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A CONTRIBUTION FROM EXCHANGE INTERACTION TO MAGNETIZATION OF A DEGENERATE ELECTRON GAS IN A QUANTUM CYLINDER

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The exchange energy of an electron gas on a cylindrical surface in a constant magnetic field is calculated. Analytical formulas describing the contribution from exchange interaction to magnetization of a quantum cylinder are derived. It is shown that the magnetic response of the system undergoes the Aharonov–Bohm oscillations.

INTRODUCTION

The model of a carbon nanotube in the form of a two-dimensional electron gas rolled in a cylinder finds wide application in theoretical investigations of physical properties of such nanostructures as quantum cylinders and quantum bracelets [1–3]. In this connection, much attention is given to studying the quantum effects induced by the external electrical-magnetic field not only in flat but also in curved low-dimensional layers of an electron gas. Of special interest are the oscillation effects. One can refer here, for example, an examination of oscillations of photoconductivity of a two-dimensional electron gas in the magnetic field, magnetotransport studies within the Hall geometry for the case of a two-dimensional electron gas on a cylindrical surface, and oscillations of magnetic resistance of low-dimensional nanostructures [4].

In this work, we have calculated the energy of exchange interaction of a two-dimensional electron gas on a cylindrical surface in the presence of magnetic field directed along the cylinder axis and derived explicit analytical formulas describing the contribution from exchange interaction to magnetization oscillations of a quantum cylinder for the case of a degenerate electron gas. We have also studied the dependence of the obtained results on the characteristic parameters of the problem.

1. EXCHANGE ENERGY

The energy of exchange interaction of an electron gas can be written as the following expression [5, 6]:

$$V = -\frac{e^2}{2} \sum_{\alpha_1 \neq \alpha_2, \sigma=\pm 1} n_{\mathrm{F}}(\alpha_1, \sigma) n_{\mathrm{F}}(\alpha_2, \sigma) \times \int \psi^*_{\alpha_1}(r_1) \psi_{\alpha_2}(r_1) \frac{1}{|r_1 - r_2|} \psi^*_{\alpha_2}(r_2) \psi_{\alpha_1}(r_2) dr_1 dr_2, \quad (1)$$

where summation is performed over all quantum numbers and spin projections of electronic-state pairs, $\psi_{\alpha_1}(\boldsymbol{r}_1)$ and $\psi_{\alpha_2}(\boldsymbol{r}_1)$ are the wave functions of electronic stationary states taken at various points with the radius-vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, $n_{\mathrm{F}}(\alpha, \sigma)$ is the occupation number of the given quantum state of electrons, and e is the electron charge. The vector

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potential of a uniform magnetic field directed along the axis z coinciding with that of the cylinder is chosen as

$$A_x = -\frac{yH}{2},\ A_y = \frac{xH}{2},\ A_z = 0 . \tag{2}$$

The Hamiltonian $\hat{H}$ of a nonrelativistic Pauli equation commutes with the operators of electron-spin projection, an orbital momentum and an electron momentum projection onto the direction of the magnetic field $H \uparrow\uparrow OZ$

$$\left[\hat{H}, \hat{S}_z\right] = \left[\hat{H}, \hat{L}_z\right] = \left[\hat{H}, \hat{p}_z\right] = 0 . \tag{3}$$

As a result, we get the following formulas for a normalized wave function and electron-energy levels in field (2):

$$\psi_{\alpha,\sigma}(r) = \frac{e^{in\varphi + ip_3 z}}{\sqrt{2\pi RL}} C , \tag{4}$$

$$E(n, p_3, \sigma) = \varepsilon\left(n + \frac{\Phi}{\Phi_0}\right)^2 + \frac{p_3^2}{2m} + \mu_0 H\sigma . \tag{5}$$

