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Enhancement of valley splitting in (100) Si MOSFETs at high magnetic fields

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ABSTRACT

We report the density and magnetic field dependence of the valley splitting of two-dimensional electrons in (100) Si metal-oxide-semiconductor field-effect transistors, as determined via activation measurements in the quantum Hall regime. We find that the valley activation gap can be greatly enhanced at high magnetic fields as compared to the bare valley splitting. The observation of strong dependence of the valley activation gap on orbital Landau level occupancy and similar behavior of nearby spin gaps suggest that electron-electron interactions play a large role in the observed enhancement.

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Recent interest in using Si as a material for solid state quantum computing applications [1,2] has led to renewed interest in the question of the magnitude of valley splitting in a two-dimensional electron gas (2DEG) in Si. In particular, 2DEGs in Si are of interest as a host for quantum bits (qubits) based on the spin of electrons in electrostatically confined quantum dots [2]. Coherent manipulation of electron spins in quantum dots has been experimentally demonstrated in GaAs/AlGaAs heterostructures [3,4]. In GaAs, coupling between the electronic and nuclear spins of the host material are a major source of electron spin decoherence [3,4]. Silicon is thought to be a potentially better host material than GaAs for long electron spin coherence times due to the reduced density of nuclear spins, especially since the nuclear spin density in Si can be reduced by using isotopically enriched ²⁸Si, an isotope which has zero nuclear spin. However, an open question still lingers about the suitability of Si due to the unknown magnitude of the valley splitting. Degenerate valley states or even a finite, but small, valley splitting, $\Delta_V \lesssim kT$, will be detrimental to the operation of a spinbased qubit. For $\Delta_V \gg kT$, it is proposed that a spin qubit can be operated by appropriately adjusting the Zeeman energy E_z so that $\Delta_V > E_z$ [5]. Thus, the crucial question is whether the condition $\Delta_V \gg kT$ can be met for reasonable experimental conditions (i.e., $T \lesssim 100$ mK in a typical dilution refrigerator).

The band structure of bulk Si gives rise to six degenerate conduction band valleys. Confinement at the (100) interface lifts this degeneracy due to the difference in the transverse and longitudinal effective masses, causing the two valleys with heavy mass along the direction perpendicular to the interface to have the lowest energy. These two remaining valleys are nearly degenerate; however, a coupling between these two valleys can occur due to confinement at the Si/SiO₂ Si metal–oxide–semiconductor field–effect transistor (MOSFET) interface [6]. Theoretical work also emphasizes that Δ_V depends sensitively on the details of the interface structure [6–8]. Thus, experimental measurements of Δ_V in actual Si MOSFET devices are important in order to verify that the magnitude of the valley splitting is large enough for spin-based quantum computing applications.

The valley splitting in a Si MOSFET is typically too small to measure at zero magnetic field. Early experimental studies of the magnitude of Δ_V in (100) Si MOSFETs were made by detailed analyses of the lineshape of Shubnikov–de Haas (SdH) oscillations of the conductivity under application of perpendicular and parallel magnetic fields [9–12]. More recently, magnetocapacitance measurements were used to extract the magnitude of Δ_V in the quantum Hall regime [13]. Valley splitting for 2DEGs in large perpendicular magnetic fields has also been observed in other Si systems, such as (111)-oriented MOSFETs [14], 2DEGs formed at the H-passivated Si (111) surface [15], and in Si/SiGe heterostructures [16–18]. However, due to the possible sensitivity of Δ_V to details of the interface, direct comparison between these other materials and (100) Si MOSFETs may not be justified. Takashina et al. recently published a

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Fig. 1. (a) Longitudinal resistance R_{xx} versus *B* for sample B, at T = 0.3 K. Inset: schematic diagram indicating the LL structure at various filling factors, including valley, spin, and orbital splitting. (b) Semilog plot of R_{xx} versus 1/T data with Arrhenius fit (dotted line), yielding an activation gap $\Delta = 2.6$ K.

zero magnetic field valley splitting measurement in a (100) Si MOS-FET [19] where the 2DEG was located near the back interface of a SIMOX (separation by implantation of oxygen) silicon-on-insulator wafer. Compared to the usual thermal Si/SiO₂ interface on bulk Si, the observed magnitude of the valley splitting in the presence of this SOI interface is much larger [19]. However, it is not yet known why this additional interface appears to give rise to such large valley splittings.

In this report, we present measurements of the valley splitting in (100) Si MOSFETs in large perpendicular magnetic fields, via measurement of the activation energy gap at valley-split quantum Hall (QH) states. To the best of our knowledge, our data represent the first determination of the density (*n*) and magnetic field (*B*) dependence of the valley splitting in Si (100) MOSFETs via direct measurements of activation energy gaps in the QH regime. Consistent with previous theoretical [20,21] and experimental [13] studies, we find that Δ_V is enhanced in this regime. The observed increase of the measured gaps with decreasing orbital Landau level (LL) occupancy (*N*) and similar increasing enhancement of nearby spin gaps with decreasing *N* suggest that electron–electron interactions play a large role.

