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Effect of the Fermi surface shape on the de Haas-van Alphen oscillations in layered conductors

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In this paper we theoretically analyze the effects of the Fermi surface (FS) shape on the magnetic oscillations in quantizing magnetic fields in quasi-two dimensional layered conductors. The theory is developed basing on a phenomenological model for the electron energy spectra introduced in the paper. The model enables to take into consideration various Fermi surface profiles, and this gives it the advantage over the commonly used tight-binding approximation. It is shown that when the FS curvature becomes zero at an effective cross-section with maximum/minimum cross-sectional area, this could significantly affect amplitude, shape and phase of the oscillations as well as the field dependence of the amplitude.

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In the last two decades quasi-two-dimensional (Q2D) materials with metallic-type conductivity (e.g. organic metals, intercalated compounds and some other) have attracted a substantial interest, and extensive efforts were applied to study their electron characteristics. Magnetic quantum oscillations are frequently used as a tool in these studies [1, 2]. A theory of magnetic oscillations in Q2D materials was proposed in several works (see e.g. Refs. [3 – 10]). Significant progress is already made in developing the theory but there still remain some points not taken into account so far. The purpose of the present work is to contribute to the theory of de Haas-van Alphen oscillations in Q2D conductors by analyzing one of these points, namely, the effect of the Fermi surface (FS) curvature on the amplitude and shape of the oscillations.

This effect could be easily given a physical explanation (see e.g. Refs. [11, 12]). In general, quantum oscillations in various observables are specified with contributions from vicinities of effective cross-sections of the FS. Those are cross-sections with minimum and maximum sectional areas. When the FS curvature becomes zero at an effective cross- section, the number of electrons associated with the latter increases, and their response enhances. This may significantly strengthen the oscillations originating from such cross- section and change their shape and phase.

The Fermi surfaces of Q2D metals are known to be systems of weakly rippled cylinders. Ignoring the anisotropy of the energy spectrum in conducting layers planes, the latter could be written out as follows [13, 14]:

$$E(\mathbf{p}) = \frac{\mathbf{p}_\perp^2}{2m_\perp} - 2t\sum_{n=1}^{\infty}\epsilon_n \cos\left(\frac{np_z d}{\hbar}\right) \equiv \equiv \frac{\mathbf{p}_\perp^2}{2m_\perp} - 2t\epsilon\left(\frac{p_z d}{\hbar}\right). \tag{1}$$

Here, z axis is assumed to be perpendicular to the conducting layers, $\mathbf{p}_\perp, p_z$ are the quasimomentum projections on the layer plane and on the z axis, respectively; $m_\perp$ is the effective mass corresponding to the motion of quasiparticles in the layers plane; and d is the interlayer distance. The sum of the Fourier series $\epsilon(p_z d/\hbar)$ is an even periodic function of p_z whose maximum and minimum values equal ± 1. The parameter t in this expression (1) is the interlayer transfer integral whose value determines how much the FS is warped. When t goes to zero the FS becomes perfectly cylindrical.

By introducing this expression we get opportunities to describe Q2D FSs of various profiles (see Fig.1). In particular, assuming that $\epsilon_1 = 1$ and all remaining coefficients ϵ_n in the Fourier series in Eq. (1) equal zero, we arrive at the well known tight-binding approximation:

$$E(\mathbf{p}) = \frac{\mathbf{p}_\perp^2}{2m_\perp} - 2t\cos\left(\frac{p_z d}{\hbar}\right). \tag{2}$$

The latter corresponds to a simple cosine warping of the FS. The adopted model (1) enables us to analyze the influence of the FS profiles on magnetic oscillations in strong (quantizing) fields. As shown below, these studies bring some nontrivial results which could not be obtained within the tight-binding approximation.

