We study transport properties of a MoS$_2$ monolayer in the presence of a perpendicular magnetic field $B$. We derive and discuss its band structure and take into account spin and valley Zeeman effects. Compared to a conventional two-dimensional electron gas, these effects lead to new quantum Hall plateaus and new peaks in the longitudinal resistivity as functions of the magnetic field. The field $B$ leads to a significant enhancement of the spin splitting in the conduction band, to a beating of the Shubnikov–de Haas (SdH) oscillations in the low-field regime, and to their splitting in the high-field regime. The Zeeman fields suppress significantly the beating of the SdH oscillations in the low-field regime and strongly enhance their splitting at high fields. The spin and valley polarizations show a similar beating pattern at low fields and are clearly separated at high fields in which they attain a value higher than 90%.

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I. INTRODUCTION

Recent developments in the experimental realization of two-dimensional (2D) transition-metal dichalcogenides $MX_2$ ($M = Mo, W$; $X = S$, Se) have drawn much attention due to potential applications [1--10]. MoS$_2$ is a semiconducting material with strong spin-orbit coupling $2\lambda' = 150$ meV and a large intrinsic band gap $2\Delta = 1.66$ eV. These properties of $MX_2$ contrast sharply with those of graphene, the first stable 2D material with promising technological applications in various fields [11], which has a negligible band gap and a very weak spin-orbit coupling (SOC). MoS$_2$ has the honeycomb structure of graphene but provides a mass to the Dirac fermions [5,6,10]. As a consequence, preliminary results indicate a high potential for valleytronics because the dispersion can be manipulated in a flexible manner for optoelectronic applications [6--9]. Spin and valley Hall effects have been predicted in an experimentally accessible temperature regime [5], the former arising from the strong SOC and the latter from the broken inversion symmetry. Some experimental results for MoS$_2$ and WSe$_2$ [7,8,12,13] suggest that monolayers of $MX_2$ could be used for integrated valleytronic devices. From a fundamental point of view, many efforts have focused on different properties of MoS$_2$ and other group-VI dichalcogenides in the absence of a magnetic field. To see the effects of such a field and the corresponding Landau levels (LLs), magnetotopical properties [14--16] have been theoretically studied.

The integer quantum Hall effect (QHE) of a 2D electron gas (2DEG) is epitomized by steps in the Hall conductivity of height $2(n+1)e^2/h$ where $h$ is the Planck constant, $e$ the electron charge, and $n$ an integer, and the vanishing of the longitudinal conductivity (dissipationless current) at these steps. In graphene [17--19], the QHE plateaus appear at $4(n+1/2)e^2/h$ and the fourfold degeneracy is associated with the spin and valley degrees of freedom. More recently, the QHE has been assessed for silicene/germanene [20,21] in which the SOC rearranges the LLs in two groups and the plateaus appear at $2(n+1/2)e^2/h$ due to the valley degeneracy except for the $n = 0$ LL in which the fourfold degeneracy is lifted. Quantum transport measurements to observe the QHE and Shubnikov–de Haas oscillations (SdH) in high mobility MoS$_2$ have been performed very recently [22]. Although an unconventional QHE [23] has been predicted for MoS$_2$ through its band structure, we are aware only of the limited study of ballistic transport in Ref. [24], i.e., in the absence of scattering, but not of any detailed magnetotransport studies that take scattering into account. As clearly stated in Ref. [24], though, trigonal warping contributes a Zeeman-type term to the valley splitting but does not affect much the band structure which depends strongly on the linear term in the magnetic field $B$ [see Sec. II after Eq. (3)].

In this work, we study quantum magnetotransport through a monolayer MoS$_2$. We derive and discuss the corresponding band structure in the presence of a perpendicular magnetic field and include the spin and valley Zeeman terms. The study of transport is based on general conductivity expressions, derived within the linear-response theory [25], and cast explicitly in terms of single-particle eigenstates and eigenvalues. Using them, we investigate the influence of a magnetic field on the spin and valley Hall conductivity, and show that the plateaus exhibit an unusual sequence. In addition, we evaluate the longitudinal conductivity, and compare the results with those for graphene and silicene or germanene.

The paper is organized as follows. In Sec. II, we present the one-electron eigenstates, eigenvalues, and the corresponding density of states (DOS). In Sec. III, we evaluate the Hall and longitudinal conductivities and discuss our numerical results. Summary and concluding remarks follow in Sec. IV.

