Valley Splitting in Si-Inversion Layers at Low Magnetic Fields

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We report novel manifestation of the valley splitting for the two valley electron system in (100) Si-inversion layers at low carrier density. We found that valley splitting causes almost 100% modulation of the Shubnikov de Haas oscillations in very low magnetic fields, almost on the bound of the quantum interference peak of the negative magnetoresistance. From the interference pattern of oscillations we determined the valley splitting in the $B = 0$ limit which appears to vary within a factor of 1.3 over the density range $(3-7) \times 10^{11}$ cm$^{-2}$. Within the same range of densities, level broadenings in both electron valleys differ only by $\leq 3\%$. The latter result shows that the inter-valley scattering is not responsible for the strong (six fold) ‘metallic-like’ changes of the resistivity with temperature.

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The apparent ‘metallic-like’ temperature dependence of the resistivity is in the focus of current research interest. A number of microscopic mechanisms have been proposed for explaining the two major features of the resistivity: (i) strong metallic-like changes with temperature and magnetic field. In addition to the spin-related sub-bands [1–6], and (ii) strong changes with in-plane magnetic field. If the carriers mobility strongly depends on the Fermi energy $E_F$, the minority subband(s) may have a mobility essentially lower than that for the majority subband(s). The intersubband scattering may thus cause strong changes in the resistivity with temperature and magnetic field. In addition to the spin-related subbands, $n$-(100)-Si system has two minima in the conduction band. The minima originate from six equivalent valleys located close to the X-points in the Brillouin zone. Four of them shift up in energy by about (20-40) meV due to the confinement potential. At low densities, only the two lowest valleys are filled; the sharp Si/SiO$_2$ interface causes their additional splitting by $\Delta_v \gtrsim 1 \text{K}$. Therefore, apriori, the remarkable strength of the metallic-like conduction in Si-samples might be related to the valley multiplicity.

The ‘metallic’ temperature changes in the resistivity and the ‘metal-insulator’ transition (MIT) in 2D systems are most pronounced in high-mobility samples where they take place in the regime of low carrier density and strong electron-electron interaction (the ratio of the Coulomb interaction energy to Fermi energy, $r_s$, is of order of 3-10). The interaction is expected to enhance both, spin- and valley-splitting; a possibility of a spontaneous polarization, caused by interactions, was discussed earlier and was recently recalled again in connection with the problem of the MIT in 2D.

In strong quantizing magnetic fields $B_\parallel (\omega_c \tau \gg 1)$, valley splitting is known to be enhanced by exchange interaction between energy levels and was directly measured from Shubnikov-de Haas (ShdH), quantum Hall (QHE) effect, and chemical potential oscillations. In particular, in Ref. [18], valley splitting was found to be almost density independent and to increase linearly with magnetic field, $\Delta_v(B) = \Delta_v^0 + \alpha B$, where $\alpha = 0.6 \text{K/T}$ and the sample dependent $\Delta_v^0 \approx 2 \text{K}$. The latter renormalization is intrinsic only to the strong field regime of well separated energy levels and is irrelevant to the problem of metallic conduction at $B = 0$; valley splitting in Si-structures at $B \to 0$ remained so far unexplored.

In the current work we have found that valley splitting manifests itself in high mobility Si-samples not only at high fields, but also at low magnetic fields, $B < 0.8 \text{T}$, giving rise to beatings in the ShdH oscillations. Such beatings were discussed theoretically in Ref. [15] but have not been observed experimentally. Due to very high mobility of the samples we traced the oscillations down to the fundamental limit of $\approx 0.2 \text{T}$, given by the onset of the quantum interference (i.e., weak negative magnetoresistance). From this novel beating pattern we determined the zero-field valley splitting as a function of the carrier density. We found that $\Delta_v$ varies only weakly in the range of low densities, $n = (3-7) \times 10^{11}$ cm$^{-2}$. Almost 100% amplitude of modulation in the beating pattern evidences that the scattering times in the two valleys are about equal. This observation demonstrates that the inter-subband scattering mechanism is not responsible for the strong ‘metallic-like’ temperature dependence of the conduction in Si-inversion layers.

