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Combination quantum oscillations in canonical single-band Fermi liquids

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Chemical potential oscillations mix individual-band frequencies of the de Haas–van Alphen and Shubnikov–de Haas magnetooscillations in canonical low-dimensional multiband Fermi liquids. We predict a similar mixing in canonical single-band Fermi liquids, which Fermi surfaces have two or more extremal cross sections. Combination harmonics are analyzed using a single-band almost two-dimensional energy spectrum. We outline some experimental conditions allowing for resolution of combination harmonics.

Magnetic quantum oscillations of magnetization [de Haas–van Alphen (dHvA) effect] and resistivity [Shubnikov–de Haas (SdH) effect] are unequivocal hallmarks of the Fermi liquid, providing most reliable and detailed Fermi surfaces,\textsuperscript{1} in particular, in layered organic metals\textsuperscript{2,3} and almost two-dimensional (2D) superconductors such as Sr\textsubscript{2}RuO\textsubscript{4}.\textsuperscript{4} An interesting feature of dHvA and/or SdH oscillations is a difference between canonical and grand canonical ensembles. While it is negligible in three-dimensional metals,\textsuperscript{5} the quantum fluctuations of two thermodynamically identical ensembles are very different in 2D multiband metals. In particular, there are combination frequencies in dHvA and/or SdH oscillations of a 2D multiband metal with fixed electron density \( n_e \) (canonical ensemble), predicted by Alexandrov and Bratkovsky (AB),\textsuperscript{6} and studied numerically\textsuperscript{6–11} and analytically.\textsuperscript{12–14} The effect has been experimentally observed in different low-dimensional systems.\textsuperscript{3,15,16} Obviously, there are no mixing of the fundamental single-band frequencies, if the chemical potential \( \mu \) is fixed by a reservoir (grand-canonical ensemble). Importantly, samples are normally placed on nonconducting substrates with no electrodes attached, so the system is closed in actual dHvA experiments.

As it happens the fundamental frequency mixing due to the chemical potential oscillations (AB effect) may be obscured by mixing due to the magnetic breakdown\textsuperscript{17} (MB effect), as discussed by Kartsovnik.\textsuperscript{5} The MB effect is the switching of two close electron orbits in different bands on the Fermi surface (FS) at sufficiently strong magnetic fields. Here, we predict a mixing of two or more fundamental frequencies in a canonical single-band Fermi liquid with a few extremal FS cross sections, where the MB is nonexistent.

To illustrate the point, we consider an anisotropic single band, with the dispersion \( E(k) \) in zero magnetic field,

\[
E(k) = \frac{\hbar^2 k^2}{2m} - 2 t_\perp \cos(k_\perp d),
\]

which is a fair approximation for a band in layered metals.\textsuperscript{2,3} Here, \( k_\parallel \) and \( k_\perp \) are the in-plane and out-of-plane quasimomenta, \( t_\perp \) is the interplane hopping integral, and \( d \) is the interplane distance.

When the magnetic field \( B \) is applied, the spectrum [Eq. (1)] is quantized as\textsuperscript{18}

\[
E_n(k_\parallel) = \hbar \omega_c (n + 1/2) - 2t \cos(k_\perp d) \pm g \mu_B B/2,
\]

where \( \omega_c = eB \cos(\theta)/m \) is the cyclotron frequency (\( n = 0, 1, 2, \ldots \), \( t = 1, J_0(k_F d \tan(\theta)) \) [\( J_0(x) \) is the Bessel function], \( \theta \) is the angle between the field and the normal to the planes, \( g \) is the electron g factor, and \( \mu_B \) is the Bohr magneton. The spectrum [Eq. (2)] is perfectly 2D at the Yamaji angles\textsuperscript{19} found from \( J_0(k_F d \tan(\theta))=0 \), where \( k_F = (2m \mu)^{1/2} \) is the Fermi momentum in pure 2D case, but otherwise there are two extremal semiclassical orbits. They give rise to beats in dHvA/SdH oscillations with two fundamental Fourier-transform (FT) frequencies, \( F_{l,i} = \hbar A_{l,i}/2 \pi e \cos(\theta) \), revealing modulations of the cylindrical FS along the perpendicular direction (Fig. 1), as observed, e.g., in Sr\textsubscript{2}RuO\textsubscript{4}.\textsuperscript{4,16}

