Editors' Suggestion

Strong Spin-Orbit Contribution to the Hall Coefficient of Two-Dimensional Hole Systems

Hong Liu,[‡] E. Marcellina,[*,‡] A. R. Hamilton, and Dimitrie Culcer[†]
School of Physics and Australian Research Council Centre of Excellence in Low-Energy Electronics Technologies, UNSW Node, The University of New South Wales, Sydney 2052, Australia

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Classical charge transport, such as longitudinal and Hall currents in weak magnetic fields, is usually not affected by quantum phenomena. Yet relativistic quantum mechanics is at the heart of the spin-orbit interaction, which has been at the forefront of efforts to realize spin-based electronics, new phases of matter, and topological quantum computing. In this work we demonstrate that quantum *spin* dynamics induced by the spin-orbit interaction is directly observable in classical *charge* transport. We determine the Hall coefficient R_H of two-dimensional hole systems at low magnetic fields and show that it has a sizable spin-orbit contribution, which depends on the density p, is independent of temperature, is a strong function of the top gate electric field, and can reach ~20% of the total. We provide a general method for extracting the spin-orbit parameter from magnetotransport data, applicable even at higher temperatures where Shubnikov–de Haas oscillations and weak antilocalization are difficult to observe. Our work will enable experimentalists to measure spin-orbit parameters without requiring large magnetic fields, ultralow temperatures, or optical setups.

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Quantum mechanical effects in charge transport, such as weak localization [1] and the Altshuler-Aronov corrections to the conductivity [2,3], manifest themselves in the diffusive regime and require ultralow temperatures for clear experimental observation. By contrast, for weak momentum scattering, charge transport is well described by the Drude conductivity and the ordinary Hall coefficient, $R_H = 1/(pe)$, where p is the carrier density and e the elementary charge [4]. These classical expressions are so reliable that R_H has long been the standard experimental tool for measuring carrier densities.

Recent years have witnessed the development of structures whose operation depends on relativistic quantum mechanics, such as the spin-orbit interaction, which couples a carrier's spin to its orbital degrees of freedom. Specifically, low-dimensional hole systems have attracted considerable attention in nanoelectronics and quantum information [5–16]. Holes exhibit strong spin-orbit coupling but a weak hyperfine interaction, allowing low-power electrical spin manipulation [17–19] and long coherence times [20–23]. Their effective spin-3/2 [24] brings about physics inaccessible in electron systems [25–30], allowing access to the highly complex intermediate regime, in which the spin-orbit energy is very large but still less than the kinetic energy, so that spin precession and interband dynamics are possible [31]. Significant tuning of the band structure is possible via strain [32], while topological properties can be calibrated by an in-plane magnetic field. Strong coupling to ferromagnets opens new avenues for spin torques [33]. In addition to recently reported hole superconductivity [34], strongly spin-orbit coupled systems paired with superconductors may enable topological superconductivity hosting Majorana bound states and non-Abelian particle statistics relevant for topological quantum computation [35–39]. Whereas in the past fabricating high-quality hole structures was challenging, recent progress has been outstanding [20,32,40–58]. The availability of strongly spin-orbit coupled state-of-the-art devices hints at the intriguing possibility that relativistic quantum mechanics, such as spin-orbit induced spin dynamics, could be probed directly in experiments traditionally associated with classical charge transport.

In this work we identify a strong signature of relativistic quantum mechanics in classical transport which is observable for weak momentum scattering and is temperature independent in this regime. We predict that the spin-orbit interaction has a sizable, density-dependent effect on the low-field magnetotransport of a two-dimensional hole system (2DHS). Our central result (Fig. 1) is the low-field Hall coefficient

$$R_H = \frac{1}{pe}\left[1 + \left(\frac{64\pi m^{*2}\beta^2}{\hbar^4}\right)p\right], \quad (1)$$

where β is the cubic Rashba spin-orbit coefficient, arising from the application of an electric field $\boldsymbol{F} = F_z\hat{z}$ across the quantum well, m^* is the heavy-hole effective mass at $\beta = 0$, and p is the hole density [59]. The term outside the brackets is the classical result for R_H, to which most experiments are fitted in order to extract p. We find that the spin-orbit corrections can reach more than 10% in GaAs and Ge quantum wells, and ~20% in InAs and InSb quantum wells