Here, we analyze quantum oscillations in the magnetization (de-Haas – van Alphen effect) so we start from

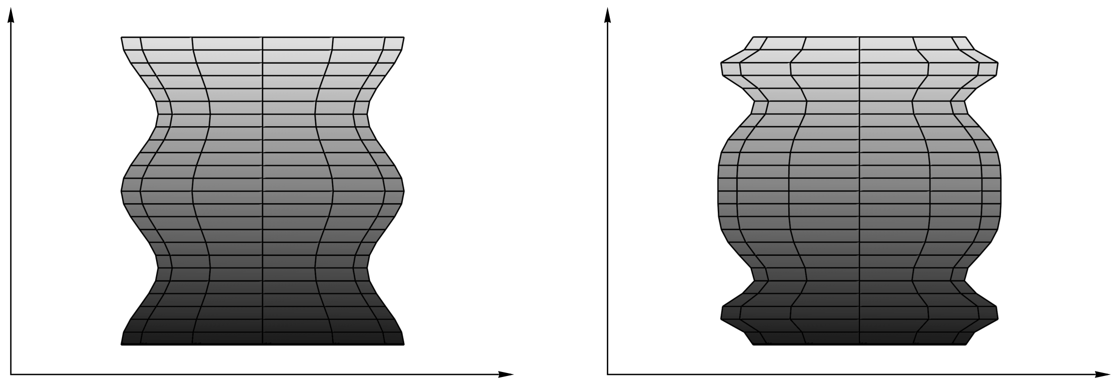

Fig.1. Schematic plots of a Fermi surface with a cosine warping corresponding to the tight-binding model (left), and a Fermi surface of a complex profile including cross- sections with maximum areas where the FS curvature becomes zero (right)

the standard expression for the longitudinal magnetization:

$$M_{||}(B,T,\mu) \equiv M_z(B,T,\mu) = -\left(\frac{\partial\Omega}{\partial B}\right)_{T,\mu}. \quad (3)$$

The magnetization depends on the temperature T and the chemical potential μ. The expression for the thermodynamic potential could be written out in a usual fashion:

$$\Omega(B,T,\mu) = -T\sum \ln\left\{1 + \exp\left[(\mu - E)/T\right]\right\}. \quad (4)$$

In this expression the summation is carried over all possible states of quasiparticles. When a strong magnetic field is applied the quasiparticles have the Landau energy-spectrum, so the expression (1) takes the form:

$$E_{n,\sigma}(p_z) = \hbar\omega\left(n + \frac{1}{2}\right) + \sigma\hbar\omega_0 - 2t\epsilon\left(\frac{p_z d}{\hbar}\right). \quad (5)$$

Here, ω is the cyclotron frequency, $\omega_0 = \beta B$; β is the Bohr magneton, and σ is the spin quantum number. In further consideration we assume as usually, that the cyclotron quantum $\hbar\omega$ is small compared to the chemical potential μ. Then the expression for the thermodynamic potential could be presented as a sum of a monotonous term Ω_0 and an oscillating correction $\Delta\Omega$:

$$\Delta\Omega = \frac{i}{4\pi^2\hbar\lambda^2}\sum_\sigma\sum_{r=1}^{\infty}\frac{(-1)^r}{r}\int_0^\infty \frac{I_r(E_\sigma)dE}{1 + \exp[(E_\sigma - \mu)/T]}. \quad (6)$$

The function $I_r(E_\sigma)$ is given by:

$$I_r(E_\sigma) = 2\mathrm{Im}\int \exp\left[ir\frac{\lambda^2}{\hbar^2}A(E_\sigma, p_z)\right]dp_z \quad (7)$$

where λ is the magnetic length, and $A(E_\sigma, p_z)$ is the cross- sectional area.

Until this point we followed the well-known Lifshitz and Kosevich (LK) theory in derivation of the expression for $\Delta\Omega$. As a result we arrived at Eqs. (6),(7) which are valid for conventional 3D metals as well as for Q2D and perfectly 2D conductors. Diversities in the expressions for $\Delta\Omega$ appear in the course of calculations of the function $I_r(E_\sigma)$. These calculations bring different results for different FS geometries. In deriving the standard LK formula it is assumed that the FS curvature is nonzero at the effective cross-sections with the extremal areas A_{ex}, and $I_r(E_\sigma)$ is approximated using the stationary phase method. In the case of Q2D conductors we can use this method when the FS warping is not too small ($t \gg \hbar\omega$). As a result we get:

$$\Delta M_{||} = -2N\beta\sqrt{\frac{\hbar\omega}{2\pi^2 t}}\sum_{r=1}^{\infty}\frac{(-1)^r R(r)}{\pi r^{3/2}} \times \\ \times \sin\left(2\pi r\frac{F}{B}\right)\cos\left(\frac{4\pi r t}{\hbar\omega} - \frac{\pi}{4}\right). \quad (8)$$

Here, $F = cA_{ex}/2\pi\hbar e$; N is the density of charge carriers, and $R(r)$ accounts for the effects of temperature, scattering and spin splitting:

$$R(r) = R_T(r)R_D(r)R_S(r). \quad (9)$$

The damping factors $R_T(r), R_D(r)$ and $R_S(r)$ are written in their usual form [15].