Since there are no different bands, one might expect neither AB nor MB mixing of the fundamental frequencies \( F_l \) and \( F_i \) in the single-band model [Eq. (1)], in contrast with canonical multiband systems.\textsuperscript{6,17} Actually, as we show below, \( F_l \) and \( F_i \) turn out mixed, if \( n_e \) is constant, so that a combination frequency \( F_c = F_l + F_i \) appears similar to the AB combination frequency\textsuperscript{6} in two-band canonical Fermi liquids. Using conventional Poisson’s summation and integrals,\textsuperscript{1} the grand canonical potential per unit volume,

\[
\Omega = -\frac{k_B T e B \cos(\theta)}{4 \pi^2 \hbar} \sum_n \int_{-\pi/d}^{\pi/d} d k_\perp \ln[1 + e^{\mu - E_n(k_\parallel)/k_B T}],
\]

is given by \( \Omega = \Omega_0 - m \mu^2 / 2 \pi d^2 \hbar^2 \), where

![FIG. 1. (Color online) Large, \( A_1 = 2 \pi m (\mu + 2t)/\hbar^2 \), and small, \( A_2 = 2 \pi m (\mu - 2t)/\hbar^2 \), extremal cross sections of a layered-metal Fermi surface.](image-url)
\[ \Omega = \frac{e^2 B^2 \cos^2(\Theta)}{4 \pi^2 m_d} \sum_{r=1}^{\infty} R_f(r) \cos \left[ \frac{\pi r \mu m}{m_e \cos(\Theta)} \right] \left( -\frac{R}{r} \right) J_0 \left( \frac{4 \pi r \mu}{h \omega_c} \right) \times \cos \left( \frac{2 \pi r \mu}{h \omega_c} \right) \]

is its quantum part with the conventional temperature, \( R_f(r) = (2 \pi r k_B T / h \omega_c) \sinh(2 \pi r k_B T / h \omega_c) \), and Dingle collision damping factor \( R \), as derived in Ref. 13 (0 < \( R_f(r) \), \( R \leq 1 \)). Differentiating \( \Omega \) with respect to the magnetic field at constant \( \mu \), one obtains the oscillating part of the magnetization, \( \tilde{M} = -\partial \tilde{\Omega} / \partial B \),

\[ \tilde{M} = \frac{e \mu \cos(\Theta)}{2 \pi^2 h d} \sum_{r=1}^{\infty} \frac{(-R') R_f(r)}{r^{3/2}} \left[ \sin \left( \frac{2 \pi r F_f}{B} - \frac{\pi}{4} \right) \right] \]

where we neglect small terms of the order of \( 2t/\mu \ll 1 \), and take \( g = 0 \) for more transparency.

We are interested in the regime \( h \omega_c \ll 4 \pi \), where three-dimensional corrections to the spectrum are significant, rather than in the opposite ultraquantum limit,\(^{13}\) where the quantized spectrum is almost 2D. In our intermediate-field regime, one can replace the Bessel function in Eq. (5) by its asymptotic, \( J_0(x) \approx (2 / \pi x)^{1/2} \cos(x - \pi / 4) \) at large \( x \) to obtain

\[ \tilde{M} = \frac{e \mu \cos(\Theta)}{2 \pi^2 h d} \left( \frac{2 B}{\pi B_1} \right)^{1/2} \sum_{r=1}^{\infty} \frac{(-R') R_f(r)}{r^{3/2}} \left[ \sin \left( \frac{2 \pi r F_f}{B} - \frac{\pi}{4} \right) \right] \]

where \( B_1 = 4 \pi n t / e h \cos(\Theta) \gg B \).

