Spin-valley relaxation and quantum transport regimes in two-dimensional transition metal dichalcogenides

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Quantum transport and spintronics regimes are studied in p- and n-doped atomic layers of hexagonal transition metal dichalcogenides (TMDCs), subject to the interplay between the valley structure and spin-orbit coupling. We find how spin relaxation of carriers depends on their areal density and show that it vanishes for holes near the band edge, leading to the density-independent spin diffusion length, and we develop a theory of weak localisation/antilocalisation, describing the crossovers between the orthogonal, double-unitary and symplectic regimes of quantum transport in TMDCs.

Interplay between spin-lattice relaxation and quantum transport leads to a crossover between orthogonal and symplectic classes of quantum disordered systems,1,2 manifested in measurements as weak localisation3 (WL) and weak anti-localisation4 (WAL) magnetoresistance (MR). This interplay acquires an additional twist in two-dimensional (2D) conductors with a multi-valley band structure.5–9 For electrons in the valleys centred, e.g., at the Brillouin zone corners $K_{\pm}$ of a hexagonal crystal, spin-orbit (SO) coupling leads to spin splitting which suppresses spin relaxation, whereas lattice defects and deformations mimic time-inversion symmetry breaking for the intravalley propagation of carriers (though the true time-inversion symmetry is preserved because it involves interchanging the valleys). Below, we study the interplay between SO coupling and multi-valley properties in the quantum transport in monolayers of semiconducting transition metal dichalcogenides10 (TMDCs), recently implemented in the field-effect transistors.11–13

The effective-mass Hamiltonian for electrons and holes in semiconducting monolayer TMDCs,14–19
\[
\mathcal{H} = \frac{|\mathbf{p}|^2}{2m^*} + \mu \left( p_z^2 - 3p_x p_y \right) \tau_z + \frac{\lambda}{2} \tau_z s_z + \delta \mathcal{H}(r), \quad (1a)
\]
takes into account trigonal warping, $\mu$ of their dispersion (inverted in $K_{\pm}$ valleys: $\tau_z$ is a valley space Pauli matrix) and SO splitting, $\lambda$ (large/small in the valence/conduction band16–18,20–23). The last part in Eq. (1a),
\[
\delta \mathcal{H}(r) = u_0(r) + u_z(r) \tau_z s_z + \left\{ \mathbf{p}, \mathbf{a}_y(r) \right\} \tau_z + \left\{ \mathbf{p}, \mathbf{a}_2(r) \right\} s_z + \mathbf{u}_{sf}(r) \cdot \mathbf{s} \tau_z + \sum_{\alpha=x,y} \left\{ \mathbf{p}, \mathbf{w}_\alpha(r) \right\} s_\alpha + \mathbf{u}_1(r) \cdot \mathbf{\tau} + \sum_{\alpha=x,y} \left\{ \mathbf{p}, \mathbf{w}_{z\alpha} \right\} \tau_\alpha s_z + \sum_{\alpha,\beta=x,y} \left\{ \mathbf{p}, \mathbf{w}_{\alpha\beta} \right\} \tau_\alpha s_\beta, \quad (1b)
\]
describes imperfections in the 2D crystal. Here, the first two terms stand for intravalley disorder, sensitive to the allowed spin state of the electron in each valley. The next two terms account for both lattice deformations (responsible for a valley/spin-dependent pseudo-magnetic field15,16) and the Berry curvature specific for the bands at the corners of the Brillouin zone. Their $\mathbf{k} \cdot \mathbf{p}$ theory derivation is described in Supplementary Material.24 The presence of the last two terms in the first line, with spin operators $(s_x, s_y) \equiv \mathbf{s}$, requires $z \rightarrow -z$ symmetry breaking, e.g., by flexural deformations of the 2D crystal.25

The second line in Eq. (1b), with valley Pauli matrices $(\tau_x, \tau_y) \equiv \mathbf{\tau}$, describes intervalley disorder due to atomic defects in the crystal. The first two terms account for intervalley scattering without spin-flip; the last term represents the only intervalley spin-flip perturbation permitted by the time-inversion symmetry in the lowest-order $\mathbf{k} \cdot \mathbf{p}$ expansion around $K_{\pm}$. The momentum dependence of such a term suggests that the intervalley spin-flip scattering is absent for the carriers at the band edge.26