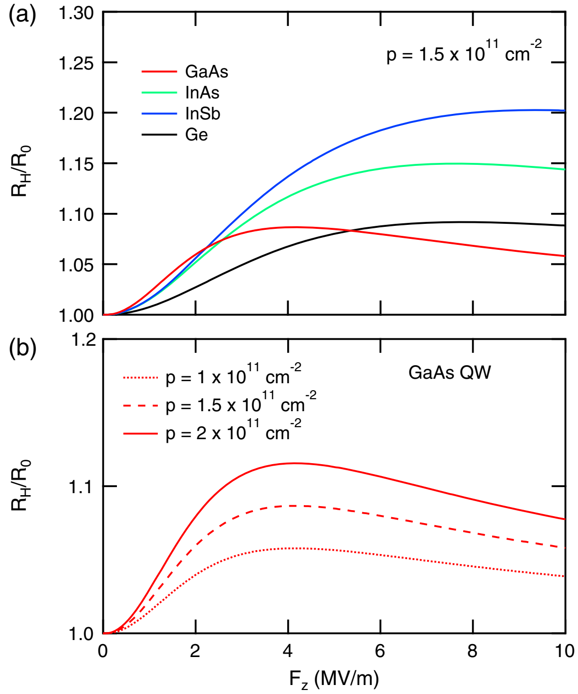

FIG. 1. Spin-orbit correction to the Hall coefficient R_H for various 15 nm quantum wells as a function of the perpendicular electric field F_z, where $R_0 \equiv 1/pe$ is the bare Hall coefficient. Panel shows results for (a) different materials at $p = 1.5 \times 10^{11}$ cm^{-2} and (b) GaAs quantum wells at different densities.

[Fig. 1(a)]. This is because the spin-orbit interaction is cubic in wave vector and it affects the group velocity of holes to an even larger extent than the Fermi energy. The magnitude of the spin-orbit corrections in hole systems increases with density [Fig. 1(b)]. At the low magnetic fields we consider, the Zeeman interaction is overwhelmed by scattering and the Berry curvature is zero; hence, there is no topological term in the conductivity. The terms $\propto \beta^2$ in Eq. (1) are due to several mechanisms. Spin-orbit coupling affects the occupation probabilities, band energies, and density of states. There are two Fermi surfaces with different Fermi velocities (see Supplemental Material, Figure S2 [60]). An in-plane electric field shifts the band with faster Fermi velocity by a larger amount than the slower band, enhancing the overall group velocity and, hence, Lorentz force $e\boldsymbol{v} \times \boldsymbol{B}$. Scattering between spin-split subbands renormalizes this result. Finally, Rashba spin-orbit generates a current-induced spin polarization of first order in β [61] with a feedback on the charge current, which accounts for approximately a quarter of the spin-orbit term in R_H.

A full quantitative understanding of spin-orbit coupling is vital for spintronics and quantum devices [62]. For example, holes in an out-of-plane magnetic field are a prime candidate for electrically driven spin resonance [17] in quantum computing. However, experimental measurement of spin-orbit parameters is challenging [63]. They are usually estimated from weak antilocalization [64–67], Shubnikov–de Haas oscillations, and spin precession in large magnetic fields (up to 2 T) [68–71], scanning tunneling spectroscopy [72], and optical measurements [73,74]. Yet many techniques yield only the ratio between the Rashba and Dresselhaus terms or allow the determination of only one type of spin splitting, and we are not aware of any Kerr spectroscopy [75–77] in indirect gap systems such as silicon [78]. Current-induced spin polarizations are small and their relationship to theoretical estimates is ambiguous [30,61,79,80], while spin-Hall currents [81] can only be identified via an edge spin accumulation [82–84]. Lastly, the interpretation of experiments involves crude approximations, such as estimating the dephasing time in weak antilocalization. The alternative approach for measuring spin-orbit parameters we present is of great utility, since it does not require large magnetic fields, ultralow temperatures, or optical setups.

We consider a 2DHS in the presence of a constant in-plane electric field $\boldsymbol{E} = E\hat{\boldsymbol{x}}$, a perpendicular magnetic field $\boldsymbol{B} = B_z\hat{\boldsymbol{z}}$, and a perpendicular gate electric field $\boldsymbol{F} = F_z\hat{\boldsymbol{z}}$. The full Hamiltonian is $\hat{H} = \hat{H}_0 + \hat{H}_E + \hat{U} + \hat{H}_Z$, where the band Hamiltonian $\hat{H}_0$ is defined below in Eq. (2), $\hat{H}_E = -e\boldsymbol{E}\cdot\hat{\boldsymbol{r}}$ represents the interaction with the external electric field, $\hat{\boldsymbol{r}}$ is the position operator, and $\hat{U}$ is the impurity potential. The Zeeman term is $H_Z = 3\kappa\mu_B\boldsymbol{\sigma}\cdot\boldsymbol{B}$, where κ is a material-specific parameter [25], μ_B the Bohr magneton, and $\boldsymbol{\sigma}$ the vector of Pauli spin matrices. The band Hamiltonian at $\boldsymbol{B} = 0$ is thus [85]

