

Anomalous Magneto-Oscillations in Two-Dimensional Systems

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The frequencies of Shubnikov-de Haas oscillations have long been used to measure the unequal population of spin-split two-dimensional subbands in inversion asymmetric systems. We report self-consistent numerical calculations and experimental results which indicate that these oscillations are not simply related to the zero-magnetic-field spin-subband densities.

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Spin degeneracy of the electron states in a solid is the combined effect of inversion symmetry in space and time. Both symmetry operations change the wave vector \mathbf{k} into $-\mathbf{k}$, but time inversion also flips the spin so that combining both we have a twofold degeneracy of the single particle energies, $\mathcal{E}_+(\mathbf{k}) = \mathcal{E}_-(\mathbf{k})$ (Ref. [1]). When the potential through which the carriers move is inversion asymmetric, however, the spin-orbit interaction removes the spin degeneracy even in the absence of an external magnetic field B . This $B = 0$ spin splitting is the subject of considerable interest because it concerns details of energy band structure that are important in both fundamental research and electronic device applications ([2–13] and references therein).

The spin splitting of the single particle energies yields two spin subbands with different populations N_{\pm} . The frequencies f_{\pm}^{SdH} of longitudinal magnetoresistance oscillations in small magnetic fields perpendicular to the plane of the system, known as Shubnikov-de Haas (SdH) oscillations, have often been used [2–7] to measure the $B = 0$ spin-subband densities N_{\pm} following

$$N_{\pm} = \frac{e}{h} f_{\pm}^{\text{SdH}}. \quad (1)$$

Here e is the electron charge and h is Planck's constant. Equation (1) is based on a well-known semiclassical argument due to Onsager [14] which relates the cyclotron motion at $B > 0$ with extremal cross sections of the Fermi surface at $B = 0$. In this paper, we test both experimentally and theoretically the validity of this procedure. We obtain good agreement between experimental and calculated SdH oscillations. On the other hand, the calculated $B = 0$ spin splitting differs substantially from the predictions of Eq. (1). We will show that this difference reflects the inapplicability of conventional Bohr-Sommerfeld quantization for systems with spin-orbit interaction.

The subjects of our investigation are two-dimensional (2D) hole systems in modulation-doped GaAs quantum wells (QW's). We use GaAs because high quality samples can be grown which allow the observation of many SdH oscillations, and because the band-structure parameters are well known [15,16] so that accurate numerical calculations

can be performed. The crystal structure of GaAs is zinc blende, which is inversion asymmetric. Furthermore, a QW structure can be made asymmetric if an electric field E_{\perp} is applied perpendicular to the plane of the well. Therefore, at a given 2D hole density, the $B = 0$ spin splitting in these systems has a fixed part due to the bulk inversion asymmetry (BIA), and a tunable part due to the structure inversion asymmetry (SIA).

Figure 1 highlights the main findings of our paper. It shows the Fourier spectra of the calculated [Fig. 1(a)] and measured [Fig. 1(b)] SdH oscillations as well as the expected peak positions $(h/e)N_{\pm}$ according to the calculated spin split densities N_{\pm} at $B = 0$ [open circles in Fig. 1(a)] for a 2D system with constant hole density $N = N_{+} + N_{-} = 3.3 \times 10^{11} \text{ cm}^{-2}$ but with varying E_{\perp} . Even around $E_{\perp} = 0$, when we have only BIA but

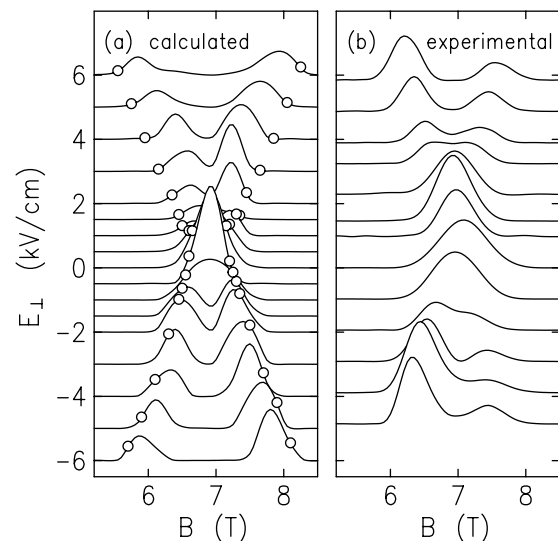


FIG. 1. Fourier spectra of the (a) calculated and (b) measured SdH oscillations versus magnetic field B for different values of electric field E_{\perp} for a 200 Å wide GaAs-Al_{0.3}Ga_{0.7}As QW with growth direction [113] and 2D hole density $N = 3.3 \times 10^{11} \text{ cm}^{-2}$. The open circles show the expected Fourier transform peak positions $(h/e)N_{\pm}$ according to the calculated spin splitting N_{\pm} at $B = 0$.

