consider the case in which the system is doped by a single charge carrier. In the one-band scheme, in the absence of hybridization ($\mathbf{P}\equiv 0$), Eqs. (40) were solved by Brazovskiĭ.[23] In the two-band model, in contrast to the one-band model, the wave functions depend not only on the modulus, but also on the direction of quasimomentum $\mathbf{k}$. Moreover, in Eqs. (40), gradient linearization in the direction of the inhomogeneity (37') in valid everywhere except in a narrow region in the vicinity of the plane $k_F=0$. The phase volume of this region is of the same order as the volume of the region where the energy dependence of the density of states becomes significant, and it may be neglected in terms of the parameter $\tilde{\omega}/\varepsilon_F$, where $\tilde{\omega}$ is the cutoff energy in Eq. (39).

We specify the antisymmetric boundary condition

$$\Delta(\pm\infty)=\mp\Delta_0.$$

For a given direction $\mathbf{k}$ we have the following soliton solution of Eqs. (40) and (39):

$$\Delta_0(x)=-\Delta_0\operatorname{th}\frac{\Delta_0}{v_F}x,\quad \Delta_0=2\tilde{\omega}e^{-1/g}. \tag{42}$$

In the energy spectrum for the potential (42), there is one discrete state with energy $\mathscr{E}_0 = 0$ and wave functions

$$v^0=0, \quad u^0=\frac{\Delta_0}{v_F}\operatorname{ch}^{-1}\frac{\Delta_0}{v_k}x \tag{43}$$

and states of the continuous spectrum

$$\mathscr{E}_{\mathbf{k}}=\mp(\varepsilon^2+\Delta_0^2)^{1/2}, \quad v_{\mathbf{k}}^0=\frac{1}{(2V)^{1/2}}e^{i\mathbf{k}\mathbf{R}},$$

$$u_{\mathbf{k}}^0=-\frac{\varepsilon-i\Delta_0(x)}{E_{\mathbf{k}}}e^{i\mathbf{k}\mathbf{R}}.$$

The amplitude of the order parameter Δ_0 is determined from the self-consistency equation (39). The level of the chemical potential is located between the level of the bound state and the conduction band.

For the opposite direction of the quasimomentum $(-\mathbf{k})$, the expressions for the wave functions are obtained from Eqs. (43) by means of the substitution $u \leftrightarrow v$, $v_F \to -v_F$. It is precisely in a narrow region near the plane $k_F = 0$, where Eqs. (40) do not hold, that a restructuring of the wave functions takes place.

The introduction of hybridization complicates the problem. In the absence of hybridization, the state with one extra electron is the limiting case of a system with a finite concentration of excess carriers that permits an exact solution. In this case, the ground state of the Hamiltonian (36), which realizes the minimum of the functional (41), is a periodic solution $\Delta(x)$ (Refs. 24 and 25), which belongs to the class of finite-band potentials.[2] Hybridization leads to the appearance of a term linear in $\Delta(x)$ in the functional. A term analogous to Eq. (41) and linear in the order parameter was discussed in a discrete one-dimensional model in Ref. 27. The authors of the latter showed that the introduction of a term of the type of (41), linear in the order parameter, violates the property of exact integrability of the model; the same paper presents arguments in favor of an infinite-band character of the spectrum. It goes without saying that exact integrability is also violated in the limiting case of a single excess charge carrier. However, to determine the induced order parameter $\delta(x)$ in an approximation linear in the field, it suffices to confine oneself to the hybridization perturbation theory with the functions (43) as the zeroth approximation.

It is pertinent to note that the explicit gauge-invariant model (36) requires both the absence of current of type (1) and the absence of the corresponding components, simply proportional to the vector potential, from the order parameter. In the microscopic scheme in the homogeneous case, the absence of nongauge components from the current and from the order parameter is demonstrated by reducing their **k**th components in momentum space to total derivatives of the expressions containing the exact value of the spectrum.[4,20] On summing over the momentum with any partition function dependent solely on energy, the nongauge components become zero. Unfortunately, for nonzero hybridization in the inhomogeneous case, we do not have an analytical expression for the spectrum. Nevertheless, having used the property of completeness of the system of finite-band potentials,[26] we can describe with any given precision the spectrum of a system with a nonintegrable perturbation (41) by finite-band potentials, for each of which the value of the spectrum is known. Thus, also in an inhomogeneous system, in the expressions for all the physical quantities such as energy, current, and order parameter, there takes place the cancellation of the gauge parts simply proportional to the vector potential, but not to its derivatives. Without resorting to expansion in finite-band potentials, we shall omit these parts everywhere below.