We performed measurements on three high mobility Si-MOS samples selected from three different wafers (whose plane coincide with (100)-crystal plane to within 1°): Si11 (peak mobility $\mu_{\text{peak}} = 3.9 \text{m}^2/\text{Vs}$ at $T = 0.3 \text{K}$), Si12 ($\mu_{\text{peak}} = 3.4$) and Si15 ($\mu_{\text{peak}} = 4.0$). All samples exhibited strong (six-fold) metallic-like fall in the resistivity with temperature, and an apparent MIT at a ‘critical density’ $n_c \approx 0.9 \times 10^{11} \text{cm}^{-2}$.

Figure 1 shows a picture of the oscillations typical for
high magnetic fields and for a relatively high carrier density, \( n = 10.24 \times 10^{11} \text{cm}^{-2} \). As the magnetic field increases, ShdH oscillations evolve into the quantum Hall effect. In quantizing fields the energy spectrum is

\[
\varepsilon = \hbar \omega_c(N + \frac{1}{2}) \pm \frac{1}{2} g^* \mu_B B \pm \frac{1}{2} \Delta_v(B),
\]

where \( g^* \) is the effective \( g \)-factor, \( \mu_B \) is the Bohr magneton, and \( N \geq 0 \) is the Landau level index.

\[
\Delta_v \approx \frac{\hbar}{e^2} \frac{\pi (n/eB)^2}{4} \quad \text{for } n < 9 \times 10^{11} \text{cm}^{-2}.
\]

For \( n < 3 \times 10^{11} \text{cm}^{-2} \), the decreasing number of oscillations in the interference pattern prevented us from making a quantitative analysis.

FIG. 1. Typical manifestation of valley splitting in diagonal resistivity at high fields and high carrier density. Arrows point at the valley gaps \( \nu = 5, 7 \), circled numbers depict filling factors for the cyclotron gaps, and \( \nu = 6, 10 \) for the Zeeman gaps. Inset illustrates the hierarchy of the energy levels in high fields.

The inset to Fig. 1 illustrates the energy spectrum Eq. (1) in the high field regime. The strongest minima in Fig. 1a (and the largest splittings) at high fields correspond to the cyclotron gaps \( \Delta_c = \hbar \omega_c - g^* \mu_B B - \Delta_\nu \); they occur at integer filling factors \( \nu = 4, 8, 12 \ldots \), where \( \nu = nh/eB_{\perp} \). The series of minima at \( \nu = 2, 6, 10, \) etc. corresponds to Zeeman-gaps, \( \Delta_\nu = g^* \mu_B B - \Delta_\nu \). Starting from \( B = 6 \text{T} \), valley gaps become resolved and produce minima in \( \rho_{xx} \) at \( \nu = 7, 5, 3, 1 \). For magnetic fields less than 6 Tesla, valley splitting is not seen in Fig. 1 at any density, to within \( \sim 1\% \) resolution.

Spin splitting (\( \nu = 6, 10, 14, \) etc) can be seen in Fig. 1 down to about 1.5 T. For lower fields, the oscillations decay exponentially in amplitude, become harmonic and obtain the anticipated periodicity \( 4Be/\hbar n \) corresponding to four degenerate levels (2 spins and 2 valleys).

Unexpectedly, in the low field range, \( B = 0.2 - 0.3 \text{T}, \) almost on the border with the quantum interference peak in \( \rho_{xx}(B) \) [3], we found beatings in the oscillatory picture, demonstrated in Figs. 2. The beatings are observed in all three samples but only at low densities.

\[
\begin{align*}
\Delta_c &= \hbar \omega_c - \Delta_Z - \Delta_\nu \approx 1.8B_\perp - 2, \\
\Delta_Z &= g^* \mu_B B_\perp - \Delta_\nu \approx 2B_\perp - 2, \\
\Delta_\nu &\approx 2 + 0.6B_\perp,
\end{align*}
\]

where all energies are in K, \( B_\perp \) is in T, \( \hbar \omega_c \approx 7 \times (0.19/m^*) \approx 5 \text{K/T} \) [3][5], and \( g^* \mu_B B \approx 2.6 \text{K/T} \) [24] for a typical density \( n = 5 \times 10^{11} \text{cm}^{-2} \).

