The origin of "high-temperature" quantum oscillations of the magnetoresistance in semimetals

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The anomalously slow temperature-induced damping of the quantum oscillations of the magnetoresistance in semimetals is shown to be caused by the constant-energy transitions of electrons with a change in the sign of the effective mass between the Landau levels.

The "high-temperature" quantum oscillations (HTO) of the magnetoresistance of bismuth and its alloys with antimony, which die out anomalously slowly [in comparison with the Shubnikov–de Haas oscillations (SdHO)] as the temperature is raised, have been observed in many experiments.[1–4] The physical cause of HTO has, however, not yet been explained. In particular, the angular oscillations and the anomalously small HTO period have not been explained.

In this letter we show that HTO are caused by constant-energy interband electron transitions between the Landau levels in semimetals and we interpret the experimental results of Refs. 1–4. The quantum theory of magnetoresistance in semimetals was derived by Davydov and Pomeranchuk[5] and Abrikosov.[6] Davydov and Pomeranchuk,[5] however, ignored the Landau quantization in the valence band and Abrikosov[6] studied the quantum limit, so that HTO dropped out of the picture.

It is known that the Shubnikov–de Haas oscillations are caused by the electrons that move along closed extremal orbits at the Fermi surface. A change in the magnetic field causes the Landau cylinders to periodically come in contact with the Fermi surface, which accounts for the periodic change in the magnetoresistance. High-temperature quantum oscillations occur in the presence of constant-energy surfaces with several extremal cross sections and are related to the transition of electrons from one extremal closed orbit to another as a result of scattering. A change in the magnetic field causes two Landau cylinders to periodically come in contact simultaneously with the constant-energy surface. The HTO reach the maximum amplitude if this surface is situated near the Fermi surface. In semimetals the foregoing remarks apply to the electron and hole sheets of the constant-energy surfaces in the valence- and conduction-band overlap interval.

The principal characteristic features of HTO can be traced in actual calculations by making use of a simple parabolic model for electrons and holes in a semimetal[6]: $\epsilon^e(\mathbf{p}) = p^2/2m_e$ and $\epsilon^h(\mathbf{p}) = \epsilon_o - (\mathbf{p} - \mathbf{p}_0)^2/m_h$, where $m_{e,h}$ are the corresponding effective masses, and ϵ_o is the overlap of the valence band and the conduction band. In the last part of this article we discuss the effects that would be encountered by going beyond the scope of this model. At $p_0^2 > 2(m_e + m_h)\epsilon_o$ we can ignore the magnetic breakdown in the relevant magnetic field range and we can use the effective-Hamilto-

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nian method. Using the Kubo equation for the transverse conductivity σ_{xx} of the electron gas in a strong magnetic field $\mathbf{H} = (0,0,H)$ in the case of a quasielastic-scattering mechanism, we find $\sigma_{xx} = \sigma_{xx}^{ee} + \sigma_{xx}^{hh} + \sigma_{xx}^{eh}$. The first two terms, which describe the intraband transitions, give rise to the Shubnikov-de Haas oscillations. The last term describes the interband transitions with a change in the sign of the effective mass. This term accounts for the high-temperature oscillations, in addition to the Shubnikov–de Haas oscillations. At $\omega_{e,h};T \ll \zeta_{e,h}$ [$\omega_{e,h} = (m_{e,h} a_H^2)^{-1}$ are the cyclotron frequencies; $a_H = \sqrt{c/eH}$ is the magnetic length; $\zeta_e = \zeta$ and $\zeta_h = \epsilon_o - \zeta$ are the electron and hole chemical potentials defined by the neutrality condition; we use a system of units with $\hbar = 1$; and T is the temperature given in energy units] we find $\sigma_{xx}^{eh} = \sigma_{\text{mon}} + \sigma_s + \sigma_{\text{HTO}}$ after summing with use of Poisson's formula. Here

$$\sigma_{\text{mon}} = \frac{4eN_i |V_{\mathbf{p}_0}|^2 m_e m_h}{3\pi^4} \left(\frac{\epsilon_o}{\omega_e + \omega_h} \right)^2, \tag{1}$$