$$H_{0\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m^*} + \frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\Omega}_{\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m^*} + \beta[k_y(k_y^2 - 3k_x^2)\sigma_x + k_x(k_x^2 - 3k_y^2)\sigma_y], \quad (2)$$

where $m^* = m_0/(\gamma_1 + \gamma_2)$, γ_1, γ_2 are the Luttinger parameters, $\boldsymbol{\Omega}_{\boldsymbol{k}}$ is the effective spin-orbit magnetic field, and $\boldsymbol{k}$ is the hole wave vector. We assume $\boldsymbol{B}$ is sufficiently small that Landau quantization can be neglected ($\omega_c\tau_p \ll 1$), and the weak disorder regime prevails ($\varepsilon_F\tau_p/\hbar \gg 1$), where $\omega_c = eB_z/m^*$ is the cyclotron frequency, τ_p is the momentum relaxation time, and ε_F is the Fermi energy.

To make experimental predictions, we consider 15-nm-wide front- and back-gated quantum wells, where F_z is the gate field and can be turned on or off at constant density, and the symmetry of the quantum well can be tuned arbitrarily. For typical experimental densities, only the lowest heavy-hole subband is occupied. To calculate the Rashba coefficient β only the lowest heavy-hole and light-hole subbands are relevant and β reads [86]

$$\beta = \frac{3\hbar^4}{m_0^2\Delta_E}\bar{\gamma}^2\langle\phi_L|\phi_H\rangle\left\langle\phi_H\left|\frac{\partial}{\partial z}\right|\phi_L\right\rangle, \quad (3)$$

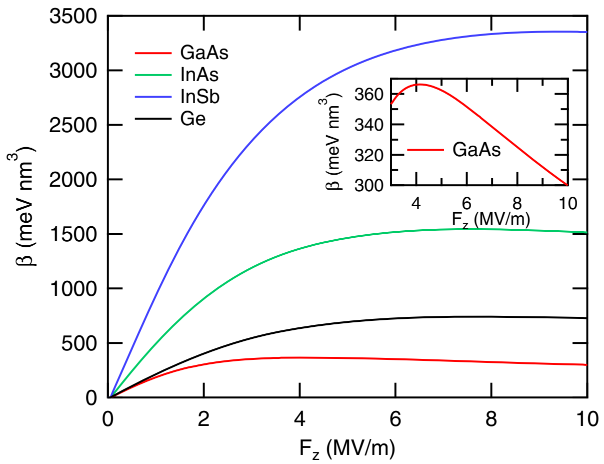

FIG. 2. The Rashba coefficient β of as a function of the net perpendicular electric field F_z for 15 nm GaAs, InAs, and InSb quantum wells. The inset shows that β for GaAs decreases by ~20% as F_z is increased from 4 MV/m to 10 MV/m, as the well becomes quasitriangular at $F_z \gtrsim 4$ MV/m.

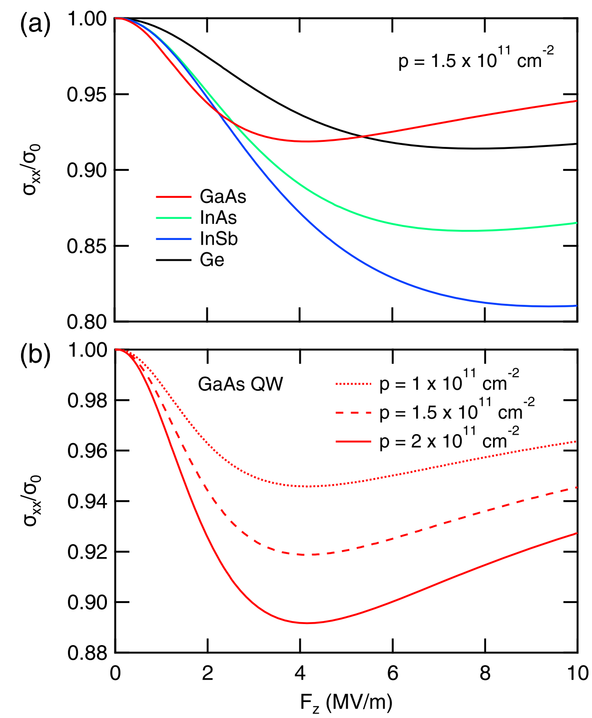

FIG. 3. Ratio of Drude conductivity at finite perpendicular electric fields (F_z) to its zero electric field value ($F_z = 0$), with the bare Drude conductivity $\sigma_0 \equiv pe\mu$, for (a) different quantum well materials at $p = 1.5 \times 10^{11}$ cm^{-2} and (b) GaAs quantum wells at different densities. The well width is 15 nm.

