Anomalous magneto-oscillations and spin precession

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A semiclassical analysis based on concepts developed in quantum chaos reveals that anomalous magneto-oscillations in quasi two-dimensional systems with spin-orbit interaction reflect the nonadiabatic spin precession of a classical spin vector along the cyclotron orbits.

If in a solid the spatial inversion symmetry is broken, spin-orbit (SO) interaction gives rise to a finite spin splitting of the energy bands even at magnetic field $B = 0$. In quasi two-dimensional (2D) systems this $B = 0$ spin splitting is frequently analyzed by measuring the magneto-oscillations at small magnetic fields $B > 0$, known as Shubnikov-de Haas (SdH) oscillations. Following a semiclassical argument due to Onsager [1] it has long been assumed [2, 3], that the frequencies $f^\text{SdH}$ of these oscillations are proportional to the unequal occupations $N_\pm$ of the spin-split subbands,

$$N_\pm = \frac{(e/2\pi \hbar)}{f^\text{SdH}} \tag{1}$$

where $e$ is the electron charge and $\hbar$ is Planck’s constant. Recently, experiments and numerical quantum mechanical calculations have shown that, in general, these oscillations are not simply related to the $B = 0$ spin-subband densities [4]. However, it has remained unclear when and why Onsager’s semiclassical argument fails. Here we use a semiclassical trace formula for particles with spin, which was only lately developed [5, 6] in the context of quantum chaos, in order to show that the anomalous magneto-oscillations reflect the nonadiabatic spin precession along the cyclotron orbits. Currently great efforts are made to obtain a deeper understanding of spin-related phenomena in semiconductor quantum structures, in particular due to possible applications in spintronics [7]. While spin is a purely quantum mechanical property with no immediate analogue in classical physics, the present analysis reveals that our understanding of spin phenomena can be greatly improved by investigating equations of motion for a classical spin vector.

In the presence of a magnetic field perpendicular to the plane of a 2D electron system the electrons condense in highly degenerate Landau levels that are regularly spaced in energy. With increasing field $B$ these Landau levels are pushed through the Fermi surface causing magneto-oscillations which reflect the oscillating density of states (DOS) at the Fermi energy $E_F$, see, e.g., [8]. Onsager’s semiclassical analysis of magneto-oscillations was based on a Bohr-Sommerfeld quantization of cyclotron orbits. However, for systems with spin there is no straightforward generalization of Bohr-Sommerfeld quantization [9, 10]. The Gutzwiller trace formula [11] provides an alternative and particularly transparent semiclassical interpretation of magneto-oscillations that is applicable even in the presence of SO interaction. Rather than giving individual quantum energies, the trace formula relates the DOS of the quantum mechanical system to a sum over all periodic orbits of the corresponding classical system. As a function of energy $E$ the individual terms oscillate proportional to $\cos[S(E)/\hbar]$ where $S(E)$ is the action of the orbit.

First we briefly discuss magneto-oscillations of electrons with effective mass $m^*$ in a 2D system without SO interaction. Here, the sum over $k$-fold repetitions of the classical periodic cyclotron orbits corresponds to a Fourier decomposition of the DOS as a function of the energy $E$, where the action of the $k$-fold revolution corresponds to the $k$th harmonic $2\pi k E/(\hbar \omega) = 2\pi k m^* E/(\hbar e B)$ of the DOS with cyclotron frequency $\omega = eB/m^*$. Thus we see that the DOS for a fixed energy $E = E_F$ oscillates as a function of the reciprocal magnetic field $1/B$ which is the origin of magneto-oscillations. In particular, we get Onsager’s formula from the first harmonic $k = 1$. Longer orbits $k > 1$, giving rise to higher harmonics in the oscillating DOS, are exponentially damped for small but nonzero temperatures [12] so that here it suffices to consider $k = 1$. In general, the Gutzwiller trace formula is an asymptotic relation that holds in the semiclassical limit $\hbar \to 0$. However, in the particular case discussed above it is an identity.