The two samples used in this study are Si MOSFET structures with a low-temperature (T = 0.3 K) peak mobility of $\mu \sim 1.5 \times 10^4$ cm²/Vs (sample A) and $\sim 1.2 \times 10^4$ cm²/Vs (sample B). For both samples, the 2DEG resides at the Si/SiO₂ interface, where the SiO₂ thickness is nominally 35 nm for sample A and 10 nm for sample B. The gate oxide is thermally grown in dry O₂ at 900 °C, with a subsequent N₂ anneal at 900 °C for 30 m, on float zone (100)-oriented high-resistivity p-type Si wafers. Both wafers have a miscut angle of less than $\pm 1^\circ$. Ohmic contacts to the 2DEG consist of n^+ Si regions formed by implantation of As and an n^+ polysilicon gate is used to induce carriers. The 2DEG resistivity is experimentally determined via standard four-terminal lock-in measurements and the density is calibrated via measurements of the Hall resistivity ity and SdH oscillations.



Fig. 2. (a) SdH oscillations at low magnetic field for sample B at a density $n = 0.9 \times 10^{12} \text{ cm}^{-2}$ and temperature T = 0.3 K. The dotted line is fit to the amplitude of the oscillations using Eq. (1). (b) Mobility versus density data for samples A and B. The shaded region indicates the μ and n range over which activation data was obtained. Inset: sketch showing the density of states (DOS) versus energy *E*, with definition of the gap Δ and the LL broadening Γ .

In Fig. 1(a) we show representative magnetotransport data for sample B, indicating several QH states and the corresponding filling factors $v \equiv nh/Be$. As sketched in the inset to Fig. 1(a), odd filling factors correspond to valley-split levels. The valley gap at v = 3 is large enough to use the temperature dependence of R_{xx} to obtain an activation gap, as shown in Fig. 1(b), which displays R_{xx} versus 1/T at v = 3, B = 12.77 T. The dotted line is a fit to the data of the Arrhenius form: $R_{xx} \propto e^{-\Delta/2T}$, where Δ is the activation gap.

The resolution of our measurement of Δ_V is limited by the disorder-induced broadening of the Landau levels. We estimate the magnitude of this broadening via the evolution of the SdH oscillations versus *B* at low magnetic fields. We define Γ as the half-width at half-maximum of the LL density of states, as sketched in the inset to Fig. 2(b). In Fig. 2(a) we show a representative low-magnetic-field R_{xx} versus *B* trace, along with a fit of the amplitude of the SdH oscillations. We fit the R_{xx} versus *B* data to the expression [6]

$$\Delta \rho_{\rm xx} \propto (X/\sinh X) e^{-\pi/\omega_c \tau},\tag{1}$$

where $X \equiv 2\pi^2 kT/\hbar\omega_c$, $\hbar\omega_c$ is the bare cyclotron splitting, and τ is the momentum relaxation time. Using this expression, we find $\Gamma \equiv \hbar/2\tau \sim 4.3$ K and 4.6 K for sample A and B, respectively, at densities near peak mobility. In Fig. 2(b) we show the mobility μ versus density *n* for samples A and B. We limit our activation measurements to the density range indicated by the shaded regions in Fig. 2(b), near peak mobility, so that μ varies by less than 10% over the range of our measurements. We restrict the data to this density range to minimize the variation of Γ with *n*, which would potentially further complicate interpretation of our activation data. The Γ obtained via the above methods is a reasonable estimate of the LL broadening at moderately low magnetic fields. However, we note that this Γ may not accurately represent the disorder broadening at higher magnetic fields, especially for very strong QH states



Fig. 3. Activation gap Δ versus *B* and *n* at $\nu = 3$ for samples A and B. Solid and open circles indicate experimental data. Solid and dashed lines are linear fits to the data, yielding $\Delta = -1.9 + 0.5 \times B$ and $\Delta = -2.5 + 0.4 \times B$ for samples A and B, respectively.

where Γ can be much larger than our low-field estimate due to the reduction in screening when the Fermi level is in a large gap in the density of states [22,23].

Fig. 3 shows our measurements of the $\nu = 3$ activation gap versus magnetic field and density, for samples A and B. We find that the data follows a linear dependence on *B* (note that $B \propto n$ for fixed ν), as demonstrated by the linear fits to the data shown as solid and dashed lines in Fig. 3. Both fits extrapolate to a negative offset in Δ at zero *B*. This may be due to the disorder-induced LL broadening, which will reduce the measured values of the QH gaps.

