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Semiclassical theory of magnetic quantum oscillations in a two-dimensional multiband canonical Fermi liquid

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The semiclassical Lifshitz-Kosevich description of quantum oscillations is extended to a multiband two-dimensional Fermi liquid with a constant number of electrons. The amplitudes of oscillations with combination frequencies, recently predicted and observed experimentally, are analytically derived and compared with the single-band amplitudes. The combination amplitudes decay with temperature exponentially faster than the standard harmonics, and this provides a valuable tool for their experimental identification.

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It has been shown[1] that the magnetic quantum oscillations in a multiband two-dimensional metal with a fixed electron density [canonical ensemble (CE)] are qualitatively different from those in an open system where the chemical potential is fixed [grand canonical ensemble (GCE)]. There is a mechanism for different bands to ''talk'' to each other in CE producing a de Haas–van Alphen (dHvA) signal with the combination frequencies, $f=f_1+f_2$ (Ref. 1) and $f=f_1-f_2$ (Refs. 2 and 3) in addition to the ordinary dHvA frequencies, $f_{1,2}$, of the individual bands in GCE. Numerical studies of oscillations showed that their amplitudes are comparable with the standard components, and they are robust with respect to a *background* (nonquantized) density of states.[2]

The frequencies have been recently observed[4] in quantum well structures. These additional components in the dHvA frequency spectrum of low-dimensional metals may provide a unique information on the Fermi surface and carrier density if detailed analytical theory is available. In this paper we develop such a theory in the framework of the semiclassical Lifshitz-Kosevich (LK) approach.[5] The Eqs. (12) and (13) are the main results of the present paper.

We first derive a convenient expression for a multiband two-dimensional thermodynamic potential in an external magnetic field H,

$$\Omega=-T\int d\epsilon\, N(\epsilon,B)\ln\left[1+\exp\left(\frac{\mu-\epsilon}{T}\right)\right], \tag{1}$$

where

$$N(\epsilon,B)=\sum_{\alpha}\sum_{n=0}^{\infty}\rho_\alpha\omega_\alpha\delta(\epsilon-\epsilon_{\alpha n}) \tag{2}$$

is the quantized density-of-states, ρ_α is the zero-field density-of-states in the band α, $\epsilon_{\alpha n}=\Delta_{\alpha 0}+\omega_\alpha(n+1/2)+g_\alpha\sigma\mu_B B$, $\omega_\alpha=eB/m_\alpha$ the cyclotron frequency with the cyclotron mass m_α, $B=H+4\pi M$ the magnetic field, $\Delta_{\alpha 0}$ the band edge in zero magnetic field, μ the chemical potential, g_α the electron g factor, $\sigma=\pm 1/2$, μ_B the Bohr magneton, and $\hbar=c=k_B=1$. The band index α includes the electron spin. In actual experiments on 2DEG, $B\approx H$ and magnetic coupling between subbands was negligible.[4]

By applying the Poisson formula[6] to the sum over n in the thermodynamic potential

$$\Omega=-T\sum_{\alpha}\rho_\alpha\omega_\alpha\sum_{n=0}^{\infty}\ln\left[1+\exp\left(\frac{\mu_\alpha-\omega_\alpha(n+1/2)}{T}\right)\right] \tag{3}$$

with $\mu_\alpha=\mu-\Delta_\alpha$ and $\Delta_\alpha=\Delta_{\alpha 0}+g_\alpha\sigma\mu_B B$, we obtain

$$\Omega=\Omega_0+\tilde{\Omega}, \tag{4}$$

where

$$\Omega_0=-T\int_0^{\infty}d\epsilon\sum_{\alpha}\rho_\alpha\ln\left[1+\exp\left(\frac{\mu_\alpha-\epsilon}{T}\right)\right] \tag{5}$$

is the ''classical'' part. In GCE it does not oscillate as a function of $1/B$, and contains the contribution due to spin susceptibility (Pauli paramagnetism). The second part is