The spin part of the electron wave function has the following form in Eq. (4):

$$C \equiv C\left(\frac{1}{2}\right) = \begin{pmatrix} 1 \\ 0 \end{pmatrix},\ C \equiv C\left(-\frac{1}{2}\right) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

for the cases where the spin is directed along ($\sigma = +1$) or opposite ($\sigma = -1$) the direction of the axis Z, respectively. In addition, in Eqs. (4) and (5), the following designations are adopted: m is the effective electron mass, n = 0, ±1, ±2, ... is the azimuthal quantum number specifying $L_z = n\hbar$, $\varepsilon = \hbar^2/2mR^2$ is the energy of dimensional quantization, $\mu_0 = |e|\hbar/2m_0 c$ is the Bohr magneton, $\Phi = \pi R^2 H$ is the magnetic flux through the cross section of a cylinder of height L and radius R, $\Phi_0 = 2\pi\hbar c/|e|$ is the magnetic-flux quantum, p_3 is the electron-momentum projection of the axis Z (hereinafter, use is made of a system of units where $\hbar = c = 1$). Thus, in Eq. (1), the stationary electronic state is specified by three quantum numbers $(\alpha;\sigma) \equiv (n, p_3;\sigma)$, and the chemical potential μ of a perfect electron gas is related to the temperature T, total number of electrons in the gas N, and magnetic-field strength by the following equation:

$$N = \frac{L}{2\pi} \sum_{\sigma=\pm 1} \int_{-\infty}^{+\infty} dp_3 \sum_{n=-\infty}^{+\infty} \frac{1}{\exp\left(\frac{E(n, p_3, \sigma) - \mu}{T}\right) + 1} . \tag{6}$$

Taking into account Eqs. (4) and (5), the energy of exchange interaction can be found from Eq. (1) as

$$V = -\frac{e^2}{2\pi L} \sum_{\alpha_1 \neq \alpha_2; \sigma=\pm 1} n_{\mathrm{F}}(\alpha_1, \sigma) n_{\mathrm{F}}(\alpha_2, \sigma) \int_0^{2\pi} e^{in\varphi} K_0\left(2pR\sin\frac{\varphi}{2}\right) d\varphi , \tag{7}$$

where $n = n_1 - n_2$, $p = |p_{1z} - p_{2z}|$, R is the cylinder radius, $K_0(x)$ is the Macdonald function, and summation is performed over the quantum states $\alpha_1 = (n_1, p_{1z})$ and $\alpha_2 = (n_2, p_{2z})$. Equation (7) also directly describes the contribution from exchange interaction to the thermodynamic potential of electron gas, and we have

$$V = \Omega^{ex} = -\frac{\pi e^2}{2L} \sum_{\alpha_1 \neq \alpha_2; \sigma = \pm 1} n_F(\alpha_1, \sigma) n_F(\alpha_2, \sigma) I_n(pR) K_n(pR) , \quad (8)$$

where I_n is a modified Bessel function of the n th order, K_n is the Macdonald function of the n th order. Thus, Eq. (8) describes the energy of exchange electron interaction on a cylindrical surface in a longitudinal magnetic field for the case where the cylinder length is big as compared with the Fermi electron wavelength. This result will further be used for calculation of the contribution from exchange interaction to magnetization of a quantum cylinder.

$$m_z^{ex} = -\left(\frac{\partial \Omega^{ex}}{\partial H} \right)_{\mu, T} . \quad (9)$$

2. A DEGENERATE ELECTRON GAS

Let us consider quantum oscillations of degenerate-gas magnetization for real situations, where the following condition is fulfilled

$$\mu(T = 0) = \varepsilon_F >> \varepsilon , \quad (10)$$

where $\varepsilon = 1/2mR^2$ is the energy of dimensional quantization. In this case, it follows from Eqs. (7) and (8), that

$$\Omega^{ex} \approx -\frac{e^2 L}{8\pi^2} \sum_{n_1, n_2 = -\infty}^{+\infty} \int_{-\infty}^{+\infty} dp_1 dp_2 \frac{1}{\sqrt{(n_1 - n_2)^2 + R^2 p^2}} n_F(n_1, p_1) n_F(n_2, p_2), \quad (11)$$

where we also neglected the dependence of electron energy in the Fermi – Dirac distribution functions on the electron spin.

