Microscopic nature of toroidal diamagnetism

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The diamagnetism of a toroidal current state is caused by a "stiffness" of the wave functions that form the toroidal moment. This stiffness results from the formation of bound states in the electron spectrum of the inhomogeneous phase and gives rise to a paramagnetic component of the response.

1. The sign of the magnetic susceptibility of magnetic materials is strictly determined only for spin systems, where it is always positive (paramagnetic).[1] In orbital magnetic materials, this situation is ambiguous.[2] Of particular interest in this regard is the toroidal current state.[3,4] In terms of the procedure of minimizing the Ginzburg-Landau functional, the response of a toroidal current state to a uniform magnetic field is zero,[5] in agreement with the result for a classical toroidal moment.[6] Phenomenological calculation schemes proposed in Refs. 7 and 8 lead to a nonzero, diamagnetic value of the magnetic susceptibility of the inhomogeneous phase of a toroidal current state. In the present letter we solve the question of the microscopic nature of the diamagnetism of a toroidal current state. For this purpose, we use an exactly solvable model for an inhomogeneous ground state to calculate the collective contribution to the magnetic susceptibility near the temperature of the transition to the toroidal current state, where the calculated results can be compared with those found by the procedure of minimizing a Ginzburg-Landau functional.

2. We consider the model of an exciton dielectric with coincident extrema of the electron and hole bands; this model describes a transition to a toroidal current state.[3] The Hamiltonian of the model in the mean-field approximation in a Luttinger-Kohn basis is

$$\hat{H}=\frac{1}{2}\left(\epsilon_1(\hat{\mathbf{k}})+\epsilon_2(\hat{\mathbf{k}})+\mu\right)I+\frac{1}{2}\left(\epsilon_1(\hat{\mathbf{k}})-\epsilon_2(\hat{\mathbf{k}})\right)\sigma_z+\left(\frac{1}{m}\mathbf{P}\hat{\mathbf{k}}+\Delta(\mathbf{r})\right)\sigma_y\,, \tag{1}$$

where $\epsilon_{1,2}(\mathbf{k})$ is the electron (hole) dispersion, $\hat{\mathbf{k}}=\nabla/i-e\mathbf{A}(\mathbf{r})$, $\mathbf{A}(\mathbf{r})$ is the magnetic vector potential ($\mathbf{B}=\mathrm{curl}\mathbf{A}$), μ is the shift of the Fermi level due to doping, $i\mathbf{P}=i\mathbf{P}^*=i\langle 1|\nabla|2\rangle$ is the interband matrix element of the momentum operator, the σ_α are the Pauli matrices, and $\Delta(\mathbf{r})$ is the singlet imaginary component of the order parameter, which determines the density of the toroidal moment $\mathbf{T}\sim\mathbf{P}\Delta$ (the density of the macroscopic current is $\mathbf{j}=\mathrm{curlcurl}\mathbf{T}$). The free-energy functional (the number of particles, n, is fixed) of system (1) is written

$$F=-2\theta\sum_{\mathbf{k}}\ln\left(2\cosh\left(E(\mathbf{k})/2\theta\right)\right)+\int d\mathbf{r}\,\frac{\Delta(\mathbf{r})^2}{|g|} \tag{2}$$

where θ is the temperature, and g is the constant of the Coulomb electron-hole interac-

tion. The spectrum $E(\mathbf{k})$ and the wave functions $u_{\mathbf{k}}(\mathbf{r})$ and $v_{\mathbf{k}}(\mathbf{r})$ in (2) are determined by the equations ($\epsilon_1 = -\epsilon_2 = \epsilon$)

$$(i\epsilon(\hat{\mathbf{k}}) + \frac{1}{m}\mathbf{P}\mathbf{k} + \Delta(\mathbf{r}))u = -i(E-\mu)v \qquad (-i\epsilon(\hat{\mathbf{k}}) + \frac{1}{m}\mathbf{P}\hat{\mathbf{k}} + \Delta(\mathbf{r}))v = i(E-\mu)u\,. \quad (3)$$

