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Roles of the surface and the bulk electronic states in the de Haas - van Alphen oscillations of two-dimentional electron gas

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Abstract

Using the Bloch approach applied to a two-dimensional metal bar we find that the Peierls result for zero-temperature magnetization of spinless electron gas consists of sum of two magnetic moments originating of the bulk and the surface electronic states.

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The theory of the two-dimensional de Haas-van Alphen effect was started by Peierls [1]. In the zero-temperature limit he obtained that the magnetization in an ideal two-dimensional electron gas has a sharp, saw-tooth form and a constant, with field, amplitude. This behavior is typical for the 2D electron system with fixed number N of particles per unit area.

In another situation when some reservoir could make variation of N possible such that the system chemical potential keeps a constant value the magnetization has sharp oscillations of so called inverse saw-tooth form [2].

The important consequence of the sharp saw-tooth shape of magnetization oscillations is an extremely slow convergence of its Fourier representation. It means practical useless of application of Poisson summation formula, so successful in 3D case. It is more convenient, therefore, to perform explicitly the summation over the Landau levels, since only two, adjacent to the Fermi energy, Landau levels are partially full. This approach has been developed in series of papers by I. Vagner and co-authors [3]. They have obtained an analytical expression for the magnetic field dependence of the chemical potential and magnetization as well for the envelope of the magnetization oscillations at finite temperature in the limit of sharp Landau levels. The problem is simplified in presence of impurities then the oscillations are smoothed and the Lifshitz-Kosevich approach to the 2D electron gas, but taking into account the chemical potential oscillations, yields the reasonable results at any temperature including zero temperature limit [4].

Usual treatment of electron gas magnetization is based on the calculation of the partition function with summation over Landau levels with fixed degree of degeneracy per unit area [5]. The Landau level energies are taken as the degenerate eigenvalues of the Schrödinger equation in the bulk of metal. The degeneracy of Landau states is lifted near the specimen boundary. So, there are the two group electrons: (i) occupying the quantum states in the bulk and (ii) in the surface of the metal. It is interesting to know what are the roles these two group of electrons play in observable physical effects.

The more subtle derivation by F.Bloch [6] takes into account both the electrons occupying the quantum states in the bulk and in the surface of the metal [7] reproduces the Landau result for the electron gas diamagnetic moment in the high temperature limit $T \gg \hbar \omega_c$. This approach developed further in the paper by the present author [8] demonstrates that two groups of electrons give equal contributions to the Landau diamagnetism. On the other hand, it was concluded that only bulk electrons produce the de Haas-van Alphen magnetization oscillations. Indeed, the oscillating part of magnetization at $\hbar\omega_c \ll \varepsilon_F$ given by the Eq. (21) in the paper [8] is determined by the bulk states. However, it depends on the strongly oscillating with magnetic field chemical potential which is determined by equation $N = -\partial\Omega/\partial\mu$ where both group of electronic states are important. Moreover, in the integer quantum Hall effect region when the distance between Landau levels $\hbar\omega_c$ is of the order of the Fermi energy ε_F both groups of electronic states give contributions to the oscillating magnetization. Hence the conclusion that only bulk electrons produce the de Haas-van Alphen magnetization oscillations is in fact incorrect.

In general, the division of bulk and surface electronic states contributions to the two dimensional electronic gas magnetic moment oscillations is nontrivial problem. It is simplified in the zero-temperature limit where one can perform explicitly the summation over the Landau levels following to the papers by Peierls [1] and Schoenberg [2]. It is done in the present

publication dedicated to the memory of Israel Vagner.

We consider the two-dimensional (2D) clean metal bar with length A in the x direction and width B in the y direction ($|y| \leq B/2$) under a perpendicular magnetic field $\mathbf{H} = (0, 0, H)$. The thermodynamic potential of the electron gas is

$$
\Omega = -T \sum_{\nu} \ln \left(1 + e^{\frac{\mu - \varepsilon_{\nu}}{T}} \right),\tag{1}
$$

where the electron energies ε_{ν} are determined as eigenvalues of the Schrödinger equation

$$
\left(\frac{\hbar^2}{2m}\left[\left(-i\frac{\partial}{\partial x} - \frac{eHy}{\hbar c}\right)^2 - \frac{\partial^2}{\partial y^2}\right] + V(y)\right)\psi_{\nu} = \varepsilon_{\nu}\psi_{\nu}.
$$
 (2)