Let us turn to the calculation of the induced order parameter $\delta(x)$. For this purpose, as follows from the structure of the self-consistency equation (39), we must determine the corrections, linear in the magnetic field, to the wave functions. We choose the vector potential $\mathbf{A}(\mathbf{R})$ parallel to the hybridization vector $\mathbf{P}$. We direct the wave vector of the field along the x axis; this corresponds to a magnetic field applied at right angles to $\mathbf{P}$ and x, i.e., at right angles to the current contours (2):

$$\mathbf{P}\|\mathbf{A}(\mathbf{R}), \qquad \mathbf{A}(\mathbf{R})=\mathbf{A}(x)=\mathbf{A}_q e^{iqx}+\mathbf{A}_{-q}e^{-iqx}. \tag{44}$$

Then the equations for the wave functions in the magnetic field are obtained from Eqs. (40) by means of the substitution $\mathbf{k}_\perp \to \mathbf{k}_\perp + e\mathbf{A}$. It can be shown that the diagonal component of perturbation $e\mathbf{A}(x)dt(\mathbf{k}_\perp)/d\mathbf{k}_\perp$ does not contribute to the terms proportional to the magnetic field, i.e., to terms linear in q. Therefore, we shall consider everywhere below only the nondiagonal component of perturbation $(e/m)\mathbf{P}\cdot\mathbf{A}(x)$.

Expressing u in terms of v by means of Eqs. (40) to first order in the vector potential and hybridization, we obtain an equation for the correction to the wave function v', linear in the field:

$$-(v_F\nabla_x)^2v'-(E^2-\Delta_0^2)v'$$

$$=-iW(x)Eu^0-[\Delta(x)-v_F\nabla_x]W(x)v^0, \tag{45}$$

$$W(x)=(e/m)\mathbf{P}\mathbf{A}(x)+\delta(x).$$

Equation (45) is in the form of a Schrödinger equation with source $h(x)$:

$$-(v_F\nabla_x)^2v'-(E^2-\Delta_0^2)v'=h(x). \tag{45'}$$

The Green's function of the corresponding homogeneous equation is well known:

$$G(x,x')=\frac{1}{i\varepsilon v_F}\exp(i\tilde{k}|x-x'|), \tag{46}$$

where $v_F\tilde{k}=\varepsilon$. Knowing the Green's function, one can also find the solution v' to the inhomogeneous equation (45'):

$$v'(x)=\int_{-\infty}^{\infty}dx'G(x,x')h(x').$$

We separate in the self-consistency equation the source $I(x)$—the part of the self-consistency equation dependent on the perturbation $(e/m)\mathbf{P}\cdot\mathbf{A}(x)$. Substituting the value of the wave function calculated from Eqs. (46) and (45) into the self-consistency equation (39), we obtain for the source

$$I(x)=\sum_k[(J_k(q)+J_k^*(-q))e^{-iqx}+\text{c.c.}]; \tag{47}$$

In writing Eq. (47), we assumed that $\mathbf{A}_{-q}=\mathbf{A}_q^*$. For the kth component of the source we have

$$J_k(q)=\frac{v_F^{-1}}{VE_k\varepsilon_k}\frac{e}{m}\mathbf{P}\mathbf{A}_q\Big\{[\varepsilon_k+i\Delta_0(x)]\int_x^\infty dy[2\Delta_0(y)-iv_Fq]$$

$$\times\exp[i2\tilde{k}(y-x)+iq(y-x)]-i\Delta_0(x)\int_{-\infty}^{x}dy[2\Delta_0(y)-iv_Fq]e^{iq\gamma}\Big\}. \tag{48}$$

Direct substitution of $J_k(\pm q)$ from Eq. (48) into Eq. (47) will show that the second term in Eq. (48) with integration from $(-\infty)$ to x in the expression for the source (47) is canceled by its complex conjugate. This circumstance considerably facilitates the calculations and is due to the simple form of the basis wave functions (43) and Green's functions (46). Omitting the second term in Eq. (48), we obtain

$$J_k(q)+J_k^+(-q)=\frac{e}{m}\mathbf{P}\mathbf{A}_q\frac{2}{VE_k}\Big\{\frac{(v_kq)^2+4\Delta_0^2(x)}{4\varepsilon_k^2-(v_Fq)^2}$$

$$-4\int_x^\infty dy\frac{\nabla\Delta_0(y)}{4\varepsilon_k^2-(v_Fq)^2}[(iv_Fq+2\Delta_0(x))\cos(2\tilde{k}(y-x)$$

$$+2\left(\varepsilon_k-\frac{2i\Delta_0(x)v_Fq}{\varepsilon_k}\right)\sin(2\tilde{k}(y-x))]e^{iq(y-x)}\Big\}. \tag{48'}$$