Minimizing (2) with respect to $\Delta(\mathbf{r})$, we find a self-consistency equation

$$\Delta(\mathbf{r}) = \frac{i}{2}|g|\sum_k \mathrm{th}\frac{E(\mathbf{k})-\mu}{2\theta}\,(u_{\mathbf{k}}(\mathbf{r})v_{\mathbf{k}}^*(\mathbf{r}) - u_{\mathbf{k}}^*(\mathbf{r})v_{\mathbf{k}}(\mathbf{r}))\,. \quad (4)$$

We set $\mathbf{A}=0$ and $\mathbf{P}=0$, and we consider the one-dimensional dispersion law $\epsilon = iV_F\nabla_x$. The problem is thereby reduced to an exactly solvable problem.[9,10] Transverse dispersion can be dealt with by a perturbation theory in $(l/m)\mathbf{P}\mathbf{k}$ (we assume $\mathbf{P}\perp X$). Excess charge carriers ($n\neq 0$, $\mu\neq 0$) lead to an inhomogeneity of the ground state. The energy spectrum contains two energy gaps $(-E_+, -E_-)$ and (E_-, E_+); the potential $\Delta_0(x)$, the wave functions, and the state density are[9,10]

$$\Delta_0(x) = -\Delta_1 Sn(x\frac{\Delta_1}{V_F\kappa}, \kappa),\quad \Delta_1 = E_+ - E_-,\quad \kappa = \frac{E_+ - E_-}{E_+ + E_-},\quad q(x) = \Delta_0^2(x) - V_F\nabla\Delta_0(x)$$

$$v_E^0(x) = \left(\frac{q(x)+b}{L(\langle q\rangle + b)}\right)^{1/2}\exp\left\{\frac{i}{V_F}\int_0^x \frac{2\sqrt{R}\,dy}{q(y)+b}\right\},\quad \langle\ldots\rangle = \frac{1}{L}\int_{-L/2}^{L/2}\ldots dx \quad (5)$$

$$b = 2E^2 - E_+^2 - E_-^2,\quad R = E^2(E^2-E_+^2)(E^2-E_-^2),\quad \rho(E) = \frac{1}{L}\frac{dN}{dE} = \left|\frac{(\langle q\rangle + b)E}{\pi\sqrt{R}}\right|,$$

where L is the length of the system along X. We find an expression for u_E^0 through the replacement $\Delta_0(x)\to -\Delta_0(x)$. Taking (5) as a zeroth approximation, we find the component of the order parameter induced by the field, $\delta(x)$ [$\Delta(x) = \Delta_0(x) + \delta(x)$]. In first order in $(e/m)PA(x)$ ($\mathbf{P}\|\mathbf{A}$, $\mathbf{P}\perp\mathbf{B}$), we find the following expression for the correction to the wave function:

$$v_E'(x) = \eta v_E^0(x) + \int g(x,x')\,(2\Delta_0(x') - V_F\nabla)\left(\frac{e}{m}PA(x') + \delta_1(x')\right)v_E^0(x')dx'; \quad (6)$$

here $g(x,x')$ is the Green's function of Eq. (3), and the constant η ensures the preservation of the normalization. Substituting (6) into Eq. (4), linearized in the magnetic field, we find $\delta_1(x)$ in a self-consistent way. We calculate $\delta_2(x)$ in an analogous manner. Equation (4) cannot be solved analytically for an arbitrary period $\Delta_0(x)$, but we can draw a conclusion regarding the nature of the magnetic response. For the free energy we find, in second order in the magnetic field,

$$F-F(B=0)=L\int\limits_{E>0} dE\,\frac{\rho(E)}{\langle q\rangle+b(E)}\Bigg[\langle\delta_1^2(x)(E_+^2+E_-^2-q(x))\rangle$$