Depending on the relative size of SO splitting and Fermi energy $\varepsilon_F$ of charge carriers, we identify three distinct spin/valley relaxation and quantum transport regimes: (A) $\lambda > \varepsilon_F$; (B) $\varepsilon_F \gtrsim \lambda$; and (C) $\varepsilon_F \gg \lambda$. Regime (A) covers lightly p-doped monolayers of MoX$_2$ and WX$_2$ (X=S, Se, Te) with holes fully spin-polarized in opposite directions in the opposite valleys.20–23 Regime (B) is specific for heavily p-doped MoS$_2$. Regime (C) is typical for n-doped MoX$_2$ monolayers.

In the transport regime (A), energy conservation and spin polarization of electrons in opposite directions ($\uparrow\downarrow$) in valleys $K_{\pm}$ do not leave any space for intravalley spin-flip and intervalley spin-conserving scatterings. This makes redundant the last two terms in the first line of
Eq. (1b) and first two terms in the second line. Then, spin-conserving intravalley disorder is characterized by the scattering rate,

$$\tau_0^{-1} = \frac{2\pi\nu(\Omega_0 + \Omega_z)}{\hbar}, \quad \nu = \frac{m^*}{2\pi\hbar^2},$$  

\[\tag{2a}\]

$$\langle u_\alpha (\mathbf{r}) u_\beta (\mathbf{r}') \rangle = \Omega_\alpha \delta_\alpha \delta_\beta (\mathbf{r} - \mathbf{r}'), \quad \alpha = (0, z).$$

The gauge-field-like part of $\delta H$ determines the rate,

$$\tau_g^{-1} = \frac{2\pi\nu\gamma_p^2(\Theta_\alpha + \Theta_{\alpha z})}{\hbar} \propto n_h,$$  

\[\tag{2b}\]

$$\langle a_\alpha^i (\mathbf{r}) a_\beta^j (\mathbf{r}') \rangle = \Theta_{\alpha z} \delta_\alpha \delta_\beta \delta_i \delta_j (\mathbf{r} - \mathbf{r}'), \quad \alpha = (g, g z),$$

which scale linearly with the hole density, $n_h$. The last term in Eq. (1b), with $(\alpha, \beta = x, y)$ is responsible for the only possible inter-valley scattering process in the regime $(A)$, accompanied by a spin-flip, which determines the hole spin relaxation rate,$^26$

$$\tau_{is}^{-1} = \frac{8\pi\nu\gamma_p^2 \Theta_{iz}}{\hbar} \propto n_h,$$  

\[\tag{2c}\]

$$\langle w^i_{\alpha z} (\mathbf{r}) w^{j'}_{\alpha' z'} (\mathbf{r}') \rangle = \Theta_{iz} \delta_{\alpha \alpha'} \delta_{\beta \beta'} \delta_i \delta_j (\mathbf{r} - \mathbf{r}'),$$

which also scales linearly with the hole density.

Rates (2) sum up into the momentum relaxation rate,

$$\tau^{-1} = \tau_0^{-1} + \tau_g^{-1} + \tau_{is}^{-1},$$

which determines the value of Drude conductivity and diffusion coefficient, $D = \frac{1}{\tau} \gamma_p^2$, and the result of Eq. (2c) suggests that in p-doped TMDCs spin-diffusion lengths

$$L_s^{(a)} = \sqrt{D\tau_{is}} \propto \sqrt{\hbar^3/2\Theta_{is} m_s^3},$$  

\[\tag{3}\]

are almost independent of the carrier density.