We presume therefore that the interference is caused by valley splitting. With this presumption, we modeled the oscillatory component of the magnetoresistance
δρ_exx(B⊥) with Lifshitz-Kosevich (LK) formulae \[21\] \[22\] for spin-degenerate carriers:

\[
\frac{\delta \rho_{xx}(B_{\perp})}{\rho(0)} = 2 \sum_s A_s^+ \cos \left( \frac{2\pi s h \nu_+}{2eB_{\perp}} - \pi s \right) + A_s^- \cos \left( \frac{2\pi s h \nu_-}{2eB_{\perp}} - \pi s \right). \tag{3}
\]

Here \( n_{\pm} = (n/2)[1 \pm \Delta_\nu/(2\pi F)] \) are the partial populations in the ± valleys. The envelope function is

\[
A_s^\pm = \exp \left( \frac{-\pi s}{\omega_c \tau_q^\pm} \right) \frac{2\pi^2 s k T / h \nu_s^*}{\sinh(2\pi^2 s k T / h \nu_s^*)} F_s(g^* m^*), \tag{4}
\]

with \( \tau_q^\pm = \hbar/(2\pi T_D^\pm) \) being the quantum life time, and \( T_D^\pm \), the Dingle temperature in each valley. The Zeeman factor, \( F = \cos(\pi s g^* \mu_B B / h \nu_s) = \cos(\pi s g^* m^* / 2m_0) \tag{23} \), and \( m^*(n), m_0 \), are the effective and free electron masses correspondingly.

\[ \text{FIG. 3. Example of fitting of the measured interference pattern with Eq. (2) for the sample Si11.} \ n = 6.04 \times 10^{11} \text{cm}^{-2}; \ T = 0.3 \text{K.} \]

In modeling, we used two fitting parameters, \( \Delta_v \) for valley splitting and \( \tau_q = (\tau_q^+ + \tau_q^-)/2 \) for quantum lifetime. The former parameter determines entirely the Fourier spectrum of oscillations and nodes location, whereas the latter one describes the absolute amplitude of oscillations and its monotonic field dependence. The difference of partial lifetimes for each valley, \( (\tau_q^+ - \tau_q^-)/\tau_q \ll 1 \) was used for a fine adjustment of the modulation depth at the node and is found to be a small parameter, < 3%, within the explored range of densities. Two other parameters of the energy spectrum, \( g^*(n) \) and \( m^*(n) \) were determined in Ref. \[23\] vs carrier density. It is important that the desired valley splitting is determined entirely by the location of the node of oscillations on the magnetic field scale (as illustrated in Fig. 3) and is almost insensitive to \( g^*, m^* \) and \( \tau_q \) values.

We emphasize that the node of beating demonstrated in Figs. 2 and 3 is the first node; this circumstance enabled us to determine unambiguously the valley splitting. The second node might be expected at magnetic fields which are at least 3 times lower; however, the oscillations vanished earlier.

We obtained more than a satisfactory fit using Eqs. (3) and (4) for modeling over a whole range of densities where the beatings are observed; an example is presented in Fig. 3. The main result of our fitting, valley splitting for two samples is presented in Fig. 4. \( \Delta_v \) appears to be sample dependent, even for the samples with similar peak mobility (same disorder).