$$\tilde{\Omega}=\frac{1}{24}\sum_{\alpha}\rho_\alpha\omega_\alpha^2+2\sum_{\alpha}\sum_{r=1}^{\infty}A_\alpha^r\cos\left(\frac{rf_\alpha}{B}+\phi_\alpha^r\right), \tag{6}$$

where the first term produces the Landau diamagnetism and the second oscillatory term is responsible for the de Haas–van Alphen effect. It is small compared with the ''classical'' part as $\tilde{\Omega}/\Omega_0\sim(\omega/\mu)^2$. The Fourier components appear with frequencies $rf_\alpha\equiv rS_\alpha/e$, where $S_\alpha=2\pi m_\alpha(\mu-\Delta_{\alpha 0})$ is the Fermi surface zero-field cross section. The amplitudes of the Fourier harmonics are

$$A_\alpha^r=\frac{T\rho_\alpha\omega_\alpha}{2r\sinh(2\pi^2 rT/\omega_\alpha)}, \tag{7}$$

and the phase $\phi_\alpha^r=r\pi(1+g_\alpha\sigma)$.

Differently from GCE, the chemical potential oscillates in CE. Hence, the classical part of Ω contributes to oscillations as well. The relevant thermodynamic potential of CE is the free energy $F=\Omega+\mu N$, with a fixed number of electrons, $N=-\partial\Omega/\partial\mu$. At low temperatures we find

$$\Omega_0=-\sum_{\alpha}\rho_\alpha\mu_\alpha^2/2, \tag{8}$$

so that

$$\mu=\frac{1}{\rho}\left(N+\sum_{\alpha}\rho_{\alpha}\Delta_{\alpha}+\frac{\partial\tilde{\Omega}}{\partial\mu}\right),\tag{9}$$

where $\rho=\Sigma_{\alpha}\rho_{\alpha}$ is the total density-of-states. Substituting this expression into Ω_0, Eq. (8), we obtain

$$F=F_0+\tilde{F},\tag{10}$$

where the smooth nonoscillatory part of the free energy is given by

$$F_0=\frac{1}{2\rho}\left(N+\sum_{\alpha}\rho_{\alpha}\Delta_{\alpha}\right)^2-\frac{1}{2}\sum_{\alpha}\rho_{\alpha}\Delta_{\alpha}^2,\tag{11}$$

while the most essential oscillatory part is

$$\tilde{F}=\tilde{\Omega}-\frac{1}{2\rho}\left(\frac{\partial\tilde{\Omega}}{\partial\mu}\right)^2.\tag{12}$$

In a more explicit form we obtain

$$\begin{aligned}\tilde{F}=&\frac{1}{24}\sum_{\alpha}\rho_{\alpha}\omega_{\alpha}^2+2\sum_{\alpha,r}A_{\alpha}^r\cos\left(\frac{rf_{\alpha}}{B}+\phi_{\alpha}^r\right)\\&-4\sum_{\alpha,\alpha',r,r'}C_{\alpha\alpha'}^{rr'}\sin\left(\frac{rf_{\alpha}}{B}+\phi_{\alpha}^r\right)\sin\left(\frac{r'f_{\alpha'}}{B}+\phi_{\alpha'}^{r'}\right).\end{aligned}\tag{13}$$

It is the last term, which yields combination Fourier harmonics with the combination frequencies $f=rf_{\alpha}\pm r'f_{\alpha'}$. Their amplitudes,

$$C_{\alpha\alpha'}^{rr'}=2\pi^2\frac{rr'A_{\alpha}^rA_{\alpha'}^{r'}}{\rho\omega_{\alpha}\omega_{\alpha'}}\tag{14}$$

are comparable with the standard single-band harmonics at low temperatures, $T<\omega_{\alpha}/2\pi^2r$, as also found in the numerical analysis[1,2] and in the experiment.[4] For example, the ratio of the combination amplitude to a single-band one for $r=r'=1$ and $T=0$ in a metal with two parabolic bands ($\rho_{\alpha}=m_{\alpha}/2\pi$) is

$$\frac{2C_{\alpha\alpha'}^{11}}{A_{\alpha}^1}=\frac{m_{\alpha}}{m_{\alpha}+m_{\alpha'}}.\tag{15}$$