$$\sigma_s = \frac{5}{4} \sigma_{\text{mon}} \sqrt{\frac{\omega_e + \omega_h}{2\epsilon_o}} \sum_{k=1}^{\infty} \frac{(-1)^k}{\sqrt{k}} \left[A\left(\frac{2\pi^2 kT}{\omega_e}\right) \cos\left(k S_e a_H^2 - \frac{\pi}{4}\right) + A\left(\frac{2\pi^2 kT}{\omega_h}\right) \cos\left(k S_h a_H^2 - \frac{\pi}{4}\right) \right], \tag{2}$$

$$\sigma_{\text{HTO}} = \frac{3}{8} \sigma_{mon} \frac{\omega_e + \omega_h}{\epsilon_o} \sum_{k,k'=1}^{\infty} \frac{(-1)^{k+k'}}{\sqrt{kk}} \left[A\left(\frac{2\pi^2 T}{\omega_{kk'}^-}\right) \sin(S_{kk'}^+ a_H^2) + A\left(\frac{2\pi^2 T}{\omega_{kk'}^+}\right) \cos(S_{kk'}^- a_H^2) \right], \tag{3}$$

where $V_{\mathbf{q}}$ is the Fourier component of the scattering potential, N_i is the concentration of the scattering centers, $A(x) = x/\sinh x$,

$$\frac{1}{\omega_{kk}^{\pm}} = \left| \frac{k}{\omega_e} \pm \frac{k'}{\omega_h} \right|, \quad S_{e,h} = 2\pi m_{e,h} \zeta_{e,h}$$

are the areas of the extremal cross sections of the electron and hole sheets of the Fermi surface, whose plane is perpendicular to the magnetic field, and $S_{kk'}^{\pm} = kS_e \pm k'S_h$. The terms (1)–(3) describe the monotonic component of the conductivity, the Shubnikov–de Haas oscillations, and the high-temperature oscillations, respectively. According to (2), there are two sets of Shubnikov–de Haas oscillations with the periods, $\Delta_{\text{SdHO}}^{e,h}(1/H) = 2\pi e/ckS_{e,h}$. At $T \gtrsim \omega_{e,h}$ the kth harmonic of the Shubnikov–de Haas oscillations dies out with increasing temperature, $\sim \exp(-2\pi^2 kT/\omega_{e,h})$. According to (3), HTO also contain oscillations with two periods $\Delta_{\text{HTO}}^{\pm}(1/H) = (2\pi e/c|S_{kk'}^{\mp}|)$, which at $T \gtrsim \omega^{\pm}_{kk'}$ die out, $\sim \exp(-2\pi^2 T/\omega^{\pm}_{kk'})$, with increasing temperature. Since $\omega^{+}_{kk'} < \omega_e/k; \omega_h/k'$, the long-period HTO damp faster than the Shubnikov–de Haas oscillations. In the case of short-period HTO, the slowest to die out with increasing temperature are the harmonics for which $\omega^{-}_{kk'}$ has the maximum value, i.e., $km_e \approx k'm_h$. The principal contribution to HTO accordingly comes from these harmonics. The oscillation period of these harmonics is $\Delta^{-}_{\rm HTO}(1/H) \approx e/ckm_e\epsilon_o \approx e/ck'm_h\epsilon_o$. At $\omega^{-}_{kk'} > T \gtrsim \omega_{e,h}$ the amplitude of the HTO harmonics that are last to die out is exponentially large in comparison with the amplitude of the Shubnikov–de Haas oscillations, while the period of these hamonics is smaller than that of the Shubnikov–de Haas oscillations. In estimating the relative amplitude of the high-temperature oscillations and Shubnikov–de Haas oscillations account must also be taken of the fact that both these types of oscillations, which are related to the interband transitions, have been weakened by a factor of $(|V_{\mathbf{p}_0}|^2/|V_{p_F}|^2) \sim (\tau_{\rm intraband}/\tau_{\rm interband})$ in comparison with the intraband Shubnikov–de Haas oscillations ($\tau_{\rm intraband}$ and $\tau_{\rm interband}$ are the intraband and interband relaxation times, respectively, and $p_F^{e,h} = \sqrt{2m_{e,h}\zeta_{e,h}} \ll p_0$).