Comparison of the $\nu = 3$ to the $\nu = 5$ QH state may provide clues to the origin magnitude of the high-magnetic-field valley splitting. We do not show measurements of the $\nu = 5$ gap; however, our transport data indicates that this gap is much smaller than the $\nu = 3$ gap for identical magnetic fields, B = 11-13 T, but larger *n* (still within 10% of peak mobility). This is in contradiction with single-particle theories that predict increasing valley splitting with increasing *n*, due to the increasing magnitude of the electronic wavefunction at the Si/SiO₂ interface. [7,8,24,25]. For sample B the $\nu = 5$ minimum is not visible (for example, see Fig. 1(a)) and for sample A, the $\nu = 5$ minimum is barely visible even at T = 0.3 K. In fact, over the entire density range of our measurements, QH states for odd $\nu > 5$ are not visible in magnetotransport. Thus, Δ_V appears to have a strong dependence on orbital LL occupancy (*N*).

An increase of Δ with decreasing *N* is expected for Coulomb exchange-enhanced gaps, and has been previously observed for spin gaps in GaAs/AlGaAs heterostructures [26]. The precise form of the Δ dependence on *N* is not understood, but the effect can be explained by the differences in the effective character of the Coulomb interaction for different *N* [27]. The main difference between the *N* = 0 and *N* = 1 LL is that the Coulomb pseudopotential for relative angular momentum *m* = 0, which will couple electrons occupying opposite valley states, is much larger for *N* = 0 than for *N* = 1.

Because the Coulomb energy E_c scales like $E_c \propto \sqrt{n}$, one might at first expect that for gap energies dominated by Coulomb interactions $\Delta \propto \sqrt{n} \propto \sqrt{B}$, for fixed v. This contradicts our observed linear dependence of Δ on B shown in Fig. 3. However, a linear dependence of Δ on B is frequently observed for Coulomb exchange-enhanced gaps for valley, spin, and fractional QH effect gaps in many material systems, including Si MOSFETs [13], and 2DEGs in Si/SiGe [17], AlAs/AlGaAs [28] and GaAs/AlGaAs [29,30, 26] heterostructures.

To further demonstrate the importance of Coulomb enhancement of the activation gaps, we show in Fig. 4 measurements of Δ



Fig. 4. Activation gap Δ versus *B* for $\nu = 2$ and $\nu = 6$ for sample A. The dashed line indicates the bare value of the spin splitting, $\Delta = g\mu B$. The inset shows representative R_{xx} versus 1/T data with Arrhenius fits.

at the spin-split QH states, $\nu = 2$ and 6. The $\nu = 2$ and 6 bare gap should be given by $\Delta = g\mu B - \Delta_V$, where g is the bare g-factor of conduction electrons and Δ_V is the bare valley splitting. Therefore, the dashed line indicating $\Delta = g\mu B$ in Fig. 4 should be larger than the bare splitting, for finite Δ_V . However, at $\nu = 2$ the measured gap is clearly enhanced above even this overestimate of the bare splitting. Even the $\nu = 6$ gap is enhanced above $g\mu B$, after accounting for disorder by addition of $2\Gamma \sim 9$ K. The data of Fig. 4 also show a dramatic dependence of the gap energies on *N*, similar to the case for the valley-split states, where the $\nu = 2$ gap, which occurs for N = 0, is much larger than the $\nu = 6$ gap, which occurs for N = 1.

QH states for odd $v \ge 5$ are barely visible over the entire *n* range of our measurements, and show minima in R_{xx} versus B that are poorly developed compared to the v = 3 minimum, even at $B \sim 7$ T, where the $\nu =$ gap is $\Delta_3 \lesssim 1$ K. This implies that the raw gap for odd $\nu \geq 5$, $\Delta_{\nu\geq 5}$, is always less than ~ 1 K. Using our measured Γ to estimate the impact of disorder on the gap, and $\Delta_{\nu>5} \lesssim 1$ K, we find an estimate for the disorder-free gap of $\Delta_{\nu>5} + 2\Gamma \lesssim 10$ K, for valley-split states. This allows us to place a rough upper bound on the bare valley splitting of \sim 10 K, consistent with theoretical estimates of the valley coupling that predict values for the bare Δ_V of up to ~10 K at a 2D density of $n \sim 10^{12}$ cm⁻², depending strongly on the nature of the disorder at the Si/SiO₂ interface [7,8,24,25,31]. Factors such as wafer miscut [8,31] and the presence of a thin transition region (1–2 monolayers) from Si to SiO₂ at the interface [6,7,32] are suggested mechanisms that can suppress valley splitting. We also note that some theories predict a dependence of the bare Δ_V on the magnetic field and/or density [7, 8,24,25,33]. In fact, for samples where terraces are present at the interface due to wafer miscut, theory predicts that the bare Δ_V can show a strong dependence on N [33]. However, in light of the importance of Coulomb interactions, as demonstrated by our spin gap measurements at v = 2 and 6, it is difficult to make quantitative comparisons to these single-particle theories.