Differentiating $\tilde{\Omega}$ in GCE and $\tilde{F}$ in CE with respect to H, one obtains the ratio of the combination and single-band amplitudes of magnetization as

$$\frac{M_{\alpha\alpha'}^{11}}{M_{\alpha}^1}=\frac{2C_{\alpha\alpha'}^{11}}{A_{\alpha}^1}\frac{f}{f_{\alpha}}=\frac{m_{\alpha}}{m_{\alpha}+m_{\alpha'}}\frac{f}{f_{\alpha}},\tag{16}$$

Differentiating twice the ratio in susceptibility is ($T=0$)

$$\frac{\chi_{\alpha\alpha'}^{11}}{\chi_{\alpha}^1}=\frac{2C_{\alpha\alpha'}^{11}}{A_{\alpha}^1}\left(\frac{f}{f_{\alpha}}\right)^2=\frac{m_{\alpha}}{m_{\alpha}+m_{\alpha'}}\left(\frac{f}{f_{\alpha}}\right)^2.\tag{17}$$

The last two ratios may be even larger than unity for the ‘‘plus’’ combination harmonic ($f=f_{\alpha'}+f_{\alpha}$) while the ‘‘minus’’ one ($f=f_{\alpha'}-f_{\alpha}$) is suppressed in magnetization and susceptibility, Fig. 1. At higher temperatures the combination harmonics are exponentially small compared with the single-band ones, as shown in Fig. 1.

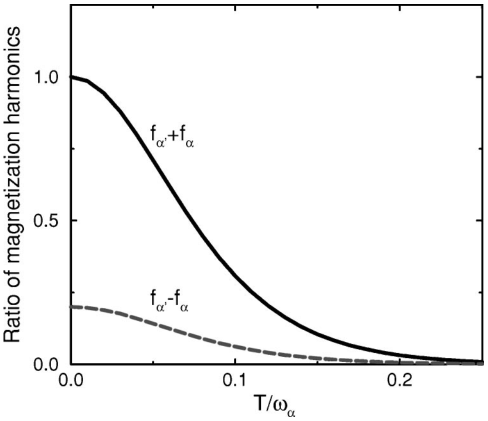

FIG. 1. The relative values of $f_{\alpha'}+f_{\alpha}$ and $f_{\alpha'}-f_{\alpha}$ combination Fourier components of magnetization for $m_{\alpha'}=1.5m_{\alpha}$ and $f_{\alpha'}=1.5f_{\alpha}$. The ratio for the parabolic bands is $M_{\alpha\alpha'}^{11}/M_{\alpha}^1=2\pi^2Tm_{\alpha'}(f_{\alpha'}\pm f_{\alpha})/[f_{\alpha}(m_{\alpha}+m_{\alpha'})\omega_{\alpha}\sinh(2\pi^2T/\omega_{\alpha'})]$.

We note that according to Eq. (13) the difference between the Fourier harmonics for open and closed systems should be seen even in a simplest single-band metal due to splitting of the band. On the other hand, in three- (and higher) band metals, a mixture of more than two different frequencies can be observed due to nonparabolic band dispersion giving rise to cubic and higher powers of the chemical potential in the expression for Ω_0, Eq. (8). In very high magnetic fields the usual magnetic breakdown and the nonlinear field dependence of magnetic subbands due to nonparabolicity of the band dispersion could also lead to combination frequencies.[7]

In conclusion we have developed the analytical semiclassical theory of magnetic quantum oscillations in multiband two-dimensional metals. We have found the amplitudes of the combination Fourier harmonics, which are comparable with the single-band harmonics at low temperatures and exponentially small at higher temperatures. Their frequencies and the temperature dependence of amplitudes provide additional information on the band structure and carrier densities of a multiband canonical Fermi liquid. Essentially different temperature dependence of the combination amplitudes compared with the standard harmonics, Fig. 1, should allow to distinguish them experimentally.

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