no SIA, the open circles indicate a significant spin splitting $\Delta N = N_+ - N_-$. However, the Fourier spectra in Figs. 1(a) and 1(b), while in good agreement with each other [17,18], deviate substantially from the zero- B spin splitting: for nearly all values of E_\perp the splitting $(h/e)\Delta N$ is significantly larger than $\Delta f = f_+^{\text{SdH}} - f_-^{\text{SdH}}$. In particular, near $E_\perp = 0$ only one SdH frequency is visible in both the measured and calculated spectra, whereas we would expect to obtain two frequencies [19]. In the following we will show how one can understand these results. We will briefly describe some details of our calculations and experiments and then discuss the physical origin of when and why Eq. (1) fails.

Our calculations are based on the methods discussed in Refs. [20–22]. A multiband Hamiltonian [23] containing the bands Γ_6^c , Γ_8^v , and Γ_7^v is used to calculate hole states in the QW. It fully takes into account the spin splitting due to BIA and SIA. The Poisson equation is solved self-consistently in order to obtain the Hartree potential. We obtain two spin-split branches of the energy dispersion $\mathcal{E}_\pm(\mathbf{k}_\parallel)$ as a function of in-plane wave vector \mathbf{k}_\parallel . However, we do not call these branches spin-up or spin-down because the eigenstates are not spin polarized; i.e., they contain equal contributions of up and down spinor components. (This reflects the fact that for $B = 0$ the system has a vanishing magnetic moment.) From $\mathcal{E}_\pm(\mathbf{k}_\parallel)$ we obtain the population N_\pm of these branches [21].

For the calculation of SdH oscillations we use the very same Hamiltonian [23] discussed above so that the results for $B = 0$ and $B > 0$ are directly comparable. We introduce the magnetic field by replacing the in-plane wave-vector components with Landau raising and lowering operators in the usual way [22,23]. From the Landau fan chart, using a Gaussian broadening, we obtain the oscillatory density of states at the Fermi energy which is directly related to the electrical conductivity [24]. In order to match the experimental situation the Fourier spectra in Fig. 1(a) were calculated for B between 0.20 and 0.85 T (B^{-1} between 1.17 and 5.0 T $^{-1}$). We note that the positions of the peaks in the Fourier spectra in Fig. 1(a) depend only on the Landau fan chart as determined by the multiband Hamiltonian [25]. A single peak in the Fourier spectrum corresponds to the situation that at the Fermi energy the spacing between Zeeman-split Landau levels is a fraction α of the spacing between Landau levels with adjacent Landau quantum numbers n and $n + 1$, with a constant α independent of B .

For measurements, we use Si modulation-doped GaAs QW's grown by molecular beam epitaxy on the (113)A surface of an undoped GaAs substrate. The well width of the sample in Fig. 1 is 200 Å. Photolithography is used to pattern Hall bars for resistivity measurements. The samples have metal front and back gates that control both the 2D hole density and E_\perp . Measurements are done at a temperature of 25 mK. In order to vary E_\perp while maintaining constant density we first set the front gate (V_{fg})

and back gate (V_{bg}) biases and measure the resistivities as a function of B . The total 2D hole density N is deduced from the Hall coefficient. Then, at small B , V_{fg} is increased and the change in the hole density is measured. V_{bg} is then reduced to recover the original density. This procedure changes E_\perp while maintaining the same density to within 3%, and allows calculation of the change in E_\perp from the way the gates affect the density.

In Fig. 1(b) we show the Fourier spectra for the measured magnetoresistance oscillations. Keeping in mind that we may not expect a strict one-to-one correspondence between the oscillatory density of states at the Fermi energy [Fig. 1(a)] and the magnetoresistance oscillations [Fig. 1(b)] the agreement is quite satisfactory. However, these experimental and theoretical results indicate a surprising discrepancy between f_\pm^{SdH} and $(h/e)N_\pm$. In the following we will discuss possible explanations of these results.

The common interpretation [2] of SdH oscillations in the presence of inversion asymmetry is based on the intuitive idea that for small B the Landau levels can be partitioned into two sets which can be labeled by the two spin subbands. Each set gives rise to an SdH frequency which is related to the population of the respective spin subband according to Eq. (1). However, a comparison between the (partially) spin polarized eigenstates at $B > 0$ and the unpolarized eigenstates at $B = 0$ shows that in general such a partitioning of the Landau levels is not possible. This reflects the fact that the orbital motion of up and down spinor components is coupled in the presence of spin-orbit interaction, i.e., it cannot be analyzed separately.