II. BASIC MODEL FORMULATION

We consider MoS$_2$ in the ($x,y$) plane in a perpendicular magnetic field $B$. Including two Zeeman terms in the one-electron Hamiltonian of Ref. [5] [Eq. (3)], we obtain

$$H = v_F(\eta \sigma_x \Pi_x + \sigma_y \Pi_y) + (\Delta - \lambda \eta \sigma_z + \lambda \eta s \Pi_z + s M_z - \eta M_\|).$$  

(1)
Here, $\eta = \pm 1$ for valleys $K$ and $K'$, $2\Delta \approx 1.66$ eV is the mass term which breaks the inversion symmetry and creates an intrinsic direct band gap, $\sigma_{1}$, $\sigma_{1}$, and $\sigma_{2}$ are the Pauli matrices, $\Pi = \mathbf{p} + e\mathbf{A}$ is the 2D canonical momentum with $\mathbf{A}$ the vector potential, $v_{F}$ denotes the Fermi velocity, and $\lambda = \lambda' / 2 = 37.5$ meV is the SOC strength with spin up and spin down represented by $s = +1$ and $-1$, respectively. Further, $M_{c} = g' \mu_{B} B / 2$ is the Zeeman exchange field induced by ferromagnetic order, $g'$ the Landé $g$ factor ($g' = g'_{e} + g'_{h}$), and $\mu_{B}$ the Bohr magneton [26]. Also, $g'_{e} = 2$ is the free-electron $g$ factor and $g'_{h} = 0.21$ is the out-of-plane factor due to the strong SOC in MoS$_{2}$. The last term, $M_{v} = g'_{e} \mu_{B} B / 2$, breaks the valley symmetry of the levels and $g'_{e} = 3.57$ [26]. The Zeeman field energy has been measured in very recent experiments [27–30] and is theoretically shown to be approximately 30 meV by first-principles calculations [31].

Using the Landau gauge for the vector potential $\mathbf{A} = (0, B x, 0)$ and diagonalizing the Hamiltonian (1), we obtain the eigenvalues

$$E_{n,p}^{x,s} = \eta s \lambda + s M_{c} - \eta M_{v} + p E_{n}^{x,s}, 
$$

$$= \left[ n^{2}(\omega_{c}^{2} + \Delta_{n}^{2}) \right]^{1/2},
$$

(2)

here, $\Delta_{n} = \Delta - \eta s \lambda$, $p = +(-)$ denotes the electron (hole) states, $\omega_{c} = v_{F} \sqrt{2 e B / \hbar}$ is the cyclotron frequency, and the integer $n$ labels the Landau levels (LLs). A simpler expression for the eigenvalues is obtained by noticing that $\hbar \omega_{c} \ll \Delta_{n}$. Expanding the square root gives

$$E_{n,p}^{x,s} \approx (1 - p) \eta s \lambda + s M_{c} - \eta M_{v} + p \Delta + pn \frac{\hbar^{2} \omega_{c}^{2}}{2 \Delta_{n}},
$$

(3)

This is a usual, linear in $n$ and $B$, LL spectrum. Notice that in the conduction band the first term in Eq. (3) vanishes, whereas in the valence band it does not. Using $\Delta \gg \eta s \lambda$, the last term is equal $pn(\hbar^{2} \omega_{c}^{2} / 2 \Delta)(1 + \eta s \lambda)$. This gives a spin slitting $E(s = 1) - E(s = -1) = 2M_{c} + n\eta s \lambda(\hbar^{2} \omega_{c}^{2} / \Delta)$ in the conduction band and $2n\lambda - n\eta s \lambda(\hbar^{2} \omega_{c}^{2} / \Delta)$ in the valence band. The term $n(\hbar^{2} \omega_{c}^{2} / 2 \Delta) \propto n B$ is about twice as big as $M_{c}$ and much smaller than $\lambda$. It is important in the conduction band but negligible in the valence band in which $\lambda \approx 150$ meV.

The eigenfunctions for the $K$ valley are

$$\Psi_{n,p}^{x,s} = \frac{e^{ik_{y}y}}{\sqrt{L_{y}}} \left( A_{n,p}^{x,s} \phi_{n}, B_{n,p}^{x,s} \phi_{-n-1} \right),
$$

(4)

where $A_{n,p}^{x,s} = [(p E_{n}^{x,s} + \Delta_{n}) / 2p E_{n}^{x,s}]^{1/2}$, $B_{n,p}^{x,s} = [(p E_{n}^{x,s} - \Delta_{n}) / 2p E_{n}^{x,s}]^{1/2}$, and $\phi_{n}$ is the harmonic oscillator function. The eigenfunctions for the $K'$ valley ($\eta = -1$) are obtained from Eq. (4) by exchanging $\phi_{n}$ with $\phi_{-n-1}$. The eigenvalues and eigenfunctions of the $n = 0$ LL are

$$E_{0}^{x,s} = \Delta + s M_{c} - M_{v}, \quad \Psi_{0,0}^{x,s} = \left( \phi_{0}, 0 \right),
$$