Recently it has been shown [3, 8] that in leading semiclassical order the SO interaction results in weight factors $2 \cos(ka/2)$ for the orbits in the trace formula where the angle $\alpha$ characterizes the spin precession $s = s \times B$ of a classical spin vector $s$ along the classical orbit [13]. Here $s$ is the time derivative of $s$ and $B$ is an effective magnetic field including the contributions of both SO coupling and the Zeeman interaction due to the external magnetic field $B$ felt by the spin along the orbit. After $k$ periods of the cyclotron motion the spin vector $s$ has been rotated by the angle $ka$ about an axis $n$, see Fig. [4]. We remark that the axis $n$ (but not $\alpha$) depends on the starting point of the cyclotron orbit. Like the effective field $B$, the angle $\alpha$
depends on the external field \( B \). It contains a dynamical as well as a geometric phase similar to Berry’s phase \([14]\). Apart from higher harmonics the oscillating part of the DOS at the Fermi energy \( E_F \) is proportional to

\[
\cos(\alpha/2) \cos \left[ 2\pi m^* E_F / (\hbar e B) \right]. \tag{2}
\]

We have analyzed magneto-oscillations for quasi 2D electron systems in semiconductors such as GaAs where we have two contributions to the SO coupling. The Dresselhaus term \([15]\) reflects the bulk inversion asymmetry of the zinc blende structure of GaAs. If the inversion symmetry of the confining potential of the quasi 2D system is broken, we get an additional SO coupling given by the Rashba term \([16]\). While the Dresselhaus term is fixed, the Rashba SO coupling can be tuned by applying an electric field \( E_\perp \) perpendicular to the plane of the quasi 2D system \([3]\).

In Fig. 2 we compare the Fourier spectra of the magneto-oscillations of the DOS calculated by means of a diagonalization of the quantum mechanical Hamiltonian with the spectra obtained from Eq. (2) based on an integration of the classical equations of motion for the precessing spin. We consider here a 2D electron system in a 100 Å wide GaAs-Al_{0.5}Ga_{0.5}As quantum well (QW) grown in the crystallographic direction \([113]\) with constant total density \( N = N_+ + N_- = 5 \times 10^{11} \text{ cm}^{-2} \) and with varying \( E_\perp \). For comparison, the circles mark the peak positions which one would expect according to Eq. (2) for the spin subband densities \( N_\pm \) calculated quantum mechanically at \( B = 0 \). The Fourier spectra are in strikingly good agreement. On the other hand, the peak positions deviate substantially from the positions expected according to the \( B = 0 \) spin splitting. In particular, the semiclassical analysis based on Eq. (2) reproduces the central peak that is not predicted by Eq. (1). The asymmetry in Fig. 2 with respect to positive and negative values of \( E_\perp \) reflects the low-symmetry growth direction \([113]\) (Ref. 4).

An analysis of the classical spin precession along the cyclotron orbit reveals the origin of anomalous magneto-oscillations. The spin-split states at \( B = 0 \) correspond to fixing the direction of spin parallel and antiparallel to the effective field \( \mathbf{B}(p) \) along the cyclotron orbit, where \( \mathbf{p} \) is the kinetic momentum. However, in general the precessing spin cannot adiabatically follow the momentary field \( \mathbf{B}(p) \). This can be seen in Fig. 1 where we have plotted the momentary field \( \mathbf{B}(p) \) as well as the precessing spin \( \mathbf{s} \) along a cyclotron orbit. Both the direction and the magnitude of \( \mathbf{B} \) change along the orbit. In particular, the Dresselhaus term reverses the direction of \( \mathbf{B} \) when \( |\mathbf{B}| \) has a minimum. A spin vector that is no longer parallel or antiparallel to \( \mathbf{B} \) implies that the system is in a superposition of states from both spin subbands so that the magneto-oscillations are not directly related to the \( B = 0 \) spin splitting.

For the spin, in order to be able to follow the momentary field \( \mathbf{B}(p) \) adiabatically, the orbital motion must be slow compared to the motion of the precessing spin, i.e., we must have \( B \ll |\mathbf{B}(p)| \) for all points \( p \) along the cyclotron orbit. Therefore, it is the smallest value \( E_{\text{min}} = \min |\mathbf{B}(p)| \) along the cyclotron orbit which determines whether or not the spin evolves adiabatically. This is illustrated in Fig. 1 where the parameters were chosen such that initially the spin is parallel to the effective field.
\( \mathbf{B} \). First \( s \) can follow \( \mathbf{B} \), but after a quarter period of the cyclotron orbit the effective field \( \mathbf{B} \) reaches its minimum \( B_{\text{min}} \) and \( s \) starts to “escape” from \( \mathbf{B} \). Subsequently, the spin vector \( s \) is no longer parallel to \( \mathbf{B} \) also in those regions where \( \mathbf{B} \) becomes large again. We remark that adiabatic spin precession does not imply \( \alpha = 0 \) but only that the rotation axis \( n \) is approximately parallel to the initial (and final) direction of the effective field \( \mathbf{B} \).