Naturally, the FT of Eq. (6) yields two fundamental frequencies in the grand-canonical ensemble, where \( \mu \) is fixed (Fig. 2). However, the chemical potential oscillates with the magnetic field in the canonical system,\(^{16}\) which affects quantum corrections to magnetization. Using \( n_c = -\partial \Omega / \partial \mu \), one can find the oscillating component, \( \tilde{\mu} = \mu_0 / 2 \pi \cos(\Theta) / \partial \mu \), of the chemical potential, \( \mu = \mu_0 + \tilde{\mu} \), where \( \mu_0 = d \pi h^2 n_c / m \) is its zero-field value and

\[ z = \left( \frac{B}{2 \pi B_1} \right)^{1/2} \sum_{r=1}^{\infty} \frac{(-R') R_f(r)}{r^{3/2}} \left[ \sin \left( r z + \frac{2 \pi r f_1}{B} - \frac{\pi}{4} \right) \right] + \sin \left( r z + \frac{2 \pi r f_2}{B} + \frac{\pi}{4} \right) \]

yields two first fundamental harmonics with the frequencies \( f_1 \) and \( f_2 \), identical to those of the grand-canonical system,

\[ z_1 = -R R_f(1) \left( \frac{B}{2 \pi B_1} \right)^{1/2} \left[ \sin \left( \frac{2 \pi f_1}{B} - \frac{\pi}{4} \right) \right] \]

yields two second fundamental harmonics with the frequencies \( 2f_1 \) and \( 2f_2 \), as in the grand-canonical system, and
is the mixed harmonic with the frequency $F_0 \pm f_1$, which is a specific signature of the canonical ensemble. Its amplitude is small compared with the first-harmonic amplitudes as $(B/2\pi B_\perp)^{1/2}$ in contrast with multiband systems, where the mixed-harmonic amplitudes have roughly the same order of magnitude as the fundamental-harmonic amplitudes at $R = R_0(r) = 1$. Moreover, there is no $F_0 \pm f_1$ frequency in the FT spectrum of the single-band canonical system, different from the multiband canonical systems.

To assess an accuracy of the analytical approximation [Eq. (10)] and some experimental conditions, allowing for resolution of the mixed harmonic, we present numerically exact magnetization and their FTs in Fig. 2 at $T=0$. Since convergence of the sum in Eq. (7) is poor at $T=0$, one can use its integral representation in numerical calculations as

$$z_{\text{mix}} = R^2 R_0^2 (1 - \frac{2\pi B}{2\pi B_\perp})^2 \left( \frac{2\pi F_0}{B} \sin \left( \frac{2\pi F_0}{B} \right) \right)$$

is the mixed harmonic with the frequency $F_0 = f_1 + f_2$, which is a specific signature of the canonical ensemble. Its amplitude is small compared with the first-harmonic amplitudes as $(B/2\pi B_\perp)^{1/2}$ in contrast with multiband systems, where the mixed-harmonic amplitudes have roughly the same order of magnitude as the fundamental-harmonic amplitudes at $R = R_0(r) = 1$. Moreover, there is no $F_0 = f_1 - f_2$ frequency in the FT spectrum of the single-band canonical system, different from the multiband canonical systems.

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In conclusion, we have found the combination frequency in the quantum magnetic oscillations of the single-band canonical layered Fermi liquid. The difference between quantum oscillations of the canonical and grand-canonical ensembles is tiny (Fig. 2), but not obscured by the MB effect, which is absent in the single-band case in contrast with the multiband systems. We have also shown that the analytical (perturbation) FT amplitudes are numerically accurate even at zero temperature and in clean samples (i.e., for $R=1$) as they are in the multiband analytical theory.$^{10,12}$ A wide magnetic-field window is essential for experimental resolution of the combination $dHvA/SdH$ frequency.