(5)

$$E_{0}^{-,s} = -\Delta + s M_{c} - M_{v} + 2s \lambda, \quad \Psi_{0,0}^{-,s} = \left( 0, \phi_{0} \right).
$$

(6)

For a better appreciation of the spectrum given above, one can contrast it with that for $B = 0$ given by

$$E_{p}^{x,y} = s \eta \lambda + p(\sqrt{\lambda^{2} \hbar^{2} k^{2} + (\Delta - \lambda \eta s)^{2}})^{1/2},
$$

(7)
of the spin down (up) at the K’ valley and show a spin and valley polarization in contrast with the zero magnetic field limit in which they are the same [5]. (iv) For \( M_z \neq 0 \) and \( M_x = 0 \) the spin splitting in the conduction band for \( n = 5 \) is 2.2 meV at \( B = 10 \) T and 4.3 meV at \( B = 20 \) T, respectively. (v) In contrast to the \( B = 0 \) case [5], the spin splitting in the conduction band is about 10 meV for \( B = 30 \) T (\( M_z \neq 0, M_x \neq 0 \)) and can become larger by increasing \( B \). A 10-meV spin splitting in the conduction band has been realized in recent experiments [22]. On the other hand, in the valence band the spin degeneracy is spin nondegenerate for \( M_z = 0, M_x \neq 0 \) (\( M_z \neq 0 \)) and can become larger by increasing \( B \). The Fermi level results in Fig. 3 in the presence of \( M_z \neq 0 \) correspond to the fourfold-nondegenerate LLs. This is also shown separately in Fig. 4 for a clearer understanding.

The Fermi energy is obtained from the electron concentration \( n_e \) given by

\[ n_e = \int_{-\infty}^{\infty} D(E) f(E) dE = \frac{g_s}{D_0} \sum_{\alpha, \eta, s} f(E_{\alpha, \eta, s}), \tag{8} \]

where \( D(E) \) is the density of states (DOS), with \( D_0 = 2\pi^2 \) and \( g_s \) is the spin (valley) degeneracy. Further, \( f(E_{\alpha, \eta, s}) = (1 + \exp(\beta(E_{\alpha, \eta, s} - E_F)))^{-1} \), with \( \beta = 1/k_B T \), is the Fermi-Dirac function. We use \( g_s = g_v = 1 \) due to the lifting of the spin and valley degeneracies. The DOS is given in the Appendix.

The magenta solid curve in Fig. 3 shows the Fermi level, obtained numerically from Eq. (8), as a function of \( B \); the LLs shown are the same as those in Fig. 2, i.e., spin and valley dependent, since the magnetic field lifts the spin and valley degeneracies of the \( n \geq 1 \) LLs. To appreciate the difference between the case \( M_z = M_x = 0 \), shown in the top panel, and the case \( M_z \neq 0, M_x \neq 0 \), we plot the spectrum in the lower panel of Fig. 3, versus the field \( B \), for \( M_z = 0, M_x = 0 \). The additional intra-LL small jumps result from the lifting of the spin and valley degeneracies; the solid and dashed curves (\( n \geq 1 \)) are, respectively, for spins up and spins down in the K valley, respectively. For the K’ valley the spins are reversed, e.g., for \( n \geq 1 \), the spin-up electrons in the K valley have the same energy as the spin-down ones in the K’ valley. For \( n \geq 1 \), the fourfold degeneracy, due to spin and valley, of all LLs is lifted while the \( n = 0 \) LL in the conduction band is valley degenerate. The Fermi level results in Fig. 3 in the presence of \( M_z, M_x (M_z, M_x \neq 0) \) correspond to the fourfold-nondegenerate LLs. This is also shown separately in Fig. 4 for a clearer understanding.

Another worth noticing feature is the beating of the oscillations for \( B \) fields up to about 10 T with a giant splitting of the LLs at higher fields due to the spin and valley Zeeman terms. As we show in the following, such a beating pattern also appears in the DOS and other transport quantities.

The DOS is evaluated in the Appendix [see Eq. (A2)]. We show it in Fig. 5 as a function of the magnetic field \( B \) for an electron density \( n_e = 5 \times 10^{16} \) m\(^{-2} \) and a Fermi velocity \( v_F = 5.3 \times 10^5 \) m s\(^{-1} \). We plot the dimensionless DOS \( D(E_F)/D_0 \) in the top and bottom panels for the conduction band. For low and high fields \( B \) we observe a beating pattern and a splitting of the SdH oscillations, respectively. Both are due to the closeness of the frequencies.
of the spin-up and -down states that result from the splitting of the LLs due to the SOC. The beating is suppressed at very low fields and the splitting of the oscillations becomes more pronounced at high fields. The beating pattern vanishes in the conductive band in the limit \( B \to 0 \) since so does the SOC splitting in this limit [5].