For many years, anomalous magneto-oscillations have been explained by means of magnetic breakdown. Underlying this approach is a rather different semiclassical picture where each spin-split subband is associated with an energy surface with separate classical dynamics. In our treatment, on the other hand, there is only one energy surface complemented by the dynamics of a classical spin vector. It is the essential idea within the concept of magnetic breakdown that in a sufficiently strong external magnetic field \( B \) electrons can tunnel from a cyclotron orbit on the energy surface of one band to an orbit on the energy surface of a neighboring band separated from the first one by a small energy gap. For spin-split bands the separation of these bands is proportional to the effective field \( \mathbf{B} \), i.e., magnetic breakdown occurs most likely in regions of a small effective field \( \mathbf{B} \). This approach implies that the anomalous magneto-oscillations are essentially determined by the breakdown regions only. (These breakdown regions can be identified with mode conversion points.) We want to emphasize that here our approach differs fundamentally from these earlier models: In the present ansatz spin continuously precesses along the cyclotron orbit, i.e., the angle \( \alpha \) in Eq. (1) is affected by the nonadiabatic motion of \( s \) in the regions of both small and large \( \mathbf{B} \) (see Fig. 2).

In the adiabatic regime \( B \ll B_{\text{min}} \) the angle \( \alpha \) is given by the integral of the modulus of the momentary field \( \mathbf{B} \) along the orbit plus a Berry phase [4],

\[
\alpha = \int_0^T |\mathbf{B}| \, dt + \alpha_B, \tag{3}
\]

where \( T = 2\pi/\omega \) is the period of the cyclotron motion. In the limit of small external fields \( (B \to 0) \) the Berry phase \( \alpha_B \) converges towards a constant and the integrand in Eq. (3) can be expanded with respect to a small Zeeman term, \( |\mathbf{B}| \approx B_0 + B_1 B \), where the coefficients \( B_0 \) and \( B_1 \) are \( T \)-periodic in time. Thus in the limit of small external fields we obtain \( \alpha(B) \approx \alpha_0/B + \alpha_1 \) with constants \( \alpha_0 \) and \( \alpha_1 \) independent of \( B \). Inserting the last relation in Eq. (3) we thus retrieve Eq. (1), i.e., only in the limit of adiabatic spin precession magneto-oscillations are directly related to the \( B = 0 \) spin splitting. By changing the crystallographic growth direction of the QW, it is possible to tune the value of \( B_{\text{min}} \). In particular, for a QW grown in the crystallographic direction \([110]\) the Dresselhaus term vanishes for \( p \) parallel to the in-plane directions \([001]\) and \([00\bar{1}]\). Thus for a symmetric QW without Rashba SO coupling we have \(|\mathbf{B}(p)| = B \) for these values of \( p \) which implies that there is no adiabatic regime and one always observes anomalous magneto-oscillations.

For a system with Rashba SO coupling but no Dresselhaus term both the classical equations of motion for the precessing spin and the quantum mechanical problem can be solved analytically. Here the Gutzwiller trace formula exactly reproduces the quantum mechanical density of states for \( B > 0 \). For this system, the effective magnetic field \( \mathbf{B}(p) \) along the cyclotron orbit has a constant magnitude \( B \) and for small external fields \( B \to 0 \) the exact solution turns into the adiabatic solution so that we get no anomalous magneto-oscillations in agreement with an earlier quantum mechanical analysis [6].

Finally, we note that the concepts developed here are rather general and, in particular, are not restricted to spin-1/2 systems. Indeed, an analogous semiclassical analysis can be carried out for any system with (nearly) degenerate subbands. These bands can be identified with a single band with a SO coupling acting on an effective spin degree of freedom similar to Lipari and Baldareschi’s treatment [13] of the multiply degenerate valence band edge in semiconductors with diamond or zinc blende structure. In particular, we expect that our approach can be applied to the interpretation of de Haas-van Alphen experiments on ultrahigh-purity samples [20] that had called in question the established concepts of magnetic breakdown.

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The relation between the angle $\alpha$ and the previously defined angles $\theta$ and $\eta$ is given by $\cos(\alpha/2) = \cos(\theta/2) \cos \eta$.

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