where Δ_E is the energy difference between the lowest heavy-hole and light-hole subbands, $\bar{\gamma} = (\gamma_2 + \gamma_3)/2$ is the cubic Luttinger parameter, and $\phi_{H,L}(z)$ represents the *orbital* component of the heavy-hole and light-hole wave functions, respectively, in the $\hat{z}$ direction. We approximate $\phi_{H,L}(z)$ with a modified infinite square well wave function containing F_z [87], see Section I of the Supplemental Material [60].

The Rashba coefficient β, as a function of F_z, for 15 nm hole quantum wells is shown in Fig. 2. For GaAs, at low F_z ($F_z \ll 4$ MV/m), the Rashba coefficient increases with F_z, in accordance with the trends reported in Ref. [88]. As F_z is increased, β saturates, and, at larger electric fields ($F_z > 4$ MV/m), the quantum well becomes quasitriangular and the Rashba coefficient β decreases with increasing F_z. The decrease of β as a function of F_z in quasitriangular wells is consistent with the experimental findings of Ref. [89]. For different materials, β saturates at different values of F_z, and β is larger in materials with a higher atomic number [86].

Given the dependence of β (Fig. 2), and hence the Hall coefficient R_H (Fig. 1), on F_z, we outline how β can be deduced experimentally. Using a top- and back-gated quantum well [55,88,89], the well is initially tuned to be symmetric so that $\beta = 0$ and the hole density can be measured accurately. One subsequently increases F_z (to ~4 MV/m for the GaAs well above), while keeping the density constant. This results in an appreciable increase in β, and, hence, a large change in R_H as a function of F_z.

The dependence of β on F_z affects the longitudinal conductivity $\sigma_{xx} = \sigma_0(1 - 60\pi m^{*2}\beta^2 p/\hbar^4)$ (Fig. 3). The spin-orbit corrections are larger in InAs and InSb [Fig. 3(a)] than in GaAs. As the density increases, σ_{xx} decreases faster with F_z [Fig. 3(b)]. Yet it is difficult to single out the dependence of σ_{xx} on β experimentally. As the shape of the wave functions changes with F_z, spin-orbit independent scattering is also altered, which introduces a large correction to σ_{xx} [90]. In fact, the spin-orbit independent corrections can alter the carrier mobility by ~20% even in electron quantum wells [55].

The analytical work presented here is of practical use for making experimental predictions and interpreting experimental data. Since, for a realistic 2DHS, higher subbands are only occupied at extremely high densities, and the spin-orbit energy $2\beta k_F^3 \gg k_B T$, our theory applies for a wide range of densities and temperatures (Table I) [91]. Moreover, from the computational standpoint, our approach offers significant advantages for two main reasons. First, Eq. (1) is general and can be applied for any 2DHS, provided the wave function in the growth direction is known. In this work we have neglected the wave function

TABLE I. The maximal hole densities p_{max} and temperatures T for which our theory is applicable for 15-nm-wide quantum wells (see Section V of the Supplemental Material [60]). Densities in units of 10^{11} cm^{-2} and temperature in K.

	GaAs	InAs	InSb	Ge
p_{max}	6.20	2.77	1.60	5.82
T	$\ll 50$	$\ll 80$	$\ll 80$	$\ll 120$

penetration into the barrier, which we expect to be very small (< 1 nm), and will not change the main result of Eq. (1), i.e., the quadratic dependence of R_H on β. Second, since Hall transport under strong spin-orbit coupling is strongly influenced by the interplay between intrinsic interband coherence effects and intraband response limited by scattering, a full transport calculation would be computationally expensive, especially in the dc limit. By contrast, in this work we use the quantum Liouville equation to solve for the hole density matrix, with the scattering term included in the first Born approximation, as described below.