As shown in Fig. 5, the amplitude is modulated by \( \cos(2\pi\beta/\hbar^2\epsilon_{\text{r}r}^2) \) and nodes occur at \( \delta/\hbar^2\epsilon_{\text{r}r}^2 = \pm 0.5, \pm 1.5, \ldots \) [see Eq. (A4)]. We also note that the amplitude modulation occurs only when both the SOC and the field \( B \) are finite. Further, the threshold magnetic field where beating is seen depends on both \( \lambda \) and \( \Delta \).

The beating persists in the conduction band for magnetic fields up to about 10 T. Above this value, it is quenched and the SDH oscillations are split. This behavior is explained by the closeness of the oscillation frequencies of the SOC-split LLs. The magnetic-field-enhanced splitting in the conduction band mixes the spin-up and -down states of neighboring LLs into two unequally spaced energy branches. The beating appears when the subband broadening is of the order of \( \hbar \omega_{\text{c}} \). For high magnetic fields, the SOC effects weaken and the beating pattern is replaced by a splitting of the peaks, which persist due to the SOC and Zeeman energies.

The giant splitting of the SDH oscillations in the high-field regime can be understood by the term \( \cos[4\pi(G_{\text{r}}\Delta + \eta\lambda M_0)/\hbar^2\epsilon_{\text{r}r}^2] \) with and without the Zeeman terms \( M_0 \) and \( M_0 \). Normally this term exhibits SDH oscillations without the terms \( M_0 \) and \( M_0 \); thus, the giant splitting at high fields is purely caused by their presence in the Fermi energy and DOS. Noting that the cyclotron energy is \( \hbar \omega_{\text{c}} = 19 \text{ meV} \) at \( B = 1 \text{ T} \), the observation of the LL splitting and the discussed consequences require that the temperature and level broadening are smaller than the splitting due to the SOC.

### III. Linear-Response Conductivities

In the linear-response formalism of Ref. [25], the many-body Hamiltonian of the system is written as \( H = H_0 + H_1 - \mathbf{R} \cdot \mathbf{F}(t) \), where \( H_0 \) is the unperturbed part, \( H_1 \) a binary interaction of electrons, e.g., with impurities or phonons, \( -\mathbf{R} \cdot \mathbf{F}(t) \) is the interaction of the system with an external time-dependent field \( \mathbf{F}(t) \), \( \mathbf{R} = \sum_i \mathbf{r}_i \), and \( \mathbf{r}_i \) the position operator of electron \( i \). For electrical transport we have \( \mathbf{F}(t) = N\mathbf{e}\mathbf{E}(t) \), where \( \mathbf{E}(t) \) is the electric field. In the representation in which \( H_0 \) is diagonal the many-body density operator \( \rho = \rho^d + \rho^{\text{ad}} \) has a diagonal \( (\rho^d) \) and a nondiagonal \( (\rho^{\text{ad}}) \) part. Accordingly, the conductivity tensor \( \sigma_{\mu\nu} \) has a diagonal \( (\sigma_{\mu\nu}^d) \) and a nondiagonal \( (\sigma_{\mu\nu}^{\text{ad}}) \) part; the full tensor is \( \sigma_{\mu\nu} = \sigma_{\mu\nu}^d + \sigma_{\mu\nu}^{\text{ad}} \).

#### A. Longitudinal conductivity, polarizations

In general, two mechanisms contribute to the current, diffusion, and hopping, but usually only one of them is present. When a magnetic field is present, we have only the hopping contribution since the diffusive one, involving only diagonal elements of the velocity operator [25], vanishes. For weak electric fields and weak scattering potentials the longitudinal conductivity \( \sigma_{\mu\mu}^d \) due to hopping has the form [25]

\[
\sigma_{\mu\mu} = \frac{e^2}{2}\sum_{\xi} f(E_\xi)(1 - f(E_\xi))W_{\mu\mu}(X_\xi - X_\xi)^2, \tag{9}
\]

with \( f(E_\xi) = f(E_\xi^{\text{ad}}) \) and \( S_0 = L_xL_y \), the area of the sample. Further, \( W_{\mu\mu} \) is the transition rate between the one-electron states \( |\xi\rangle \) and \( |\zeta\rangle \) and \( e \) the charge of the electron. For elastic scattering, we have \( f(E_\xi) = f(E_\xi) \) and conduction occurs by hopping between the orbit centers \( X_\xi \) and \( X_\zeta \), with \( X_\xi = \langle \zeta | X | \xi \rangle = \ell k_y \).