The analysis of quantum transport characteristics of TMDCs is based on the diagramatic perturbation theory calculations,$^{24}$ similar to those performed earlier in graphene.$^{7,8,27}$ Similarly to other multi-valley conductors without inter-valley scattering, lattice defects$^{5-8,27}$ and trigonal warping in the valley dispersion$^{7,8}$ suppress the low-temperature part of the quantum correction to conductivity caused by the interference of phase-coherent diffusive waves encircling the same random walk trajectory in the reversed directions. This is because inhomogeneous deformations generate a random pseudo-magnetic field with the opposite sign in $K_x$ valleys, whereas trigonal anisotropy splits hole’s wavenumber for the opposite Fermi velocity directions, hence inducing a random phase difference for the clockwise and anticlockwise propagating waves. Fig. 1 (top) (with the opposite sign in the opposite valleys). The cumulative effect of these two factors determines the decay rate $\tau_{-1}$ of valley-polarised Cooperons$^{7,8,27}$ in the set of triplet and singlet two-hole correlation functions corresponding to the Kramers doublet $(K_+; \uparrow; K_-, \downarrow)$,

$$\tau_{-1}^{-1} = 2 \tau_g^{-1} + \frac{15 \mu^2 \gamma_p^2 \tau}{4 \hbar^2} \propto n_h + C n_h^3.$$  

\[\tag{4}\]

Without inter-valley scattering, this places the system in the double-unitary symmetry class$^{2,28}$ with a WL peak saturated at a temperature such that $\tau_e(T) \sim \tau_s$, and this interplays with spin-flip inter-valley scattering which drives the system to the WAL regime. The resulting behaviour of magnetoresistance (MR), $\Delta \rho \equiv \rho(B) - \rho(0)$, is illustrated in Fig. 1, plotted from analytical expressions$^{24}$ for quantum correction to conductivity,

$$\delta g = \frac{e^2}{\pi \hbar} \left[ \ln \left( \frac{\tau_e^{-1}}{\tau_s^{-1}} \right) - \frac{1}{\tau_s^{-1} + \tau_{is}^{-1}} \right],$$  

\[\tag{5a}\]

$$-2 \ln \left( \frac{\tau_e^{-1}}{\tau_s^{-1} + \tau_{is}^{-1}} \right),$$

and its variation as a function of an out-of-plane magnetic field $B$ (MR),

$$\frac{\Delta \rho (B)}{\rho^2} = \frac{e^2}{\pi \hbar} \left[ \frac{F(B/B_c)}{F(B/B_c + 2B_{is})} - 2F(B/B_c + 2B_{is} + B_s) \right],$$  

\[\tag{5b}\]

$$F(z) \equiv \ln (z) + \psi \left( \frac{1}{2} + \frac{1}{z} \right), \quad B_s \equiv \frac{\hbar/e}{4D\tau_s}.$$  

Here, $\psi(z)$ is the digamma function. From the density dependence of relaxation rates $\tau_e^{-1}$ and $\tau_s^{-1}$, $B_{is}$ and $B_s$ should be finite at $n_h \to 0$, in contrast to $B_c \sim n_h^{-1}$, hence, we conclude that magnetoresistance displays a crossover from WL to WAL behavior upon increasing the hole density. Here, the form of MR would be dependent on the amount of atomic defects responsible for the spin-flip inter-valley scattering: for a virtually defectless crystal, MR would display a two-step crossover, from suppressed WL to WAL (this behaviour is exactly the reverse of the WAL-WL crossover in monolayer graphene$^7$). In regime $(B)$, where some minority spin carrier are present on the top of majority spin Fermi seas in both valleys,$^{29}$ both intra-valley spin-flip and spin-conserving inter-valley scattering are permitted for carriers at the Fermi level. Those are characterized by the inter-valley, $\tau^{-1}$, and spin-flip intravalley, $\tau_{sf}^{-1}$, scattering rates,

$$\tau_{-1/sf}^{-1} = \frac{4\pi\nu}{\hbar} [\gamma_{s sf} + p_F^2 \Xi_{e/sf}],$$  

\[\tag{6}\]

parameterised by the correlation functions,

$$\langle u_{s sf}^i (\mathbf{r}) u_{s sf}^j (\mathbf{r}') \rangle = \gamma_{s sf} \delta_{ij} \delta (\mathbf{r} - \mathbf{r}'),$$