$$-4\,\frac{(\langle\Delta_0(x)\delta_1(x)\rangle)^2}{\langle q\rangle+b(E)}\,E^3\frac{d}{dE}$$

$$+\int dE'\frac{\rho(E')}{\langle q\rangle+b(E')}\,\frac{|\langle E|(2\Delta_0(x)-V_F\nabla)\delta_1(x)|E'\rangle|^2}{E'^2-E^2}\Bigg]\frac{1}{E}\left(\tanh\frac{E-\mu}{2\theta}+\tanh\frac{E+\mu}{2\theta}\right). \tag{7}$$

The integration in (7) is over the allowed bands. All the terms in (7) are strictly greater than zero [$\max q(x)=E_+^2-E_-^2$], i.e., diamagnetic. If the soliton lattice $\Delta_0(x)$ is sufficiently sparse, the induced order parameter can be calculated independently for each soliton. In (1), (6), and (7) we should take the limit

$$\kappa\to 1,\ \Delta_0(x)\to-\Delta_0\tanh\frac{x\Delta_0}{V_F},\ v_E^0\to\frac{1}{\sqrt{L}}e^{\frac{ix\sqrt{E^2-\Delta_0^2}}{V_F}},$$

in the phase diagram, this limit corresponds to a region near the line of the transition from a commensurate phase [$\Delta_0(x)=\text{const}$] to a soliton phase. As a result, near the temperature (θ_c) of the transition to the toroidal current state we find

$$\delta_1(x)=-\delta_1(-x);\qquad \max\delta_1(x)\approx\frac{e}{m}PB\xi_\theta$$

$$x\to 0:\ \delta_1(x)=o(x);\ x\gg\xi_\theta:\ \delta_1(x)\approx 2\,\frac{e}{m}PBxe^{-2x/\xi_\theta} \tag{8}$$

Here $\xi_\theta=\xi_0(\theta_c/\Delta_0)$ is the temperature-independent correlation length; the scale dimension of the inhomogeneity in the spontaneous order parameter is on the order of $\Delta_0(x)$ [$\Delta_0\sim\sqrt{\theta_c(\theta_c-\theta)}$]; and $\xi_0=V_F/\theta_c$. The susceptibility $\chi=-(\partial^2F/\partial B^2)$ is given in this limit by

$$\chi=\nu f\chi_L(P\xi_0)^2 \tag{9}$$

and appears abruptly at the transition point [χ_L is the Landau diamagnetic susceptibility of the noninteracting electron gas; $f\sim 1$ is a form factor; $\nu=\xi_\theta/l\sim[\kappa\ln(1-\kappa^2)]^{-1}$, and $2l$ is the period of the soliton lattice]. By virtue of the exponential dependence of the soliton interaction energy on the distance between solitons, the soliton lattice can be regarded as sparse even at $\nu\lesssim 0.5$. The jump in the susceptibility in (9) at the transition point stems from the root singularity in the temperature in the amplitude $\delta_1(x)$ in (8).

3. What is the physical interpretation of this result? In the magnetic response of a toroidal current state, as in any system, we can distinguish diamagnetic and paramagnetic components. Since the magnetic ordering in a toroidal current state is of an orbital nature (i.e., the time average of the local current density, formed by the or-

dered motion of the collectivized electrons, is nonzero), the response to the magnetic field of the toroidal current state is naturally interpreted in terms of a deformation of current loops. The paramagnetic component of the response is described by a change in the area of the projection of the loop onto the magnetic field direction, while the diamagnetic component is described by a change in the current density of the loop. In the presence of a macroscopic inhomogeneity, there is the possibility that the paramagnetic component will be suppressed by a pinning of the current loops by inhomogeneities, without any change in the diamagnetic component. It was shown above that the formation of bound states in the electron spectrum emerges as the microscopic reason for the pinning.