At very low temperatures, the dominant scattering mechanism is that of electrons scattered by charged impurities in similar, graphenelike systems (see Ref. [32] for more details). We model the impurity potential as that of a screened charge \( U(r) = (e^2/4\pi\varepsilon_0\varepsilon_0)\rho e^{-k_xr} \), where \( k_s \) is the screening wave vector, \( \varepsilon_0 \) the relative permittivity, and \( \varepsilon_0 \) the permittivity of the vacuum. The Fourier transform of \( U(r) \) is then given by \( U(q) = U_0/(q^2 + k_s^2)^{1/2} \), with \( U_0 = e^2/2\varepsilon_0\varepsilon_0 \). Further, if the impurity potential is short ranged (of the Dirac \( \delta \)-function type), one may use the approximation \( k_s \gg q \) and obtain \( U(q) \approx U_0/k_s \). The transition rate is given by

\[
W_{\zeta\zeta} = \frac{2\pi n_i}{S_0\hbar} \sum_{\zeta'} |U(q)|^2 J_{\zeta\zeta}(u)^2 \delta(E_\zeta - E_{\zeta'})\delta(k_x + q_x), \tag{10}
\]

with \( u = l^2(q_x^2 + q_z^2)/2 = l^2q_y^2/2 \) and \( n_i \), the impurity density. \( J_{\zeta\zeta}(u) = |\zeta| \exp(\mathbf{q} \cdot \mathbf{r}) \) are the form factors and \( \zeta \equiv |\mu,\nu,\ell,k_y\rangle \). For elastic impurity scattering, we neglect LL mixing, i.e., we take \( n = n' \). Further, we note that \( \sigma_{xx} = \sigma_{xy} \) and that for \( k_x \gg q \) we can ignore the factor \( q^2 \) in \( U(q) \). We have
(X_\xi - X_\xi')^2 = l^2 q_x^2 and q_x = q \sin \phi. Since the wave function oscillates around x_0 = l^2 k_x and 0 \leq x_0 \leq L_{\xi}, the sum over k_x gives a factor S_0/2\pi l^3 and that over q is evaluated in cylindrical coordinates. The standard evaluation of |J_{\xi}(u)|^2, for n \neq n', gives |J_{n}(u)|^2 = \exp(-u)|A_{n}^{0,0}\xi|^{2}L_n(u) + |B_{n}^{0,0}\xi|^{2}L_{n-1}(u)^2. Further, \delta(E_{n} - E_{n'}) = (2A_{n}\xi/h^2\omega_{C})\delta_{n,n'}. Inserting these factors in Eq. (9) and evaluating the integral over u, the longitudinal conductivity can be written as

$$\sigma_{xx} = \frac{e^2}{h} \beta n_{\xi} T^2 \sum_{n,s} \Delta_{n,s} I_{n,s}^{\xi} \left[ f(E_{n,s}^{\xi}) - f(E_{n,s}^{\xi}) \right],$$

where

$$I_{n,s}^{\xi} = \int_{0}^{\infty} u |J_{n,s}(u)|^2 du. \quad (12)$$

The integration in Eq. (12) is carried out using the orthogonality of the polynomials L_n(u) and their recurrence relation (n + 1)L_{n+1}(u) - (2n + 1 - u)L_n(u) + nL_{n-1}(u) = 0. It gives

$$I_{n,s}^{\xi} = (2n + 1)|A_{n,s}^{0}\xi|^{4} - 2n|A_{n,s}^{0}\xi|^{2}|B_{n,s}^{0}\xi|^{2}$$

$$+ (2n - 1)|B_{n,s}^{0}\xi|^{4}. \quad (13)$$

As expected, the conductivity obtained from Eq. (11) exhibits SdH oscillations when B is varied. We show that in Fig. 6 for the following parameters [5, 22, 33]: n_i = 1 \times 10^{13} m^{-2}, \mu_B = 5.788 \times 10^{-7} eV/T, T = 1 K, n_e = 5 \times 10^{16} m^{-2}, k_0 = 1 \times 10^{-7} m^{-1}, u_F = 5.3 \times 10^5 m/s, and \epsilon_r = 7.3 [34]. In contrast with graphene [19] or silicene [21], we find a beating pattern in the SdH oscillations for a B field up to about 8 T and a splitting after this value. Figure 6 shows the SdH oscillations of \sigma_{xx} for zero (black) and finite (red) Zeeman field energies. For high magnetic fields, the beating pattern disappears and the SdH oscillations are split (see top and bottom panels in Fig. 6). It is a giant splitting and in agreement with the Fermi energy and DOS results shown in Figs. 3–5. The beating pattern is controlled by the magnetic field. It occurs when the subband broadening is of the order of the LL separation h\omega_{C}. For high fields B the SOC effects weaken and the beating pattern is replaced by a splitting of the magnetoconductivity peaks.