$$\langle w_{s}^{i} (\mathbf{r}) w_{s}^{j'} (\mathbf{r}') \rangle = \Xi_{s sf} \delta_{ij} \delta (\mathbf{r} - \mathbf{r}'),$$

$$\langle u_{sf}^i (\mathbf{r}) u_{sf}^j (\mathbf{r}') \rangle = \gamma_{sf} \delta_{ij} \delta (\mathbf{r} - \mathbf{r}'),$$

$$\langle w_{sf}^{i} (\mathbf{r}) w_{sf}^{j'} (\mathbf{r}') \rangle = \Xi_{sf} \delta_{ij} \delta (\mathbf{r} - \mathbf{r}').$$

In the crystals with short-range (atomic) defects, these rates are independent of the carrier density, whereas in a
Firing up new scattering processes at the carrier density threshold \( n_c = n_h(\varepsilon_F = \lambda) \) reduces both the mean free path of carriers and their spin-diffusion length (now, limited by the intravalley spin-flip). The reduction of the mean free path by additional scattering channels leads to a step change in the resistivity and spin relaxation upon the increase of the density across the threshold,

\[
\rho(n_h) \approx \rho(n_c) + \frac{m}{e^2 n_h} (\tau_v^{-1} + \tau_s^{-1}) \theta(n_h - n_c),
\]

followed by a gradual decrease of resistivity, with a slope determined by the mobilities of majority- and minority-spin carriers.

An abrupt change also occurs in the behavior of the quantum correction to conductivity of defected TMDCs. In short, opening intervalley and spin-flip intravalley scattering channel, with finite rates already at \( n_h \geq n_c \), drives the system deeper into the symplectic symmetry class. This statement is based on the calculation where we take into account two groups of 4 Cooperons, corresponding to singlet and triplet combinations built separately of two Kramers doublets \( (K_+, \uparrow; K_-, \downarrow) \) and \( (K_+, \downarrow; K_-, \uparrow) \). Cross-doublet Cooperons are neglected due to the large SO splitting \( (\lambda \sim \varepsilon_F) \) in each valley. The resulting quantum correction to conductivity and magnetoresistance can be described as

\[
\delta g = \frac{e^2}{\pi \hbar} \ln \left( \frac{\tau^{-1}}{\tau^{-1} + 2\tau_{sf}^{-1}} \right),
\]

\[
\frac{\Delta \rho(B)}{\rho^2} = \frac{e^2}{\pi \hbar} F \left( \frac{B}{B_{c_1}} \right)
\]

\[
\frac{e^2}{96\pi \hbar} \left[ \frac{15B^2}{(B_v + B_{sf})^2} + \frac{B^2}{B_v} + \frac{B^2}{B_{sf}} \right],
\]

\[
\tau^{-1} = \frac{\lambda^2 \tau}{\hbar^2} + \frac{4\pi \nu \Omega}{h},
\]

where \( B_{c_1} = \hbar/(4e\tau_{\alpha}D) \). Note that in this regime intravalley spin-flip processes do not lead immediately to WAL. This happens because the 4\(^{th}\) term in the 1\(^{st}\) line of Eq. (1b) looks like intravalley magnetic disorder which suppresses WAL effect coming from intravalley spin-flip scattering, similarly to how trigonal warping and Berry curvature (accounted by \( \tau^{-1} \) in Eq. (5)) suppress WL in the transport regime (A).

In the transport regime (C), the crossover between WL and WAL behaviour of magnetoresistance takes the most complicated form, especially when \( \lambda / \hbar \), since one has to take into account all 16 Cooperons built using valley-spin quartet \( (K_+; \uparrow; K_-; \downarrow; K_+; \downarrow; K_-; \uparrow) \). Similarly to graphene, one can classify Cooperons as singlets and triplets in terms of both spin and valley indexes, with intrinsic SO splitting acting as an effective Zeeman coupling making the electron spin precess around the axis perpendicular to the crystal plane in the opposite direction for electrons in the opposite valleys. SO splitting and spin-dependent disorder determine the rate,

at which 8 of these 16 Cooperons decay, and SO splitting also couples them by precession (with the rate \( \lambda / \hbar \)), similarly to how real Zeeman coupling mixes singlet/triplet Cooperon modes in a simple disordered metal. The general formulae for \( \delta g \) and \( \Delta \rho(B) \) presented in the Supplementary Material lead to the generic behaviour of MR in a TMDC monolayer, which depends on its crystalline quality: (i) material where scattering is dominated by lattice defects and (ii) defect-free TMDC.