The first term in Eq. (48') contains only components quadratic in q. This is the term responsible for the paramagnetic component, discussed in Ref. 20, of the response of the current state to an inhomogeneous field. This term is different from zero both above [where $\Delta_0(x)=0$] and below the point of transition to the state with an imaginary order parameter and is weakly dependent on the inhomogeneity of the order parameter. The second term arises only in the state with spontaneous current, since its existence is wholly due to the inhomogeneity of the spontaneous order parameter. It contains linear powers of q, i.e., describes the reaction of the system to a homogeneous magnetic field.

The self-consistent part of the self-consistency equation is calculated like the source:

$$D(x)=-\frac{1}{V}\sum_k\frac{2v_F^{-1}}{E_k}\int_x^\infty dy[2\delta(y)\Delta_0(y)-v_F\nabla\delta(y)]$$

$$\times\Big[\cos(2\tilde{k}(y-x))-\frac{\Delta_0(x)}{\varepsilon_k}\sin(2\tilde{k}(y-x))\Big]. \tag{49}$$

The induced order parameter $\delta(x)$ is determined by equating $D(x)$ and $I(x)$. For sufficiently large $x(x>\xi_0$, where $\xi_0=v_F/\Delta_0$ is the correlation length of the order parameter), one can obtain the expression for $\delta(x)$ in the form of a series:

$$\delta(z)=\sum_{n=0}d_n(z)e^{-nz}, \tag{50}$$

where we introduce the dimensionless variable $z=x/\xi_0$.

Using the well-known expansion of the spontaneous order parameter

$$\Delta_0(z)=-\Delta_0(1-2(e^{-2z}-e^{-4z}+e^{-6z}-\ldots)),\quad z>0 \tag{51}$$

and performing the summation over momentum in Eqs. (48) and (49), we obtain for the coefficients in Eq. (50) in an approximation linear in q

$$d_0=0,\qquad d_{2n+1}=0,$$

and d_{2n} is determined by the recurrence relation

$$d_2(x)=2(e/m)x([\mathbf{P}\times\mathbf{B}]\mathbf{n}_x),\quad n=1$$

$$d_{2n}(x)=(d_{2n}^{(1)}x+d_{2n}^{(2)})(e/m)([\mathbf{P}\times\mathbf{B}]\mathbf{n}_x),\quad n>1,$$

where

$$d_{2n}^{(1)}=\frac{1}{n-1}\Big\{\sum_{m=1}^{n-1}(-1)^m d_{2(n-m)}^{(1)}-\frac{1}{L_1(n)(n+1)}\sum_{m=1}^{n-1}(-1)^m$$

$$L_1(n-m)\Big[2d_{2(n-m)}^{(1)}(n-1)-\sum_{l=1}^{n-m}(-1)^l d_{2(n-m-l)}^{(1)}\Big]\Big\};$$

$$d_{2n}^{(2)}=\frac{\xi_0}{2(n-1)}d_{2n}^{(1)}+\frac{1}{n+1}\Big\{2\sum_{m=1}^{n-1}d_{2(n-m)}^{(2)}-\frac{1}{(n+1)L_1(n)}$$

$$\times\Big[\sum_{m=1}^{n-1}(-1)^m L_1(n-m)$$

$$\times\Big(2(n-1)d_{2(n-m)}^{(2)}-\xi_0 d_{2(n-m)}^{(1)}-4\sum_{l=1}^{n-m}(-1)^l d_{2(n-m-l)}^{(2)}\Big)$$

$$+(-1)^n\xi_0\Big(4n(1+2n)L_2(n)-L_1(n)-\frac{1}{4}$$

$$+8\sum_{m=1}^{n-1}mL_2(m)\Big)\Big]\Big\}; \tag{52}$$

here

$$L_1(1)=1/2,\qquad L_2(1)=2/3,$$

and for $n>1$

$$L_1(n)=\frac{1}{4}\frac{1}{n(n^2-1)^{1/2}}\ln\frac{n+(n^2-1)^{1/2}}{n-(n^2-1)^{1/2}},$$

$$L_2(n)=-\frac{1}{8}\frac{d}{dn}L_1(n),$$

n_x being the unit vector in the x direction.