The beating pattern can be understood analytically as follows. For very low temperatures, one can make the approximation \beta f(E_{n,s}^{\xi})(1 - f(E_{n,s}^{\xi})) \approx \delta(E_F - E_{n,s}^{\xi}), in Eq. (11), to broaden the \delta function, and carry out the sum over n as outlined in the Appendix. Then, similar to the case of the DOS, the beating pattern is described by the two close-in-frequency cosine terms in Eq. (A3) with the replacement E \rightarrow E_{xx}. We believe that these results for monolayer MoS_2, and presumably other group-VI dichalcogenides, can be observed by existing experimental techniques [22]. We notice in passing that such a beating pattern, entirely due to the SOC, has been observed experimentally [35] in the conventional 2DEG and treated theoretically [36]. In both cases, the LL spectrum is linear in the field B whereas in graphene or silicene it is proportional to B^{1/2}.

Equation (11) contains all spin and valley contributions to the longitudinal conductivity. Extracting them from there one can study the spin \sigma_{xx} and valley \sigma_{yy} polarizations defined by

$$P_s = \frac{\sigma_{xx}^{K,\uparrow} + \sigma_{xx}^{K,\downarrow} - (\sigma_{xx}^{K,\uparrow} + \sigma_{xx}^{K,\downarrow})}{\sigma_{xx}^{K,\uparrow} + \sigma_{xx}^{K,\downarrow} + (\sigma_{xx}^{K,\uparrow} + \sigma_{xx}^{K,\downarrow})}. \quad (14)$$

and

$$P_v = \frac{\sigma_{xx}^{K,\uparrow} + \sigma_{xx}^{K,\downarrow} - (\sigma_{xx}^{K,\uparrow} + \sigma_{xx}^{K,\downarrow})}{\sigma_{xx}^{K,\uparrow} + \sigma_{xx}^{K,\downarrow} + (\sigma_{xx}^{K,\uparrow} + \sigma_{xx}^{K,\downarrow})}. \quad (15)$$

We plot P_s and P_v versus the field B in Fig. 7; the parameters are the same as those used for producing the red curve in Fig. 6. As expected and can be seen, here too we have beating patterns at relatively low B fields and a clear separation.
between $P_1$ and $P_2$ at strong fields with both attaining more than 90% above $B = 20$ T.

**B. Hall conductivity and magnetoresistivities**

Within linear-response theory, the Hall conductivity $\sigma_{yx}$ is given by [19,25]

$$\sigma_{yx}^{\text{nd}} = \frac{ie^2}{h} \sum_{\xi'\nu\xi} \left( f_{\xi} - f_{\xi'} \right) \nu_{\xi'\xi} v_{\mu'\xi} v_{\mu\xi'},$$

(16)

where $v_{\nu'\xi} v_{\mu'\xi'}$ are the nondiagonal matrix elements of the velocity operator, $\mu, \nu = x, y$, and $S_0 = L_xL_y$. The sums run over all quantum numbers of the states $\xi \equiv \eta, s, n; \eta' \equiv \eta, s, n'$. The Zeeman splitting, the fourfold degeneracy is lifted. In the conduction band, this lifting is due to the magnetic field. The matrix elements of the Hamiltonian $(1)$, $v_1 = \partial H/\partial p_x$, and $v_2 = \partial H/\partial p_y$. We obtain $v_{\eta}s = v_{\eta}A_{\eta}s$, and, using Eq. (4), the matrix elements

$$\langle \xi'| v_{\nu} | \xi \rangle = u(A^0_{\eta,s} B^0_{\eta',p} \delta_{\eta,n-1} + B^0_{\eta,s} A^0_{\eta',p} \delta_{\eta,n-1}),$$

(17)

$$\langle \xi'| v_{\nu} | \xi \rangle = -i\eta u(A^0_{\eta,s} B^0_{\eta',p} \delta_{\eta,n-1} - B^0_{\eta,s} A^0_{\eta',p} \delta_{\eta,n-1}).$$

(18)

For the $K'$ valley $n$ and $n'$ must be interchanged only in the Kronheimer deltas.

The matrix elements between the $n = 0$ and the $n \geq 1$ LLs are obtained in a similar way. For the $K'$ valley, the $(n, 0)$ matrix elements are

$$\langle \xi'| v_{\nu} | \xi \rangle = v(A^0_{\eta,s} B^0_{\eta',p} \delta_{\eta,n-1} - B^0_{\eta,s} A^0_{\eta',p} \delta_{\eta,n-1}),$$

(19)

those for the $(0, n)$ ones are given by Eq. (19) upon changing $n'$ to $n$ and $i$ to $-i$. The results for the $K$ valley are obtained by replacing $A^0_{\eta,s}$ with $B^0_{\eta,s}$.