As seen from Fig. 4, over the explored interval of densities, \( n = (7.5 - 3) \times 10^{11} \text{cm}^{-2} \), the changes in \( \Delta_v \) are about a factor of 1.15 – 1.3, much bigger than the error bar, \( \sim (2 - 5)\% \). The changes though are not reminiscent at all of a critical behavior, \( \Delta_v \propto 1/(n - n_0) \), which might be expected for the spontaneous valley polarization at a certain density \( n_0 \approx n_c \). It is noteworthy that over the same interval of densities both, the electron effective mass \( m^* \) and \( g^* \)-factor were found \[20\] to change monotonically by a factor of about 1.2.

\[ \text{FIG. 4. Valley splitting versus carrier density for two samples. Filled symbols are for} \ \Delta_v, \text{open symbols are for} \ \Delta_0. \text{The uncertainty is represented either by error bar or the symbols size.} \]

Our measurements were performed in very low though finite fields, \( B \approx 0.3 \text{T.} \) It is not clear whether the empirical field dependence Eq. (2) remains valid down to \( B = 0 \) or \( \Delta_v \) decreases more rapidly as levels starts overlapping in low fields. The accuracy of our data was insufficient to determine this experimentally though we found the fitting to be better with field dependent \( \Delta_v(B) \) (as in Eq. (2)). Given Eq. (2) is applicable at \( B \to 0 \), it contributes about 20% to the obtained \( \Delta_v \) values. We present therefore in Fig. 4 the results of both fitting, with field independent \( \Delta_v \) and with field dependent \( \Delta_v = \Delta_0 + 0.6B \). The two results have the meaning of the upper and lower estimates, correspondingly, for the true \( \Delta_v(B = 0) \) value; their difference is about equal to \( 0.6B_{\text{node}} \ [\text{K/T}] \), where \( B_{\text{node}} \) is the location of the 1st node of oscillations on magnetic field.
The sought-for $\Delta(B=0)$ value is thus within the interval from $\Delta_v$ to $\Delta_v^0$. Both, $\Delta_v$ and $\Delta_v^0$ exhibit a weak non-monotonic dependence whose origin is unclear. Our analysis of the ShdH oscillations in the two-valley system performed up to $r_s = 5$ didn’t reveal any deviation from the LK-formulae. This justifies the assumption of the conventional Fermi-liquid behavior which we used in the analysis above.

An additional important result follows from our fitting. We found the quantum lifetime $\tau_q$ to be almost the same in the two electron valleys, the maximal difference being only $(\tau_q^+ - \tau_q^-)/\tau_q \approx 3\%$ for the density of $3 \times 10^{11} \text{cm}^{-2}$. The proximity of $\tau_q^\pm$ values manifests in Figs. 2 as deep falls in the oscillations amplitude at the beating nodes. The transport time (momentum relaxation) for Si-inversion layers is very close to $\tau_q$. It is therefore very likely that the partial transport times and partial mobilities in both valleys are almost equivalent. This is in contrast to the big, six-fold, changes of the resistivity with temperature at zero field, $(\rho(T_{\text{high}}) - \rho(T_{\text{low}}))/\rho(T)$ which the sample exhibit at the same density \[12\]. From the proximity of the quantum life times in both valleys, we conclude therefore that the inter-valley scattering mechanism \[12\] is not responsible for the strong metallic-like temperature variation of the resistivity in Si-inversion layers.

To summarize, in high mobility (100)Si-inversion layers, the system which exhibits very strong ‘metallic-like’ features in conduction, we observed a novel manifestation of valley splitting: it causes unexpected beatings in Shubnikov-de Haas oscillations in low magnetic fields, \(0.15 - 0.4\) T, right on the bound of the negative magnetoresistance peak. From the beatings pattern of oscillations we determined the valley splitting $\Delta_v$ in the $B = 0$ limit. We found that $\Delta_v$ varies with density rather weakly and doesn’t display a critical behaviour in the range of densities \((3 - 7.5) \times 10^{11} \text{cm}^{-2}\) or $r_s = 3 - 5$. We determined also the individual quantum lifetimes, $\tau_q^\pm$ in both valleys, which appear to differ by less than 3%. This insignificant difference in $\tau_q$ demonstrates that the semiclassical mechanism of mobility changes related to the inter-valley scattering is not the origin of the strong metallic-like temperature dependence of the resistivity in Si-inversion layers. The findings set novel constraints on the microscopic models developed to explain the ‘metallic’-conduction.