Finally, we summarize our transport formalism, in the spirit of Ref. [92]. We begin with a set of time-independent states $\{\boldsymbol{k}s\}$, where s represents the twofold heavy-hole pseudospin. The terms $\hat{H}_0$, $\hat{H}_E$, and $\hat{H}_Z$ are diagonal in wave vector but off-diagonal in band index while for elastic scattering in the first Born approximation $U^{ss'}_{\boldsymbol{k}\boldsymbol{k}'} = U_{\boldsymbol{k}\boldsymbol{k}'}\delta_{ss'}$. Without loss of generality, here we consider short-range impurity scattering. The impurities are assumed uncorrelated and the average of $\langle \boldsymbol{k}s|\hat{U}|\boldsymbol{k}'s'\rangle\langle \boldsymbol{k}'s'\hat{U}|\boldsymbol{k}s\rangle$ over impurity configurations is $(n_i|\bar{U}_{\boldsymbol{k}'\boldsymbol{k}}|^2\delta_{ss'})/V$, with n_i the impurity density, V the crystal volume, and $\bar{U}_{\boldsymbol{k}'\boldsymbol{k}}$ the matrix element of the potential of a single impurity.

The central quantity in our theory is the density operator $\hat{\rho}$, which satisfies the quantum Liouville equation,

$$\frac{d\hat{\rho}}{dt} + \frac{i}{\hbar}[\hat{H},\hat{\rho}] = 0. \tag{4}$$

The matrix elements $\hat{\rho}_{\boldsymbol{k}\boldsymbol{k}'} \equiv \hat{\rho}^{ss'}_{\boldsymbol{k}\boldsymbol{k}'} = \langle \boldsymbol{k}s|\hat{\rho}|\boldsymbol{k}'s'\rangle$ can be decomposed as $\rho_{\boldsymbol{k}\boldsymbol{k}'} = f_{\boldsymbol{k}}\delta_{\boldsymbol{k}\boldsymbol{k}'} + g_{\boldsymbol{k}\boldsymbol{k}'}$, where $f_{\boldsymbol{k}}$ is diagonal in wave vector, while $g_{\boldsymbol{k}\boldsymbol{k}'}$ is off-diagonal in wave vector. The quantity of interest in determining the charge current is $f_{\boldsymbol{k}}$ since the current operator is diagonal in wave vector. The quantum Liouville Eq. (4), rewritten in terms of $f_{\boldsymbol{k}}$, reads

$$\frac{df_{\boldsymbol{k}}}{dt} + \frac{i}{\hbar}[H_{0\boldsymbol{k}} + H_Z, f_{\boldsymbol{k}}] + \hat{J}(f_{\boldsymbol{k}}) = \mathcal{D}_{E,\boldsymbol{k}} + \mathcal{D}_{L,\boldsymbol{k}}, \tag{5}$$

where $\hat{J}(f_{\boldsymbol{k}})$ is the scattering term in the Born approximation

$$\hat{J}(f_{\boldsymbol{k}}) = \left\langle \frac{1}{\hbar^2}\int_0^\infty dt'[\hat{U}, e^{-iH_0t'/\hbar}[\hat{U},\hat{f}(t)]e^{iH_0t'/\hbar}] \right\rangle_{\boldsymbol{k}\boldsymbol{k}}, \tag{6}$$

and the driving terms

$$\mathcal{D}_{E,\boldsymbol{k}} = -\frac{e\boldsymbol{E}}{\hbar}\cdot\frac{\partial f_{\boldsymbol{k}}}{\partial \boldsymbol{k}}, \tag{7a}$$

$$\mathcal{D}_{L,\boldsymbol{k}} = \frac{e}{2\hbar}\left\{\hat{\boldsymbol{v}}\times\boldsymbol{B}, \frac{\partial f_{\boldsymbol{k}}}{\partial \boldsymbol{k}}\right\}, \tag{7b}$$