The potential $V(y)$ is negligible everywhere except near the edges, where it increases up from zero at $|y| = B/2 - \Delta$ to infinity at $|y| = B/2$. The length Δ is chosen much larger than magnetic length $\lambda_H = \sqrt{\hbar c/eH}$:

$$
\lambda_H \ll \Delta \ll B \tag{3}
$$

The search of a solution in the standart form

$$
\psi_{\nu} = \exp(iqx)\varphi_{\nu}(y),\tag{4}
$$

where $q = 2\pi Q/A$ and Q is an integer, leads us to the following eigenproblem

$$
\hat{H}\varphi_{\nu} = \varepsilon_{\nu}\varphi_{\nu}, \n\hat{H} = \frac{\hbar^2}{2m} \left[\left(q - \frac{eHy}{\hbar c} \right)^2 - \frac{\partial^2}{\partial y^2} \right] + V(y).
$$
\n(5)

It is clear that if the "equilibrium position" $y_0 = \hbar c q / eH$ is limited by

$$
-\frac{B}{2} + \Delta \le \frac{\hbar c q}{eH} \le \frac{B}{2} - \Delta,\tag{6}
$$

then to a quite good approximation the eigen functions of Eq. (5) are Landau wave functions

$$
\varphi_{nq}(y) = \frac{1}{\sqrt{2^n n! \sqrt{\pi} \lambda_H}} \exp[-(y - y_0)^2 / 2\lambda_H^2] H_n[(y - y_0) / \lambda_H]
$$

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with *q*-independent eigenvalues

$$
\varepsilon_n = \hbar \omega_c \left(n + \frac{1}{2} \right),\tag{7}
$$

 $\omega_c = eH/m$. If y_0 is out the interval (6) then the eigenvalues $\varepsilon_{\nu} = \varepsilon_{qn}$ are not so simple: they are q dependent and tend to infinity when $|q| \rightarrow eHB/2\hbar c$.

Applying the standart notations for quantum mechanical averages $\langle \hat{A} \rangle_{\nu} = \int dy(\varphi_{\nu}\hat{A}\varphi_{\nu})$ we obtain the following equality:

$$
-H\frac{\partial \varepsilon_{nq}}{\partial H} = q\frac{\partial \varepsilon_{nq}}{\partial q} - \frac{(eH)^2}{mc^2} \langle (y - y_0)^2 \rangle_{\nu},\tag{8}
$$

where

$$
-\frac{\partial \varepsilon_{nq}}{\partial H} = -\left\langle \frac{\partial \hat{H}}{\partial H} \right\rangle_{\nu} = \langle \hat{M}_z \rangle_{\nu},\tag{9}
$$

and

$$
\frac{\partial \varepsilon_{nq}}{\partial q} = \left\langle \frac{\partial \hat{H}}{\partial q} \right\rangle_{\nu} = \hbar \langle \hat{v}_x \rangle_{\nu}.
$$
 (10)

For the equlibrium value of the system magnetic moment at given temperature we have

$$
M = -\left(\frac{\partial\Omega}{\partial H}\right)_{\mu} = -\sum_{nQ} \frac{\frac{\partial \varepsilon_{nq}}{\partial H}}{e^{\frac{\varepsilon_{nq}-\mu}{T}}+1} = -\frac{A}{2\pi} \int_{-eH B/2\hbar c}^{eH B/2\hbar c} dq \sum_{n=0}^{\infty} \frac{\frac{\partial \varepsilon_{nq}}{\partial H}}{e^{\frac{\varepsilon_{nq}-\mu}{T}}+1}.
$$
\n(11)

The integral over q can be written as

$$
\int_{-eH B/2\hbar c}^{eH B/2\hbar c} dq = \begin{cases} e^{H(B/2-\Delta)/\hbar c} & -e^{H(B/2-\Delta)/\hbar c} \\ \int_{-eH(B/2-\Delta)/\hbar c} + \int_{-\infty}^{+\infty} + \int_{e^{H(B/2-\Delta)/\hbar c}}^{+\infty} dq, \quad (12) \end{cases}
$$

where the infinite limits are taken due to fast exponential convergency of the integral when $\varepsilon_{nq} \to \infty$ for q outside the interval (6). Correspondingly the magnetic moment presents the sum of three terms

$$
M = M_1 + M_2 + M_3 \tag{13}
$$

For the first term the energy levels have the q independent value (7); hence

$$
M_1 = -\frac{eS}{2\pi\hbar c} \sum_{n=0}^{\infty} \frac{\varepsilon_n}{e^{\frac{\varepsilon_n - \mu}{T}} + 1},\tag{14}
$$