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I. APPENDIX: ENERGY SPECTRUM IN SI-INVERSION LAYER AT LOW MAGNETIC FIELDS

The results on the valley splitting presented above shed a light on the energy spectrum of the two-valley electron system in (100)Si-inversion layers in low fields. We plotted in Fig. 5 the energy for three lowest Landau levels, N = 0, 1, 2, according to Eqs. (1) and (2) (from the main section). In high fields, the cyclotron splitting is the largest and the sequence of energy levels corresponds to the inset to Fig. 1. Counting from the lowest Fermi energy, the 1st gap in the energy spectrum (filling factor ν = 1) corresponds to valley splitting; ν = 2 is for the reduced Zeeman splitting, ν = 3 is again for the valley splitting and ν = 4 is the reduced cyclotron gap. This picture was verified in numerous experiments [1,2].

Due to the nonzero valley splitting at B = 0, as magnetic fields decreases, the energy levels start crossing each other at B ≲ 1 T [3]. In the region of crossing, this single-electron picture fails and the repulsion between levels should be taken into account. There is almost no experimental data available on the details of the energy spectrum in Si in low fields. It is well known only that in low fields/low density regime quantum oscillations are missing for ν = 3, 4, 5 and remain pronounced for ν = 1, 2 and for ν = 6 and 10; this result was recently confirmed in ref. [4].

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FIG. 5. Schematic magnetic field dependence of the energy spectrum (in the single-electron approximation) for two valley electron system in Si and for three lowest Landau levels. The parameters of the spectrum correspond to Eqs. (1) and (2); Δe = 2 K, as for the sample Si12.

In fields B < 0.7 T, the sequence of energy levels changes as shown in the inset to Fig. 5. For example, at B = 0.6 T, the 1st splitting, ν = 1, corresponds to the Zeeman gap, ν = 2 is the cyclotron gap (reduced by the spin flip energy), ν = 3 is a combination of the valley and cyclotron splitting etc. In this simplified picture, at some field values (B = 0.45 T and 0.25 T in the inset to Fig. 5) a number of energy levels coincide. We don’t think though that the simplified single-electron picture of Fig. 5 may predict exact location of the level crossing regions.

The identification of each energy splitting in low field/low density regime is not transparent and requires more thorough theoretical calculations of the spectrum and much more detailed experiments. As an example, on the n−B plane in Fig. 6 we reproduce from Ref. [5] a Landau fan diagram of oscillations in the low density limit; similar data were reported recently in Ref. [6]. In Fig. 6, the ρxx-minima at ν = 6 can be traced without interruption down to the field B = 0.55 T, through the ‘metal-insulator’ boundary, however the origin of this splitting may change from ‘Zeeman gap’ at high fields to any other one, e.g. ‘valley gap’ or ‘cyclotron gap’ at low fields. By now, there is no firm physical background to identify ν = 6 oscillation in low fields with spin splitting. For example, one can see from the inset to Fig. 5, that in the single-electron approximation the ν = 6 gap at B = 0.6 T corresponds to the transition with changing valley (but is reduced by the spin flip energy) and ν = 4 gap is the combined gap with changing both, the cyclotron number and the spin projection.

In Ref. [6], from the estimated ratio of the two gaps, at ν = 6 (which authors of Ref. [5] assumed to be the spin-gap) and at ν = 4 (was assumed to be the cyclotron gap), a conclusion was drawn on the unexpectedly strong enhancement of the g∗-factor at low electron densities. Taking into account vanishing Δe in the crossing region and ill-defined splittings at low field, we find this argument
unjustified. Recent direct measurements of the Zeeman energy in low fields vs carrier density [8] show that the Zeeman energy increases smoothly as density decreases down to \( n_c \), in agreement with the anticipated Fermi liquid renormalization and with recent results by Okamoto et al. [9], without any unexpected deviations or divergence in the range of densities \( n = (1 - 90) \times 10^{11}\text{cm}^{-2} \).

It is noteworthy that for the weak field interference pattern which we analyzed above, the interpretation of each oscillation is not important and does not influence on the conclusion about the valley origin of the interference and on the results of our analysis.

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