For many years, anomalous magneto-oscillations have been explained by means of magnetic breakdown [26]. In a sufficiently strong magnetic field B electrons can tunnel from an orbit on one part of the Fermi surface to an orbit on another, separated from the first by a small energy gap. The tunneling probability was found to be proportional to $\exp(-B_0/B)$, with a breakdown field B_0 , similar to Zener tunneling [26]. This brings into existence new orbits which, when quantized, correspond to *additional* peaks in the Fourier spectrum of the SdH oscillations. However, if the anomaly of the SdH oscillations reported in Fig. 1 were due to magnetic breakdown, for $E_\perp = 0$ we would expect several frequencies f^{SdH} with different values rather than the observed *single* frequency. In a simple, semiclassical picture a single frequency could be explained by two *equivalent* orbits in \mathbf{k}_\parallel space as sketched in Fig. 2. However, the latter would imply that the tunneling probabilities at the junctions j_1 and j_2 are equal to one (and thus independent of B). We remark that de Andrada e Silva *et al.* [13] studied anomalous magneto-oscillations for spin-split electrons in a 2D system. Their semiclassical analysis based on magnetic breakdown failed to predict B_0 by up to a factor of 3 and ΔN by up to 17% (see Table III in Ref. [13]).

In order to understand the deviation from Eq. (1) visible in Fig. 1 we need to look more closely at Onsager's semiclassical argument [14] which is underlying Eq. (1). It is

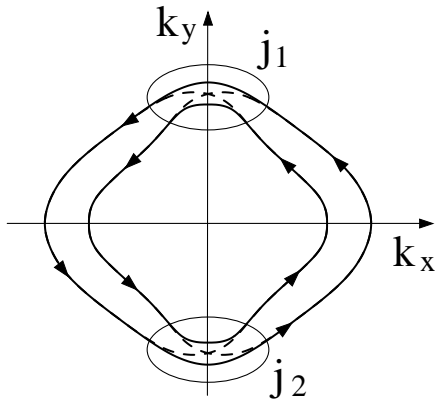


FIG. 2. Qualitative sketch of the spin-split Fermi contours in \mathbf{k}_{\parallel} space for a QW with growth direction [113] (solid lines). In a simple semiclassical picture the observation of a single peak near $E_{\perp} = 0$ in the Fourier spectra of Fig. 1 can be explained by trajectories in \mathbf{k}_{\parallel} space which follow the dashed lines at the junctions j_1 and j_2 .

based on Bohr-Sommerfeld quantization of the semiclassical motion of Bloch electrons, which is valid for large quantum numbers. However, spin is an inherently quantum mechanical effect, for which the semiclassical regime of large quantum numbers is not meaningful. Therefore Bohr-Sommerfeld quantization cannot be carried through in the usual way for systems with spin-orbit interaction. In a semiclassical analysis of such systems we have to keep spin as a discrete degree of freedom so that the motion in phase space becomes a multicomponent vector field [27,28]; i.e., the motion along the spin-split branches of the energy surface is coupled with each other and cannot be analyzed separately. In this problem geometric phases like Berry's phase [29] enter in an important way which makes the semiclassical analysis of the motion of a particle with spin much more intricate than the conventional Bohr-Sommerfeld quantization.

One may ask whether we can combine the older idea of magnetic breakdown with the more recent ideas on Bohr-Sommerfeld quantization in the presence of spin-orbit interaction. Within the semiclassical theory of Ref. [27] spin-flip transitions may occur at the so-called mode-conversion points which are points of spin degeneracy in phase space. Clearly these points are related to magnetic breakdown. However, mode-conversion points introduce additional complications in the theory of Ref. [27] so that this theory is not applicable in the vicinity of such points.

Clearly we can circumvent the complications of the semiclassical theory by doing fully quantum mechanical calculations as outlined above. We have performed extensive calculations and further experiments which confirm that the results reported here are quite common for 2D systems. In Ref. [6] spin splitting of holes was analyzed for two GaAs QW's which had only a front gate. Here V_{fg} changes both the total density $N = N_+ + N_-$ in the well, as well as the asymmetry of the confining potential.

For these QW's we obtain excellent agreement between the measured and calculated frequencies f_{\pm}^{SdH} versus N including the observation of a single SdH frequency near $N = 3.8 \times 10^{11} \text{ cm}^{-2}$ when the QW becomes symmetric. However, there is again a significant discrepancy between Δf and $(h/e)\Delta N$.

Our results apply to other III-V and II-VI semiconductors whose band structures are similar to GaAs in the vicinity of the fundamental gap [16]. Our calculations indicate that the deviations from Eq. (1) are related to the anisotropic terms in the Hamiltonian. If the Hamiltonian is axially symmetric Eq. (1) is fulfilled. This is consistent with the semiclassical analysis of spin-orbit interaction in Ref. [27] where it was found that in three dimensions no Berry's phase occurs for spherically symmetric problems. We note that for holes in 2D systems the anisotropy of $\mathcal{E}_{\pm}(\mathbf{k}_{\parallel})$ is always very pronounced [9]. It is also a well-known feature of the Hamiltonian for electrons, in particular for semiconductors with a larger gap [10]. Up to now most experiments have analyzed spin splitting and SdH oscillations for 2D electron systems [3–5]. To lowest order in \mathbf{k} the SIA induced spin splitting in these systems is given by the so-called Rashba term [8,10] which has axial symmetry. For this particular case it can be shown analytically that Eq. (1) is fulfilled.