For sufficiently large $x(x>\xi_0)$, only the first term can be kept in the sum (50), and we thus obtain for the order parameter when $x\to\infty$

$$\delta(x)\approx 2\frac{e}{m}([\mathbf{P}\times\mathbf{B}]\mathbf{n}_x)x\exp\Big[-2\frac{x}{\xi_0}\Big], \tag{53}$$

which is in qualitative agreement with the behavior of the induced order parameter when $T\leqslant T_c$. Let us note that in the selected gauge (44)

$$(\mathbf{n}_x[\mathbf{P}\times\mathbf{B}])=PB.$$

The expansion (50) was obtained only for positive x. However, even without resorting to the direct solution of the integral self-consistency equation, one can establish the general property of $\delta(x)$ relative to the inversion $x\to -x$. We shall choose as the Green's function the function $\overline{G}(x,x')$, which is the complex conjugate of the function $G(x,x')$ (46). The source in the self-consistency equation $\overline{J}_k(q,-x)$, cal-

culated by means of the function $\overline{G}(x, x')$, is of the following form at the point $(-x)$:

$$\bar{J}_k(q,-x)=-\frac{v_F^{-1}}{VE_k\varepsilon_k}\frac{e}{m}\mathbf{P}\mathbf{A}_q\Big\{[\varepsilon_k-i\Delta_0(x)] \times\int_{-\infty}^{-x}dy[2\Delta_0(y)-iv_Fq]\exp[i2\tilde{k}(y+x)+iqy]\Big\}. \quad (54)$$

Changing the sign within the limits of integration in Eq. (54) and comparing with Eq. (48), we verify that such a transformation changes $\overline{J}_k(q, -x)$ into $J_k^*(q, x)$ with the substitution $\mathbf{A}_q \leftrightarrow \mathbf{A}_q^*$. This means that the terms linear in the magnetic field $\mathbf{B}$ ($\mathbf{B}$ = const) in the source $\overline{I}$ are equal to the corresponding terms in the source I and of opposite sign. Since the form of the solution to the self-consistency equation is independent of its notation, by performing a calculation similar to (34) of the self-consistent part $\overline{D}$ and requiring that $\overline{D} = -D$, we find

$$\delta(x)=-\delta(-x), \quad (55)$$

i.e., the induced order parameter $\delta(x)$ is an antisymmetric function, in accordance with the result of the phenomenological calculation (21).

We found the induced order parameter $\sigma(x)$ within the framework of perturbation theory. The applicability of perturbation theory in this case is determined by the condition $\Delta_0(x) \gg \delta(x)$ for all the values of x.[28] Since $\Delta_0(0) = 0$, the question of behavior of the induced parameter $\delta(x)$ as $x \to 0$ requires special consideration. It follows from Eq. (55) that $\delta(0) = 0$. However, the nature of the decrease of $\delta(x)$ as $x \to 0$ is significant. We rewrite the self-consistency equation, performing the summation over momenta:

$$\int_x^\infty \mathcal{K}(x,y)\varphi(y)\,dy=I(x); \quad (56)$$

Here $\varphi(y) = 2\Delta_0(y)\delta(y) - v_F\nabla\delta(y)$, and $I(x)$ is the source (47). For the kernel $\mathcal{K}(x,y)$, we have the following expression:

$$\mathcal{K}(x,y) =\frac{1}{v_F}\Big\{\Delta_0 K_0\Big(2\frac{y-x}{\xi_0}\Big)+\Delta_0(x)\frac{y-x}{\xi_0}\Big[2\frac{y-x}{\xi_0}K_0\Big(2\frac{y-x}{\xi_0}\Big) -\pi\frac{y-x}{\xi_0}\Big(H_0\Big(2\frac{y-x}{\xi_0}\Big)K_1\Big(2\frac{y-x}{\xi_0}\Big) -H_1\Big(2\frac{y-x}{\xi_0}\Big)K_0\Big(2\frac{y-x}{\xi_0}\Big)\Big]\Big\}, \quad (57)$$

where $K_{0,1}(z)$ are modified Bessel functions of imaginary argument, and $H_{0,1}$ are Strube functions.