Since $|\xi \rangle \equiv |\eta, s, n, k_x \rangle$, there will be one summation over $k_x$ which, with periodic boundary conditions for $k_x$, gives the factor $S_0/2\pi l^2$. Now, one needs to sum over all possible combinations of the matrix elements and for convenience we write $\sum_{p,p'} = \sum_{n,+} + \sum_{n,-} + \sum_{n,+} + \sum_{n,-}$. Here, the subscript $+/-$ denotes the conduction/valence band and only the $n \geq 1$ LLs are considered. The $n = 0$ LL is considered separately. This procedure is detailed in Ref. [19]. The resulting Hall conductivity is $\sigma_{yx} = \sigma_{yx} + \Delta \sigma_{yx}$, with

$$\sigma_{yx} = \frac{e^2}{h} \sum_{\eta, s, n = 1} (n + 1/2)\left(f_{n,+}^0 - f_{n+1,+}^0 + f_{n,-}^0 - f_{n+1,-}^0\right),$$

(20)

$$\Delta \sigma_{yx} = \frac{e^2}{2h} \sum_{\eta, s, n = 1} \eta \Delta \eta \left\{ \left(f_{n,+}^0 - f_{n+1,+}^0\right)E_{n,+}^0 - \left(f_{n,+}^0 - f_{n+1,+}^0\right)E_{n+1,+}^0 \right\}.$$  

(21)

The sums in Eq. (20) run from $n = 1$ to $\infty$ and the results for the $K$ and $K'$ valleys are obtained by setting $\eta = +1$ and $-1$, respectively. Then, writing explicitly the sums over $s$ one sees that the correction terms $\Delta \sigma_{yx}^K$ and $\Delta \sigma_{yx}^{K'}$ cancel each other provided both valleys in the $n$th LL are occupied; evidently they do not cancel when only one of the spins or valleys is occupied.

The total contribution of the $n = 0$ LL, including both spins and valleys, is

$$\sigma_{yx}^{0,0} = \frac{e^2}{h} \sum_{\eta} \left\{ f_{0,+}^0 - f_{0,+}^0 \right\}/2 + \left(f_{1,+}^0 - f_{1,+}^0\right)\eta \Delta \eta/2E_{1,+}^0 \right\}.$$  

(22)

Note again that the terms $\eta \Delta \eta$ cancel each other when summing the valley contributions $\sigma_{yx}^{0,K} + \sigma_{yx}^{0,K'}$, due to the opposite spin states in the two valleys. This reveals that the conductivity $\sigma_{yx}$ is essentially independent of $\eta \Delta \eta$; that is, the size of the band gap does not affect the correction terms $\Delta \sigma_{yx}^K$ in the Hall conductivity. This limit agrees with the results for gapped graphene or silicene although MoS$_2$ and other group-VI dichalcogenides are different from these materials due to a strong SOC, a large intrinsic direct band gap, and an asymmetry between the two bands (for $B = 0$ the spin splitting is 0 and 150 meV in the conduction and valence bands, respectively [5]). In the limit $|\lambda| \rightarrow 0$, this results reduce to similar ones for gapped graphene [26] and for graphene in the limit of $\Delta = \lambda = 0$ [17]. In contrast, for $\Delta \lambda \neq 0$, as in the case of MoS$_2$ and other group-VI dichalcogenides, we see a

FIG. 8. Hall conductivity as a function of the magnetic field $B$ for $T = 1$ K. The upper and lower panels differ only in the field range ($x$ axis). For further clarity, the range 5–7 T is shown in the inset to the upper panel and the range 14–25 T in that to the lower one. This inset covers the cases $M_x = M_y = 0$, $M_x = 0, M_y \neq 0$, and $M_x \neq 0, M_y = 0$. 035406-6
The longitudinal resistivity is obtained from the relation $\rho_{xx} = (B/n_e e)^2 \sigma_{xx}$ [19], where $n_e$ is the carrier concentration. We observe extra plateaus in the Hall resistivity due to the SOC and the two Zeeman terms. We find that the steps between the plateaus coincide with sharp peaks in the longitudinal resistivity. In strong magnetic fields, larger than 10 T, we find a significant splitting of the Hall plateaus and the corresponding peaks in the longitudinal resistivity due to the spin and valley Zeeman effects. In contrast, for magnetic fields less than 10 T we observe a beating pattern of the SdH oscillations. It is interesting to note that this pattern is similar to that due to the Rashba SOC in a conventional 2DEG [36]. The predicted SdH oscillations agree well with recent experiments [22] at high magnetic fields. The particular features shown here below 10 T could be tested by more detailed experiments.