For different crystallographic growth directions spin splitting and SdH oscillations behave rather differently. Moreover, these quantities depend sensitively on the total 2D hole density $N = N_+ + N_-$ in the well. In Fig. 3 we have plotted the calculated SdH Fourier spectra versus E_{\perp} for a GaAs QW with growth direction [110] and $N = 3.0 \times 10^{11} \text{ cm}^{-2}$ [Fig. 3(a)] and $N = 3.3 \times 10^{11} \text{ cm}^{-2}$

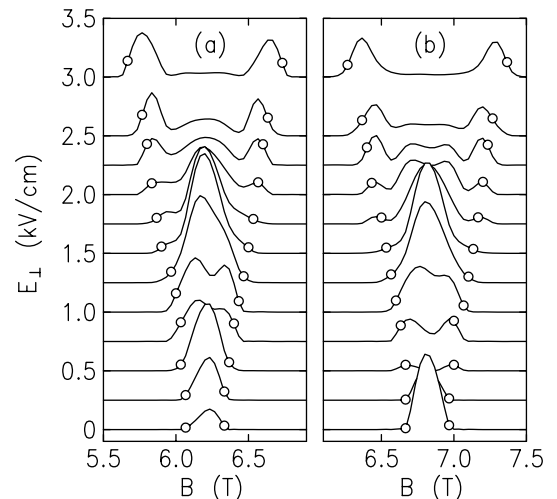


FIG. 3. Calculated Fourier spectra of the SdH oscillations versus magnetic field B for different values of electric field E_{\perp} for a 150 Å wide GaAs-Al_{0.5}Ga_{0.5}As QW with crystallographic growth direction [110] and 2D hole densities (a) $N = 3.0 \times 10^{11} \text{ cm}^{-2}$ and (b) $N = 3.3 \times 10^{11} \text{ cm}^{-2}$. The open circles show the expected Fourier transform peak positions $(h/e)N_{\pm}$ according to the calculated spin splitting N_{\pm} at $B = 0$.

[Fig. 3(b)]. Open circles mark the expected peak positions $(h/e)N_{\pm}$ according to the spin splitting N_{\pm} at $B = 0$ [17,18]. Again, the peak positions in the Fourier spectra differ considerably from the expected positions $(h/e)N_{\pm}$. Close to $E_{\perp} = 0$ there is only one peak at $(h/2e)N$. Around $E_{\perp} = 1.0$ kV/cm we have two peaks, but at even larger fields E_{\perp} the central peak at $(h/2e)N$ shows up again. At $E_{\perp} \approx 2.25$ kV/cm we have a triple peak structure consisting of a broad central peak at $(h/2e)N$ and two side peaks at approximately $(h/e)N_{\pm}$. In Fig. 3 we have a significantly smaller linewidth than in Fig. 1. Basically, this is due to the fact that for the Fourier transforms shown in Fig. 3 we used a significantly larger interval of B^{-1} (10.0 T^{-1} as compared with 3.83 T^{-1}) in order to resolve the much smaller splitting for growth direction [110]. We note that for $E_{\perp} = 0$ the SdH oscillations are perfectly regular over this large range of B^{-1} with just *one* frequency, which makes it rather unlikely that the discrepancies between Δf and $(h/e)\Delta N$ could be caused by a B dependent rearrangement of holes between the Landau levels.

Similar results like those shown in Figs. 1 and 3 have been obtained also for growth direction [001], but the spectra were more complicated with, e.g., several SdH frequencies for $E_{\perp} = 0$. Our calculations for holes are based on the fairly complex multiband Hamiltonian of Ref. [23]. We obtained qualitatively the same results by analyzing the simpler 2×2 Hamiltonian of Ref. [10]. However, this model is appropriate for electrons in large-gap semiconductors, where spin splitting is rather small, so that it is more difficult to observe these effects experimentally.

In summary, we have both measured and calculated the SdH oscillations of 2D hole systems in GaAs QW's. As opposed to the predictions of a semiclassical argument due to Onsager, we conclude that the $B = 0$ spin splitting is not simply related to the SdH oscillations at low magnetic fields [30]. This is explained by the inapplicability of conventional Bohr-Sommerfeld quantization for systems with spin-orbit interaction.

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- [30] We propose that the $B = 0$ spin splitting of 2D holes may be measured using inelastic spin-flip Raman scattering similar to the experiments for electrons in Ref. [12]. Such experiments are planned.