In conclusion, we find that Δ_V determined via thermal activation measurements can be strongly enhanced at high perpendicular magnetic field. Although several mechanisms are likely at work, electron–electron interactions appear to play a large role in the enhancement. The bare valley splitting in this regime ($n \sim 10^{12}$ cm⁻², B < 13 T) is $\lesssim 10$ K. We emphasize that Coulomb enhancement of the gap is crucial to determining Δ_V in Si 2DEGs at high magnetic field. Better quantitative understanding of the role of Coulomb interactions and disorder are required to extract the magnitude of the bare valley splitting from measurements made at high magnetic field.

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References

- [1] B.E. Kane, Nature 393 (1998) 133.
- [2] M. Friesen, et al., Phys. Rev. B 67 (2003) 121301.
- [3] J.R. Petta, et al., Science 309 (2005) 2180.
- [4] F.H.L. Koppens, et al., Nature 442 (2006) 766.
- [5] D. Culcer, et al., arXiv:0903.0863v1.
- [6] T. Ando, A.B. Fowler, F. Stern, Rev. Modern Phys. 54 (1982) 438.
- [7] A.L. Saraiva, et al., Phys. Rev. B 80 (2009) 081305(R).
 [8] M. Friesen, S. Chutia, C. Tahan, S.N. Coppersmith, Phys. Rev. B 75 (2007)
- 115318. [9] H. Köhler, M. Roos, G. Landwehr, Solid State Commun. 27 (1978) 955;
 - H. Köhler, M. Roos, Phys. Status. Solidi. B 91 (1979) 233; H. Köhler, Surf. Sci. 98 (1980) 378.
- [10] K. von Klitzing, Surf. Sci. 98 (1980) 390.

- [11] R.J. Nicholas, K. von Klitzing, Th. Englert, Solid State Commun. 34 (1980) 51.
- [12] J. Wakabayashi, et al., Surf. Sci. 170 (1986) 359.
- [13] V.S. Khrapai, A.A. Shashkin, V.T. Dolgopolov, Phys. Rev. B 67 (2003) 113305.
- [14] D.C. Tsui, G. Kaminsky, Solid State Commun. 20 (1976) 93;
 G. Dorda, I. Eisele, H. Gesch, Phys. Rev. B 17 (1878) 1785;
 D.C. Tsui, G. Kaminsky, Phys. Rev. Lett. 42 (1979) 495;
 T. Cole, B.D. McCombe, Phys. Rev. Lett. 37 (1976) 1021.
- [15] K. Eng, R.N. McFarland, B.E. Kane, Phys. Rev. Lett. 99 (2007) 016801.
- [16] P. Weitz, et al., Surf. Sci. 361 (1996) 542.
- [17] K. Lai, et al., Phys. Rev. B 73 (2006) 161301.
- [18] S. Goswami, et al., Nat. Phys. 3 (2007) 41.[19] K. Takashina, et al., Phys. Rev. Lett. 96 (2006) 236801.
- [20] T. Ando, Y. Uemura, J. Phys. Soc. Japan 37 (1974) 1044.
- [21] F.J. Ohkawa, Y. Uemura, Surf. Sci. 58 (1976) 254;
- F.J. Ohkawa, Y. Uemura, J. Phys. Soc. Japan 43 (1977) 925.
- [22] S. Das Sarma, X.C. Xie, Phys. Rev. Lett. 61 (1988) 738.
- [23] A.L. Efros, F.G. Pikus, V.G. Burnett, Phys. Rev. B 47 (1993) 2233.
- [24] F.J. Ohkawa, Y. Uemura, Surf. Sci. 58 (1976) 254;
 F.J. Ohkawa, Y. Uemura, J. Phys. Soc. Japan 43 (1977) 907;
 F.J. Ohkawa, Y. Uemura, J. Phys. Soc. Japan 43 (1977) 917.
- [25] L. Sham, M. Nakayama, Phys. Rev. B 20 (1979) 734.
- [26] O.E. Dial, et al., Nature 448 (2007) 176.
- [27] F.D.M. Haldane, E.H. Rezayi, Phys. Rev. Lett. 60 (1988) 956.
- [28] Y.P. Shkolnikov, et al., Phys Rev. Lett. 89 (2002) 226805.
- [29] G.S. Boebinger, et al., Phys. Rev. B 36 (1987) 7919.
- [30] A. Usher, et al., Phys. Rev. B 41 (1990) 1129.
- [31] T. Ando, Phys. Rev. B 19 (1979) 3089.
- [32] S.M. Goodnick, et al., Phys. Rev. B 32 (1985) 8171 and references therein.
- [33] S. Lee, P. von Allmen, Phys. Rev. B 74 (2006) 245302.