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where $S = AB$ is the bar area. For the second term, by making use the equality (8) and omiting the contribution proportional to $\langle (y - y_0)^2 \rangle_{\nu}$ which is of the order of Δ/B in comparison with other terms, we obtain

$$
M_2 = \frac{A}{2\pi H} \int_{-\infty}^{-eH(B/2-\Delta)/\hbar c} q dq \sum_{n=0}^{\infty} \frac{\frac{\partial \varepsilon_{nq}}{\partial q}}{e^{\frac{\varepsilon_{nq}-\mu}{T}}+1}
$$
(15)

$$
= -\frac{eS}{4\pi\hbar c} \int_{-\infty}^{-eH(B/2-\Delta)/\hbar c} dq \sum_{n=0}^{\infty} \frac{\frac{\partial \varepsilon_{nq}}{\partial q}}{e^{\frac{\varepsilon_{nq}-\mu}{T}}+1} = \frac{eST}{4\pi\hbar c} \sum_{n=0}^{\infty} \ln\left(1+e^{\frac{\mu-\varepsilon_n}{T}}\right).
$$

Taking into account that $M_2 = M_3$ finally we have

$$
M = M_1 + 2M_2 = -\left(\frac{\partial \Omega}{\partial H}\right)_{\mu},\tag{16}
$$

where

$$
\Omega = -\frac{eHST}{2\pi} \sum_{n=0}^{\infty} \ln\left(1 + e^{\frac{\mu - \varepsilon_n}{T}}\right). \tag{17}
$$

One can rewrite this result also as

$$
M = M_1 + 2M_2 = \left(H\frac{\partial}{\partial H} + 1\right)\left(-\frac{\Omega}{H}\right)_{\mu}
$$

$$
= \left(H\frac{\partial}{\partial H} + 1\right)\frac{eST}{2\pi}\sum_{n=0}^{\infty}\ln\left(1 + e^{\frac{\mu - \varepsilon_n}{T}}\right).
$$
(18)

As follows from the derivation, the first term here

$$
M_1 = -H \frac{\partial}{\partial H} \left(\frac{\Omega}{H}\right)_{\mu} \tag{19}
$$

originates from the electrons occupying the Landau states situated in the bulk of metal. To work at the fixed number of particles one can rewrite M_1 as

$$
M_1 = -\frac{eS}{2\pi\hbar c} \sum_{n=0}^{\infty} \frac{\varepsilon_n - H\partial\mu/\partial H}{e^{\frac{\varepsilon_n - \mu}{T}} + 1} - \frac{eSH}{2\pi\hbar c} \sum_{n=0}^{\infty} \frac{\partial\mu/\partial H}{e^{\frac{\varepsilon_n - \mu}{T}} + 1}
$$

=
$$
-H\frac{\partial}{\partial H}\left(\frac{\Omega}{H}\right) - N\frac{\partial\mu}{\partial H},
$$
(20)

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where unlike to Eq.(19) the differentiation should be performed taking into account the chemical potential field dependence.

At $T = 0$ when n is the number of Landau level occupied by electrons, such that $j = n-1$ is amount of completely filled levels, the thermodynamic potential is [2]

$$
\Omega = \frac{1}{2}gn^2 \hbar \omega_c - g\mu n,\tag{21}
$$

where $g = S/2\pi\lambda_H^2 = NH/H_0$ is the degree of degeneracy.

Hence, for the bulk states moment, taking into account $\mu = \hbar \omega_c (n+1/2)$, we obtain

$$
M_1 = \frac{e\hbar}{2mc}[gn(n+1) - N(2n+1)] = N\frac{e\hbar}{2mc} \left[\frac{H}{H_0}(j+1)(j+2) - (2j+3) \right].
$$
\n(22)

The second term

$$
2M_2 = -\frac{\Omega}{H} \tag{23}
$$

is due to the electrons filling the edge states.

Hence, for the edge states moment we obtain

$$
2M_2 = \frac{e\hbar}{2mc}gn(n+1) = N\frac{e\hbar}{2mc}\frac{H}{H_0}(j+1)(j+2)
$$
 (24)

The total magnetic moment

$$
M = M_1 + 2M_2 = N \frac{e\hbar}{2mc} \left[2\frac{H}{H_0} (j+1)(j+2) - (2j+3) \right]
$$
 (25)

coincides with derived by Peierls [1].

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