IV. SUMMARY AND CONCLUSIONS

We studied quantum magnetotransport properties of a MoS$_2$ monolayer subject to an external perpendicular magnetic field. At $B = 0$ the spin splitting energy is zero in the conduction and 150 meV in the valence band. We showed though that the magnetic field can enhance it in the conduction band by an amount $\alpha n B$ approximately twice as large as $M_0$ [see text after Eq. (3) and Fig. 2]. The combined action of the SOC and of the magnetic and Zeeman fields allows for intra-LL transitions and leads to new quantum Hall plateaus. Moreover, for fields $B$ stronger than 10 T, the peaks of the SdH oscillations of the longitudinal conductivity are doubled whereas for fields below 10 T a beating pattern is observed similar to that of a conventional 2DEG [36]. A similar beating pattern is also exhibited, at low fields, by the spin and valley polarizations. It is also worth emphasizing their oscillations in the entire range of the $B$ field covered and their higher than 90% value for $B \geq 20$ T.

The deep minima in the SdH oscillations are accompanied by Fermi level jumps and the peaks coincide with the usual singularities of the DOS. We have shown a beating and splitting of the SdH oscillations in the resistivity, which can be controlled and enhanced by increasing the magnetic field. Indeed, the magnetic field enhances the spin splitting in the conduction band [cf. last term in Eq. (3)], which in turn enhances the splitting and beating of the SdH oscillations. The spin and valley Zeeman fields lead to a giant splitting for strong magnetic fields and the lifting of the fourfold spin and valley degeneracies. We expect that these results will be tested by experiments.

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APPENDIX

The density of states (DOS) is given by $D(E) = (1/S_0) \sum_{n,p} \delta(E - E_n^p)$, where $S_0 = L_x L_y$ is the area of the system. The sum over $k_y$ is evaluated using the prescription $(k_0 = L_x/2\pi) \sum_{k_y} \rightarrow (L_x g_z g_s/2\pi) \int_{-k_0}^{k_0} dk_y = (S_0/D_0) g_z g_s$, where $D_0 = 2\pi l^2$; $g_z$ and $g_s$ are the spin and
valley degeneracies, respectively. We use $g_s = g_v = 1$ due to the lifting of the spin and valley degeneracies. Assuming a Gaussian broadening of the LLs the DOS becomes

$$D(E) = \frac{g_s^{2}}{D_0} \frac{m}{\Gamma \sqrt{2\pi}} \sum_{n,q} \exp \left[ -\left( E - E_{n,p}^{\eta} \right)^2 / 2\Gamma^2 \right]. \quad (A1)$$

where $\Gamma = 0.1 \sqrt{B}$ meV is the width of the Gaussian distribution [32].

The sum over $n$ is evaluated with the help of the Poisson summation formula [37]. The resulting DOS is

$$D(E) = \sum_{n,s} D_1 \left[ 1 + 4 \sum_{k=1}^{\infty} \left( -1 \right)^k \cos \left( 4\pi k \left( G_n - s M_\eta \right) \Delta_\eta / h^2 \omega_c^2 \right) \right] \times e^{-2\pi k \Delta_{\eta s} / h^2 \omega_c^2} \right], \quad (A2)$$

where $D_1 = \Delta_\eta / 4\pi v^2 h^2$ and $G_n = E - \Delta + \eta M_\eta$. The first term inside the curly brackets is the monotonic part and the second term the oscillatory part of the DOS. It is sufficient to retain only the term $k = 1$ since the $k > 1$ terms are strongly damped. The oscillatory part leads to a beating pattern at low fields $B$ and a splitting of the SDH oscillations at higher $B$ for $\lambda \Delta \ll E$. The pattern is due to two close-to-each other frequencies due to level splitting and its nodes occur when the summand in Eq. (A2) vanishes. Combining the terms for $s = +1$ and $-1$ shows that this occurs for

$$\cos \left[ 4\pi (G_n \Delta + \eta \lambda M_\eta) / h^2 \omega_c^2 \right] \cos \left[ 2\pi \delta / h^2 \omega_c^2 \right] = 0,$$

where $\delta = 2(\eta \lambda G_n + \Delta M_\eta)$. The nodes of the second cosine term occur for

$$2\pi \delta / h^2 \omega_c^2 = (2m + 1)\pi / 2, \text{ integer.} \quad (A3)$$

\[\text{References}\]

[34] B. Radisavljevic and A. Kis, Nat. Mater. 12, 815 (2013).