stem from the applied electric field and Lorentz force, respectively [92]. In external electric and magnetic fields one may decompose $f_{\boldsymbol{k}} = f_{0\boldsymbol{k}} + f_{E\boldsymbol{k}} + f_{EB\boldsymbol{k}}$, where $f_{0\boldsymbol{k}}$ is the equilibrium density matrix, $f_{E\boldsymbol{k}}$ is a correction to first order in the electric field (at $\boldsymbol{B}=0$), and $f_{EB\boldsymbol{k}}$ is an additional correction first order in the electric and magnetic fields. The equilibrium density matrix is $f_{0\boldsymbol{k}} = (1/2)[(f_{\boldsymbol{k}+} + f_{\boldsymbol{k}-})\mathbb{1} + \boldsymbol{\sigma}\cdot\hat{\boldsymbol{\Omega}}_{\boldsymbol{k}}(f_{\boldsymbol{k}+} - f_{\boldsymbol{k}-})]$, where $\hat{\boldsymbol{\Omega}}_{\boldsymbol{k}}$ is the unit vector of effective spin-orbit field [Eq. (2)], and $f_{\boldsymbol{k}\pm}$ represent the Fermi-Dirac distributions over subband energies $\varepsilon_{\boldsymbol{k}\pm}$. In linear response one may replace $f_{\boldsymbol{k}} \to f_{0\boldsymbol{k}}$ in Eq. (7a). On the other hand, the driving term $\mathcal{D}_{L,\boldsymbol{k}}$ vanishes when the equilibrium density matrix is substituted, so in Eq. (7b) one may replace $f_{\boldsymbol{k}} \to f_{E\boldsymbol{k}}$. Hence, in this work we perform a perturbation expansion up to first order in the electric and magnetic fields, and up to second order in the spin-orbit interaction, retaining terms up to order β^2. The solution of Eq. (5) and the evaluation of the scattering term Eq. (6) are given in Sections II-IV of the Supplemental Material [60]. Here we summarize the procedure. First, with $f_{0\boldsymbol{k}}$ known and only $\mathcal{D}_{E,\boldsymbol{k}}$ on the right-hand side of Eq. (5), we obtain $f_{E\boldsymbol{k}}$. Next, with only $\mathcal{D}_{L,\boldsymbol{k}}$ on the right-hand side of Eq. (5), we obtain $f_{EB\boldsymbol{k}}$. By taking the trace with current operator, the longitudinal and transverse components of the current are $\boldsymbol{j}_{x,y} = e\mathrm{Tr}[\hat{\boldsymbol{v}}_{x,y}f_{\boldsymbol{k}}]$, with $\hat{\boldsymbol{v}} = (1/\hbar)\partial H_{0\boldsymbol{k}}/\partial\boldsymbol{k}$. Then, with σ_{xx} and σ_{xy} the longitudinal and Hall conductivities, respectively, the Hall coefficient appearing in Eq. (1) is found through $R_H = \sigma_{xy}/B_z(\sigma_{xx}^2 + \sigma_{xy}^2)$.

Here we have restricted ourselves, to gain transparent physical insight without loss of generality, to hole systems in which the Schrieffer-Wolff approximation is applicable so that β is approximately constant [86]. In general, $\beta(k)$ is a function of wave vector k, and decreases with k at larger k. The results we have found remain true in their general closed form for hole systems at arbitrary densities provided β is replaced by $\beta(k)$. Our kinetic equation approach can be generalized to arbitrary band structures in a way suitable for fully numerical approaches [93]. Finally, we note that we have not included the Dresselhaus spin-orbit interaction as it is unlikely to affect the main results. A recent study [86] reveals that the dominant Dresselhaus terms in two-dimensional holes, i.e., the k-cubic and k-linear Dresselhaus terms [25,94], are weakly density dependent, and, together they contribute up to one order of magnitude smaller than the Rashba interaction to the total spin splitting. Moreover, Dresselhaus terms are insensitive to F_z, so they will not affect the β dependence of the conductivity.

The magnetotransport properties of 2D electrons will differ from those of 2D holes. For 2D electrons, to lowest order the spin-orbit coupling stems from $\boldsymbol{k}\cdot\boldsymbol{p}$ coupling with the topmost valence band, and the leading contribution to spin-orbit interaction is linear in k [25]. Thus, the spin-orbit interaction in electrons typically gives rise to a spin-orbit splitting up to 2 orders of magnitude smaller than that of holes [25,86]. The corrections to magnetotransport will be much smaller compared to holes, and may not be detectable within experimental resolution.

In summary, we have presented a quantum kinetic theory of magnetotransport for two-dimensional hole systems in a weak perpendicular magnetic field, and predicted that the Hall coefficient R_H, along with the longitudinal conductivity, display strong signatures of the spin-orbit interaction. We have also shown that our theory provides an excellent qualitative agreement to existing experimental trends for β. We have proposed an appropriate experimental setup using top- and back-gated quantum wells to probe the spin-orbit corrections to R_H.

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[*]Corresponding author.
elizabeth.marcellina@gmail.com
[†]Corresponding author.
d.culcer@unsw.edu.au
[‡]H. L. and E. M. contributed equally to this work.

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