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\begin{thebibliography}{10}
\bibitem{Schoenberg} D. Schoenberg, \textit{Magnetic Oscillations in Metals} (Cambridge University Press, Cambridge, 1984).
\bibitem{Singleton} J. Singleton, Rep. Prog. Phys. \textbf{63}, 1111 (2000).
\bibitem{Kartsovnik} M. V. Kartsovnik, Chem. Rev. (Washington, D.C.) \textbf{104}, 5737 (2004) and references therein.
\bibitem{Mackenzie} A. P. Mackenzie, S. R. Julian, A. J. Diver, G. J. McMullan, M. P. Ray, G. G. Lonzarich, Y. Maeno, S. Nishizaki, and T. Fujita, Phys. Rev. Lett. \textbf{76}, 3786 (1996).
\bibitem{Lifshits} J. M. Lifshits and A. M. Kosevich, Zh. Eksp. Teor. Fiz. \textbf{29}, 730 (1955) [Sov. Phys. JETP. \textbf{2}, 636 (1956)].
\bibitem{Alexandrov} A. S. Alexandrov and A. M. Bratkovsky, Phys. Rev. Lett. \textbf{76}, 1308 (1996).
\bibitem{Nakano} M. Nakano, J. Phys. Soc. Jpn. \textbf{66}, 19 (1997).
\bibitem{Alexandrov2} A. S. Alexandrov and A. M. Bratkovsky, Phys. Lett. A \textbf{234}, 53 (1997).
\bibitem{Champel} T. Champel, Phys. Rev. B \textbf{65}, 153403 (2002); \textbf{69}, 167402 (2004).
\bibitem{Alexandrov3} A. S. Alexandrov and A. M. Bratkovsky, Phys. Rev. B \textbf{69}, 167401 (2004).
\bibitem{Kishigi} K. Kishigi and Y. Hasegawa, Phys. Rev. B \textbf{65}, 205405 (2002); \textbf{72}, 045410 (2005).
\bibitem{Alexandrov4} A. S. Alexandrov and A. M. Bratkovsky, Phys. Rev. B \textbf{63}, 033105 (2001).
\bibitem{Bratkovsky} A. M. Bratkovsky and A. S. Alexandrov, Phys. Rev. B \textbf{65}, 035418 (2002).
\bibitem{Fortin} J. Y. Fortin, E. Perez, and A. Audouard, Phys. Rev. B \textbf{71}, 155101 (2005).
\bibitem{Shepherd} R. A. Shepherd, M. Elliott, W. G. Herrenden-Harker, M. Zervos, P. R. Morris, M. Beck, and M. Ilegems, Phys. Rev. B \textbf{60}, R11277 (1999).
\bibitem{Ohmichi} E. Ohmichi, Y. Maeno, and T. Ishiguro, J. Phys. Soc. Jpn. \textbf{68}, 24 (1999).
\bibitem{Harrison} N. Harrison, J. Caulfield, J. Singleton, P. H. P. Reinders, F. Herlach, W. Hayes, M. Kurmoo, and P. J. Day, J. Phys.: Condens. Matter \textbf{8}, 5415 (1996); P. S. Sandhu, Ju H. Kim, and J. S. Brooks, Phys. Rev. B \textbf{56}, 11566 (1997); J. H. Kim, S. Y. Han, and J. S. Brooks, \textit{ibid.} \textbf{60}, 3213 (1999); S. Y. Han, J. S. Brooks, and J. H. Kim, Phys. Rev. Lett. \textbf{85}, 1500 (2000); V. M. Gvozdikov and M. Taut, Phys. Rev. B \textbf{75}, 155436 (2007); D. Vignolles, A. Audouard, V. N. Laukhin, J. Beard, E. Canadell, N. G. Spitsina, and E. B. Yagubskii, Eur. Phys. J. B \textbf{55}, 383 (2007).
\bibitem{Kurihara} Y. Kurihara, J. Phys. Soc. Jpn. \textbf{61}, 975 (1989).
\bibitem{Yamaji} K. Yamaji, J. Phys. Soc. Jpn. \textbf{58}, 1520 (1989).
\bibitem{Hasegawa} R. Kubo, H. Hasegawa, and N. Hashitsume, J. Phys. Soc. Jpn. \textbf{14}, 56 (1959).
\bibitem{Champel2} T. Champel and V. P. Mineev, Phys. Rev. B \textbf{66}, 195111 (2002); \textbf{67}, 089901 (2003).
\bibitem{Grigoriev} P. D. Grigoriev, Phys. Rev. B \textbf{67}, 144401 (2003).
\bibitem{Alexandrov5} A. S. Alexandrov and V. V. Kabanov, Phys. Rev. Lett. \textbf{95}, 076601 (2005); \textbf{95}, 169902 (2005).
\end{thebibliography}