The oscillating part of magnetization is separated using the Poisson formula [7], and we get

$$\sum_{n=-\infty}^{+\infty} f(n) = \sum_{n=-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x) e^{2\pi i n x} dx . \quad (12)$$

Let us introduce the new integration variables $r_{1,2}$ and $\phi_{1,2}$ instead of $x_{1,2}$ and $p_{1,2}$

$$\begin{aligned} x_{1,2} &= r_{1,2} \sin \varphi_{1,2} \sqrt{2mR^2} , \\ p_{1,2} &= \sqrt{2m} r_{1,2} \cos \varphi_{1,2} . \end{aligned} \quad (13)$$

As a result, we derive

$$\begin{aligned} m_z = C \sum_{n_1, n_2 = -\infty}^{+\infty} e^{-2\pi i (n_1 + n_2) \frac{\Phi}{\Phi_0}} \int r_1 dr_1 d\varphi_1 r_2 dr_2 d\varphi_2 \exp\left[2\pi i \sqrt{2mR^2} \left(n_1 r_1 \sin \varphi_1 + n_2 r_2 \sin \varphi_2 \right) \right] \\ \times \frac{r_1 \sin \varphi_1}{\sqrt{r_1^2 + r_2^2 - 2 r_1 r_2 \cos(\varphi_1 - \varphi_2)}} \frac{1}{4 \cosh^2 \left(\frac{r_1^2 - \mu}{2T} \right)} \frac{1}{\exp\left[\frac{r_2^2 - \mu}{T} \right] + 1} , \end{aligned} \quad (14)$$

where

$$C = -e^2 L \frac{\mu_0}{2\pi^2} \frac{(mR)^2}{T}. \tag{15}$$

Let us calculate the integral over r_1, assuming that along with Eq. (10), the following condition is fulfilled:

$$\frac{\mu}{T} >> 1. \tag{16}$$

To this end, we go to the integration variable

$$\tau = \frac{r_1^2 - \mu}{T} \tag{17}$$

and take into account that the major contribution to the integral is made by small τ. In this case, in view of Eq. (16) we can replace the lower integration limit by $-\infty$ without high uncertainty. Restricting ourselves to the first expansion term, we get

$$m_z = C\frac{T}{2}\sqrt{\mu}\sum_{n_1 \neq n_2} e^{-2\pi i(n_1+n_2)\frac{\Phi}{\Phi_0}} \int r_2 dr_2 \sin\varphi_1 d\varphi_1 d\varphi_2 \times$$
$$\times \frac{\exp\left[2\pi i n_1 \sqrt{\frac{\mu}{\varepsilon}} \sin\varphi_1 + 2\pi i n_2 r_2 \sqrt{2mR^2} \sin\varphi_2\right]}{\sqrt{\mu + r_2^2 - 2r_2\sqrt{\mu}\cos(\varphi_1 - \varphi_2)}\left[\exp\left(\frac{r_2^2 - \mu}{T}\right) + 1\right]}. \tag{18}$$

The remaining integrals in Eq. (18) are either tabular or calculated by the method of stationary phase.

As a result, for the oscillating part of contribution from exchange interaction to magnetization of the quantum cylinder, we get the following asymptotic formula:

$$-\frac{m_z}{\mu_0} = \tilde{C}\sum_{n=1}^{\infty} \frac{\sin\left(2\pi n\sqrt{\frac{\mu}{\varepsilon}} - \frac{\pi}{4}\right)\sin\left(2\pi n\frac{\Phi}{\Phi_0}\right)}{\sqrt{n}}, \tag{19}$$

where

$$\tilde{C} = \frac{2}{\pi^2}\alpha m_0 L\left(\frac{\mu}{\varepsilon}\right)^{\frac{3}{4}}$$

and $\alpha = e^2$ is the constant of fine structure.

The expression under the sign of summation in Eq. (19) is a periodic function of fractional parts of the parameters Φ/Φ_0 and $\sqrt{\mu/\varepsilon}$, and magnetization itself is an oscillating function of these parameters.

A magnetic response of a perfect degenerate two-dimensional electron gas on a cylindrical surface in a longitudinal constant magnetic field is calculated in [1]. For example, for $\sqrt{\mu/\varepsilon} = 10.6$ and $\Phi/\Phi_0 = 0.45$ the ratio of the exchange-interaction contribution to magnetization of a quantum cylinder to a similar result obtained in [1] can be written as

$$\frac{m_z^{\text{ex}}}{m_z^{\text{id}}} \approx 2\alpha R m, \tag{20}$$

where R is the cylinder radius, m is the effective electron mass, in real nanostructures $mR >> 1$.

Thus, exchange interaction makes a significant contribution to magnetization of the quantum cylinder, and the magnetic response undergoes the Aharonov–Bohm oscillations upon varying the magnetic flux through the cross section of the nanostructure.

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