(i). In lattice-disordered TMDC, we take into account only such disorder that leads to finite scattering rates \( \tau_0^{-1} \) for electrons at the edge of conduction band. In this case, MR has a distinct WAL form, extrapolated
from the WAL behaviour in the regime (B),

\[
\frac{\Delta \rho (B)}{\rho^2} = \frac{e^2}{\pi \hbar} F \left( \frac{B}{B_\varphi} \right) - \frac{e^2}{96\pi \hbar} \left[ \frac{15B^2}{(B_\varphi + B_{sf})^2} + \frac{B^2}{B_\varphi^2} \right] + \sum_{\alpha = v, sf} \left[ \frac{32B_\alpha (B_\lambda + B_\varphi + B_{sf}) B^2}{(B_\lambda + (B_\lambda + B_{sf} + B_\varphi))^2 - B_\alpha^2} \right],
\]

where \( B_\alpha = \hbar / (4e\tau_\alpha D) \).

(ii). In a defect-free 2D crystal with scattering produced by remote charges in the substrate or smooth lattice deformations, electrons diffuse conserving their valley state \((\tau_{v, is} \to \infty)\). Then, spin-diffusion lengths,

\[
L_s (\alpha) = \frac{h p_F}{\lambda m_\alpha} \times \max \left[ \frac{\mathcal{L}}{\sqrt{2(\hbar D^2)}} \sqrt{\frac{2\pi \kappa}{K_\beta T}} \right] \propto \sqrt{n_c},
\]

is limited by either the characteristic height \( \sqrt{\langle h D^2 \rangle} \) of static wrinkles of lateral size \( \mathcal{L} \), or temperature in the case of flexural vibration modes, where \( \kappa \) is bending stiffness of the 2D crystal.\(^{25,32}\) As to the quantum transport, spurious time-inversion asymmetry for the intravalley electron propagation caused by SO coupling, Berry phase and pseudomagnetic field due to the deformations, suppress the interference correction to conductivity. As a result, MR in such high-quality 2D material would have a form of a suppressed WL effect,

\[
\Delta \rho (B) = -\frac{2e^2}{\pi \hbar} \left\{ \frac{2}{B_\varphi + B_{sf}} \right\} + \frac{1}{\sqrt{1 - \frac{\lambda^2 z f}{\hbar^2}}} \times \frac{B}{B_\varphi + B_\lambda + B_{sf}} \frac{B}{B_{sf} \sqrt{1 - \frac{\lambda^2 z f}{\hbar^2}}},
\]

where

\[
G (z_1, z_2) \equiv \left[ \pm \psi \left( \frac{1}{2} \pm \frac{1}{2} \frac{1 + z_1}{1 + z_2} \right) \mp \ln \left( \frac{1 + z_1}{1 + z_2} \right) \right].
\]

In conclusion, we analysed all possible regimes of elastic spin-lattice relaxation and quantum transport in monolayers of semiconducting TMDCs. We showed that in p-doped TMDCs spin relaxation has a rate linear in the carrier density for \( \varepsilon_F n_h < \lambda \), which leads to a density-independent spin-diffusion length, and that their MR displays a crossover from WL to WAL behaviour upon the increase in the concentration of holes. At the threshold density, \( n_c \) of the population of minority spin states in each valley, \( \varepsilon_F n_c = \lambda \), resistivity and spin relaxation rates of holes undergo a step-like increase, whereas the quantum correction to conductivity remains of a WAL type. For n-doped TMDCs, where the SO splitting is much smaller than in p-doped crystals, we find that the MR behavior is prescribed by the quality of the crystal: intervalley-scattering lattice defects lead to a distinctive WAL form of MR, whereas in structurally perfect crystals with diffusion produced by external Coulomb disorder and deformations of a 2D membrane, MR would show almost no WL or WAL effect.