For 2D metals the calculations of $I_r(E_\sigma)$ are trivial for the FS is a cylinder and the cross-sectional area does not depend of p_z. In this case we obtain [8]:

$$\Delta M_{||} = -2N\beta\sum_{r=1}^{\infty}\frac{(-1)^r}{\pi r}R(r)\sin\left(2\pi r\frac{F}{B}\right). \quad (10)$$

Within the tight-binding approximation (2) one can expand the integrand in the Eq. (7) in Bessel functions and easily carry out integration over p_z. Then $\Delta M_{||}$ takes the form [16]:

$$\Delta M_{||} = -2N\beta \sum_{r=1}^{\infty} \frac{(-1)^r}{\pi r} R(r) J_0\left(\frac{4\pi r t}{\hbar\omega}\right) \sin\left(2\pi r \frac{F}{B}\right). \quad (11)$$

When the FS warping is negligible ($t \ll \hbar\omega$) this expression passes into the previous formula (10) describing the magnetization of a 2D metal. In the opposite limit ($t \gg \hbar\omega$) one can use the corresponding asymptotic for the Bessel functions $J_0(4\pi r t/\hbar\omega)$. As a result the expression for $\Delta M_{||}$ is transformed to the form (8).

Before we proceed we remark that within the tight-binding model the FS curvature takes on nonzero values at both effective cross-sections:

$$K_{ex} = -\frac{1}{2A_{ex}}\left(\frac{d^2A}{dp_z^2}\right)_{ex} = \pm\frac{2\pi t m_\perp}{A_{ex}}\left(\frac{d}{\hbar}\right)^2. \quad (12)$$

Therefore this commonly used approximation sometimes is not suitable to analyze the effects of the FS shape in Q2D metals.

To analyze these effects we return back to our generalized energy-momentum relation (1). Then the second derivative d^2A/dp_z^2 must become zero at $p_z = p^*$ as follows from the expression for the FS curvature at the effective cross-section (12). So, using the energy-momentum relation (1) we assume that the FS curvature becomes zero at the effective cross-section at $p_z = p^*$. Then we can write the following expansion for the cross-sectional area:

$$A(E,p_z) = A_{ex}(E) + 4\pi t m_\perp \sum_{n=l} a_n(E)(p_z - p^*)^{2n} \quad (13)$$

where $l > 1$;

$$a_n(E) = \frac{1}{(n)!}\left(\frac{d^{2n}\epsilon}{dp_z^{2n}}\right)_{p_z=p^*}.$$

Assuming the series included in (13) rapidly converges [$a_{n+1}(E) \ll a_n(E)$] we may keep only the first term in this expansion in further calculations when the FS warping is pronounced so that $4\pi t a_l/t\Omega \gg 1$, we may apply the stationary phase method to compute the integrals (7). Then we arrive at the expression for the oscillating part of the magnetization:

$$\Delta M_{||} = -2N\alpha_l\beta\left(\frac{B}{F}\right)^{1/2l} \sum_{r=1}^{\infty} \frac{(-1)^r R(r)}{(\pi r)^\rho} \times \sin\left(2\pi r\frac{F}{B} \pm \frac{\pi}{4l}\right). \quad (14)$$

Here, $\rho = 1 + 1/2l$, V_0 is the FS volume in a single Brillouin zone, $\Gamma(\rho)$ is the gamma function and

$$\alpha_l = \frac{A_{ex}}{V_0}\Gamma(\rho)\left[\frac{A_{ex}}{4\pi t m_\perp a_l}\right]^{1/2l}. \quad (15)$$

The FS shape near $p_z = p^*$ is determined by the shape parameter l. When $l = 1$ the FS has a nonzero curvature at the considered cross-section. In this case Eq. (14) agrees with the LK result (8). When $l \to \infty$ Eq. (14) passes into the expression (10) describing magnetization oscillations in 2D conductors. In general, one may treat l as a phenomenological parameter whose actual value could be found from experiments. The greater is the value of this parameter the closer is the FS to a cylinder near $p_z = p^*$.