To find the asymptotic form of $\varphi(x)$ as $x^{-1} \to \infty$, we take the Laplace transform of Eq. (36). As is well known, the behavior of the function $\varphi(x)$ at small values of the argument is uniquely determined by the behavior of its Laplace transform $\varphi(p)$ at $p \to \infty$ (if the inverse transform exists). We are therefore interested in low values of the arguments in the coordinate representation. At small values of $|y - x|$, the main contribution to the kernel (57) is made by the first term on the right side: $K_0(z) \to -\ln z (z \to 0, z \to 0)$, and in the relevant region, the kernel of Eq. (56) can be replaced by a difference kernel. This makes it possible to obtain in explicit form an expression for the Laplace transform $\varphi(p)$ at large values of p:

$$\varphi(p)=I(p)/K(-p), \quad p\to\infty, \quad (58)$$

where

$$\varphi(x)=\varphi(p)=\int_0^\infty\varphi(x)e^{-px}dx, \quad I(x)=I(p),$$

$$K(-p)=\int_0^\infty K(x)e^{px}dx.$$

The analyticity regions of $I(p)$ and $K(-p)$ are half planes open to the right and left, respectively. For the inverse transform $\varphi(x)$ to exist, they must overlap. It can readily be ascertained that this is indeed the case here, since $I(z)$ and $K(z)$ damp out exponentially at large z. Separating out the far asymptotic form in Eq. (58) and performing the inverse Laplace transformation, we obtain when $x \to 0$

$$\delta(x)\sim-\frac{e}{m}\frac{x}{\ln(x/\xi_0)}([\mathbf{PB}]\mathbf{n}_x),$$

$$\frac{\delta(x)}{\Delta_0(x)}\sim\frac{([\mathbf{PB}]\mathbf{n}_x)}{\Delta_0\ln(x/\xi_0)}\xi_0\to 0. \quad (59)$$

Let us note that formula (59) was obtained for $x \ll \xi_0$, i.e., for scales on which the result (22) of the balance-of-forces scheme (12) is known to be inapplicable.

We thus found that in the TS at $\tilde{T} = 0$, a homogeneous magnetic field induces an order parameter localized in the region with spontaneous current. As in Sec. 3, the appearance of a localized induced order parameter signifies a diamagnetic character of the response of the TS. The corresponding substantiation is completely analogous to the reasoning which follows from Eq. (22).

Relations (53), (55) and (59) for an induced order parameter may be regarded as direct microscopic confirmation of the phenomenological results of Sec. 3. Let us note in this connection that although the microscopic calculation is the most consistent approach to the study of the magnetic properties of the TS, the range of application of the phenomenological balance of forces scheme is broader, and the scheme itself is physically clearer.

5. CONCLUSION

This work has shown that the response of a system with spontaneous currents to a homogeneous magnetic field is diamagnetic in character. The susceptibility can reach abnormally high values close to absolute diamagnetism; see Eq. (35). To our knowledge, this is the first model of abnormally high diamagnetism of a collective but not superconducting character. The diamagnetic state is actually an inhomogeneous phase of toroidal state.[29] It should be emphasized that high diamagnetic susceptibility is wholly and completely due to the collective interaction of electrons and is not related to the one-particle spectrum. The diamagnetism of the system increases with the effective radius of current correlations $\lambda_T(4)$. The high value of the susceptibil-

ity is due to the magnitude of this parameter and is related to a much lesser degree to the proximity of the system to the phase-transition point. Therefore, the high absolute value of the susceptibility of a diamagnetic with spontaneous current is retained when the temperature is lowered, in contrast to ferromagnetics, in which the susceptibility is high only in the vicinity of the Curie point. The TS differs from ordinary magnetics not so much in the scale of the current contours as in their characteristic structure with a total moment equal to zero. This structure in turn is caused by a specific coordinate dependence of the current on the order parameter ($j \sim q^2\Delta$, not $j \sim q\Delta$, as in ordinary magnetics). The microscopic part of the theory developed above was based on the model of the excitonic dielectric. Of importance is the fact that the procedure proposed in this work for calculating the susceptibility from the condition of balance of forces is based exclusively on the characteristic structure of the expression for current (2) and on a completely general form of the free-energy functional (3). Therefore, the results obtained here for collective diamagnetism are applicable to any microscopic model in which a spontaneous current of the type of Eq. (2) is produced.

This work completes in general outline the development of a theory of the toroidal current state. At the same time, a number of interesting problems unquestionably deserve separate consideration. These are problems of realization of the TS within the framework of specific band models, finding the structure of the TS while allowing for the real symmetry of the crystal, and microscopic analysis of diamagnetic susceptibility in the vicinity of the point of transition to the TS.

Although the conditions for formation of the TS are rather stringent[4,16] it is our view that the feasibility itself of realizing the TS is unquestionable. Of great significance for the experimental identification of TS, in addition to the specific diamagnetic properties described in this work, are the presence of the photovoltaic effect and the semiconducting character of conduction in a weak electric field below the point of transition to the TS, as well as the temperature anomaly of the magnetoelectric tensor at the transition point, all of which were studied in Ref. 29.

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