Formally, the diamagnetic response of a toroidal current state is caused, according to (7), by the appearance of an induced component of the order parameter $\delta_1(x)$ in a magnetic field. The reason for the latter is the presence of a source linear in $B = \text{const}$ in the self-consistency equation. This source comes from the term $(e/m)PA(x)\Delta_0(x)$ in (6). By following the Gor'kov procedure for deriving a Ginzburg-Landau expansion in a perturbation theory in the potential $\Delta_0(x)$, we would find in the self-consistency equation a product of matrix elements between plane waves separately from $\Delta_0(x)$ and separately from $(e/m)PA(x)$, which is zero for $B = \text{const}$. The reason for the qualitative difference between the perturbation-theory results and the results of the exact theory is the formation of bound states, which form a central band $(-E_-, E_-)$ in (5). The wave functions u and v undergo phase shifts which cannot be described by perturbation theory. The actual parameter of the expansion in the vector potential becomes the term $(e/m)PA(x)\Delta_0(x)$, which gives rise to a source in the self-consistency equation with $B = \text{const}$. The change in the structure of the wave functions in the presence of bound states may be characterized as the onset of a "stiffness." The diamagnetism of a toroidal current state due to the stiff structure of the wave functions is thus a definitely quantum-mechanical phenomenon. The magnitude of the magnetic response of the toroidal current state is determined by the radius of the bound state, which is determined in turn by the correlation length. For the microscopic model considered above, the phenomenological equations[7,8] give a qualitatively correct result for $\delta_1(x)$.

Our choice of a one-dimensional "seed" spectrum for ϵ was based solely on the simplicity with which the wave functions of the inhomogeneous system can be described in this case. All the physical conclusions derived in this letter remain valid for a spectrum of a general type, under the condition that there is a formation of states which are localized at an inhomogeneity.

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[1]A. F. Andreev and V. I. Marchenko, Usp. Fiz. Nauk **130**, 39 (1980) [Sov. Phys. Usp. **23**, 21 (1980)].
[2]L. D. Landau and E. M. Lifshitz, Élektrodinamika sploshnykh sred, §48, Nauka, Moscow, 1982 (Electrodynamics of Continuous Media, Pergamon Press, Oxford).
[3]B. A. Volkov, A. A. Gorbatsevich, Yu. V. Kopaev, and V. V. Tugushev, Zh. Eksp. Teor. Fiz. **81**, 729 (1981) [Sov. Phys. JETP **54**, 391 (1981)].
[4]V. L. Ginsburg, A. A. Gorbatsevich, Yu. V. Kopaev, and B. A. Volkov, Solid State Commun. **50**, 339 (1984).

[5]B. A. Volkov, A. A. Gorbatsevich, Yu. V. Kopaev, and V. V. Tugushev, Zh. Eksp. Teor. Fiz. **81**, 1904 (1981) [Sov. Phys. JETP **54**, 1008 (1981)].
[6]V. M. Dubovik and L. A. Tosunyan, Fiz. Elem. Chastits At. Yadra **14**, 1193 (1983) [Sov. J. Part. Nucl. **14**, 504 (1983)].
[7]B. A. Volkov, A. A. Gorbatsevich, and Yu. V. Kopaev, Zh. Eksp. Teor. Fiz. **86**, 1870 (1984) [Sov. Phys. JETP **59**, 1087 (1984)].
[8]Yu. A. Artamonov, A. A. Gorbatsevich, and Yu. V. Kopaev, Pis'ma Zh. Eksp. Teor. Fiz. **40**, 290 (1984) [JETP Lett. **40**, 1076 (1984)].
[9]B. A. Dubrovin, S. P. Novikov, and V. B. Matveev, Usp. Mat. Nauk **31**, 55 (1976).
[10]S. A. Brazovskiĭ, S. A. Gordyunin, and N. N. Kirova, Pis'ma Zh. Eksp. Teor. Fiz. **31**, 486 (1980) [JETP Lett. **31**, 456 (1980)].

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