Oscillations in magnetization described by the expression (14) may vary in magnitude, shape and phase depending on the value of the shape parameter l. This is illustrated in the Fig.2. As shown in this figure, when

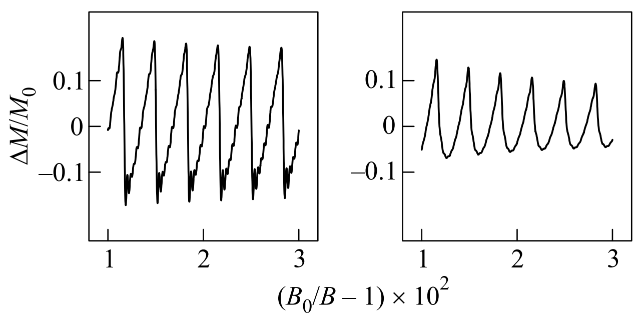

Fig.2. De Haas-van Alphen oscillations described by the Eq. (14) for $l = 4$ (left panel) and $l = 1$ (right panel). Calculations are carried out for $T = T_D = 0.5\,$K, $B_0 = 10\,$T, $F/B_0 = 300$; T_D is the Dingle temperature, and $M_0 = 2N\beta$.

there is close proximity of the FS near $p_z = p^*$ to a cylinder ($l = 4$), the oscillations are sawtoothed and resemble those occuring in 2D metals [5, 9] or originating from cylindrical segments of the FSs in conventional 3D metals [17, 18]. Here, we have intentionally chosen such a great value for the shape parameter to emphasize the difference between our result (14) and the expression (11) obtained basing on the tight-binding model. Using the latter one could easily describe sawtoothed oscillations typical for 2D metals but only for small values of the transfer integral t ($t \ll \hbar\omega$) when the FS crimping is negligible. The present result (14) shows that the oscillation shape and phase may be determined not by the value of t itself but rather by the form of the function $\epsilon(p_z d/\hbar)$ specifying the FS profile. The sawtoothed oscillations in magnetization could occur at $t \sim \hbar\omega$, when the FS curvature becomes zero at an effective cross-section. To ease the interpretation of this point one may imagine a FS shaped as a step-like cylinder. The curvature of such FS is everywhere zero, and oscillations from both kinds of the cross-sections (with minimum and maximum cross-sectional areas, respectively) should be similar to those in 2D metals. Nevertheless, the difference in the cross-sectional areas (the FS crimping) could be well pronounced, and a beat effect could be manifested. Obviously, this effect is absent when $t \ll \hbar\omega$ and the FS warping is negligible.

Speaking of realistic Q2D conductors, it would be rather uncommon to observe such close proximity of their FSs near some effective cross-sections to a cylinder as discussed above. We may rather expect the shape parameter l to take on values significantly smaller than four. Nevertheless, the main result holds, namely, that the local anomalies in the FS curvature may noticeably change the shape of the magnetization oscillations. Some features commonly expected to appear in nearly 2D metals ($t \ll \hbar\Omega$) may be manifested in magnetic oscillations in Q2D conductors at $t \sim \hbar\Omega$, originating from the specific FS profiles.

In summary, in the present work we analyze the effect of the FS shape on the de Haas – van Alphen oscillations in Q2D conductors. Such analysis is important for there exists a great deal of interest in studies of band-structure parameters and other electronic properties of these materials. Usually, the tight-binding model for the electron spectrum is employed to extract relevant information from the experiments. This approximation has its limitations, so some problems arise in interpreting the experimental data [10]. An important limitation of the current theory is that the latter misses the effects of the FS geometry assuming a simple cosine warping of the FS. Here, we lift this restriction on the FS shape. We show that the FS profile may significantly affect the quantum oscillations in magnetization if the FS curvature becomes zero at a cross-sectional area. Also, we show that main characteristics of the oscillations are determined by two different factors, namely by the FS curvature at the effective cross-sections and the transfer integral, whereas existing theory takes into account only the latter. These two factors work simultaneously, and their effects could be separated. The proposed approach could be useful in analyzing experiments on magnetization oscillations in Q2D conductors, especially those where sawtooth features in the oscillations are well pronounced (see e.g. Refs. [9, 19, 20]). It could help to extract important extra informations concerning fine geometrical features of the FSs of such materials.

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