The rate of the temperature-induced damping of the harmonics of the Shubnikov–de Haas oscillations and high-temperature oscillations is determined by the oscillation frequency of the state density (which is related to the state density near the Landau levels) in the magnetic field as a function of the energy. With increase in the temperature, the mean value of the oscillating part of the state density decreases sharply over the interval of thermally induced diffuseness of the Fermi level, while the amplitudes of the Shubnikov–de Haas oscillations and high-temperature oscillations decrease exponentially. In the case of the interband transitions, the Shubnikov–de Haas oscillations are linked with the electron transitions from (to) the specific singularities of the state density; i.e., the Shubnikov–de Haas oscillations are determined by the overlap of the monotonic and oscillating components of the state density. The oscillating frequency of the latter is high ($\sim 1/\omega_{e,h}$), and the Shubnikov–de Haas oscillations damp rapidly with increasing temperature. In contrast with the Shubnikov–de Haas oscillations, the HTO are linked with the electron transitions between the specific singularities of the state density, i.e., they are determined by the overlap of the oscillating parts of the electron and hole state densities. State density oscillations arise in this case at the combination frequencies ($\sim 1/\omega^{\pm}_{kk'}$) of both the higher (long-period) and lower (short-period HTO) inverse cyclotron frequencies. Accordingly, the rate at which the temperature-induced damping of the HTO harmonics occurs increases or decreases sharply in comparison with the harmonics of the Shubnikov–de Haas oscillations.

Going beyond the scope of the isotropic model may lead to a nonmonotonic dependence of the HTO period on the magnetic field direction. We will use a simple example to illustrate this point. Let us assume $\omega_e \approx \omega_h$ if the magnetic field is directed along a C axis. Let us also assume that the cyclotron-mass ratio $m_e(\theta)/m_h(\theta)$ decreases with increasing angle $\theta = (C\mathbf{H}$ axis). Specifically, such a situation is realized in bismuth for the trigonal axis and at least one of the electronic ellipsoids.[7] With $\mathbf{H} \| C$ the principal contribution to HTO then comes from the harmonic $k = k' = 1$ with the period $\Delta^{-}_{11}(0) = e/cm_h(0)\epsilon_o$. As θ is increased, the oscillation period increases because of the fast decrease of the cross section of the electronic ellipsoid, while the amplitude of the harmonic decreases because of the decrease in ω_{11}^{-}. As the angle θ_2, which is determined by the relation $2m_e(\theta_2) = m_h(\theta_2)$, is approached, the principal contribution to HTO begins to come from the harmonic $k = 2$, $k' = 1$ with the period $\Delta_{21}^{-}(\theta_2) = [m_h(0)/m_h(\theta_2)]\Delta_{11}^{-}(0)$. As a result, the HTO period decreases sharply. The period then begins to increase again, with the next decrease occurring near the angle θ_3, which is determined by the relation $3m_e(\theta_3) = m_h(\theta_3)$. Here we have $\Delta_{31}^{-}(\theta_3) = [m_h(0)/m_h(\theta_3)]\Delta_{11}^{-}(0)$, etc. A change in the tilt angle of the magnetic field thus causes the HTO period to oscillate near the mean value which is determined by the angular dependence of the reciprocal of the cyclotron mass of the holes, in complete agreement with the experimental data.[1-4]

To obtain the correct period of the experimentally observed HTO, we must take into account the nonparabolic nature of the electron dispersion in bismuth, setting $S_e = 2\pi m_e^0 \zeta(1 + \zeta/\epsilon_g)$, where ϵ_g is the width of the band gap, and m_e^0 is the effective mass at the bottom of the conduction band. With increase in the temperature, the last to damp is the HTO harmonic, for which $km_e(\zeta) \approx k'm_h$, with the period $\Delta_{\rm HTO}^{-}(1/H) \approx e/ck'm_h\epsilon_0$, where $m_e(\zeta) = m_e^0(1 + 2\zeta/\epsilon_g)$ and $\epsilon_0 = \epsilon_0 - \zeta^2/(2\zeta + \epsilon_g)$. At $\zeta_h = 11.7$ meV, $\zeta_e = 28.8$ meV, $\epsilon_g = 13.6$ meV, $m_h = 0.064 m_o$ (**H** is parallel to the trigonal axis),[7] and $k' = 1$ we find $\Delta_{\rm HTO}^{-}(1/H) = 0.63 \times 10^{-5}\ {\rm Oe}^{-1}$, in agreement with the results of Refs. 1–4.

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