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For spinful electrons at valleys $K_{\pm}$ time inversion is implemented by the anti-unitary operator $T = is_y\tau_3K$, where $K$ stands for complex conjugation. Therefore, $s_i\tau_j \rightarrow s_j\tau_i$ for $i, j = x, y$. As consequence, terms in the Hamiltonian that could simultaneously flip spin and scatter an electron in the same Wannier state between $K_{+}$ and $K_{-}$ are forbidden since their appearance would require breaking time-inversion symmetry. More generally, time-inversion symmetry forbids spin-flip scattering of electrons in the same Wannier state between any pair of opposite points in the Brillouin zone. To illustrate this, let us consider a free 2D electron scattering off a potential $V(r)$, for SO coupling is described by $\mathcal{H}_{SO} \propto [\nabla V(r) \times p] \cdot s$. For such a perturbation, spin-flip scattering has an amplitude $\langle k\alpha|\mathcal{H}_{SO}|k'\beta \rangle \propto i (k \times k') \cdot [s]_{\alpha\beta} V(k - k')$, which vanishes for the pairs of states related by the time-inversion transformation ($V(q)$ is the Fourier transform of $V(r)$). Hence, $|(-k - \alpha|\mathcal{H}_{SO}|k\beta)|^2 \equiv 0$. This general symmetry constraint on spin-flip scattering has been missed in the earlier studies, hence, leading to the exaggerated role of spin-flip relaxation in quantum transport in TMDCs.
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SUPPLEMENTARY INFORMATION

From two-bands $k \cdot p$ theory to single band model

We consider two-dimensional unit cells of transition metal dichalcogenides $MX_2$. The system consists on $X-M-X$ layers, where the $M$ atoms are ordered in a triangular lattice, each of them bonded to six $X$ atoms located in the top and bottom layers. A top view of the lattice is shown in Fig. 1. We discuss excitations around the two inequivalent corners $K_{\pm}$ of the Brillouin zone. Instead of dealing with degenerate states at inequivalent points one can triple the unit cell in such a way that the old $K_{\pm}$ points are now equivalent to the $\Gamma$ point of the folded Brillouin zone. From the point of view of the lattice symmetries, this means that the two elementary translations $(t_{a_1}, t_{a_2})$ are factorized out of the translation group and added to the point group $D_{3h}$, which becomes $D''_{3h} = D_{3h} + t_{a_1} \times D_{3h} + t_{a_2} \times D_{3h}$. The character table of this group is shown in Tab. 1. $D''_{3h}$ contains 24 new elements and 6 additional conjugacy classes, which leads to 6 new 2-dimensional irreducible representations (denoted by $E'_{1,2,3}$ and $E''_{1,2,3}$), the valley off-diagonal representations.

The symmetry properties of Bloch wave functions at the Brillouin zone corners are summarized in Tab. II, which gives the suitable combination of atomic orbitals and the associated irreducible representation (irreps) of $D''_{3h}$. In the case of $X$ atoms, both bonding (b) and anti-bonding (ab) combinations of orbitals from the bottom and top layers are considered. The second and third column contain the phases picked up by the wave function at each valley when a $2\pi/3$ rotation or a mirror reflection is performed.

In order to capture Berry curvature effects we consider the effective two-bands $k \cdot p$ theory describing lowest conduction and valence bands [1, 2]. Conduction and valence bands are dominated by $d$ orbitals from the $M$ atoms, in particular $(d_{x^2-y^2} \pm id_{xy})$ and $d_{3z^2-r^2}$ respectively. We consider the space of 4-vectors $\sim (E'_2, E'_1)$ whose entries represent the projection of the Bloch wave function at conduction and valence states at the Brillouin zone corners. In

Figure 1: Lattice, unit cell and Brillouin zone of $MX_2$ monolayers.
order to construct the effective \( \mathbf{k} \cdot \mathbf{p} \) Hamiltonian acting on this subspace we must consider the possible 16 hermitian operators, whose reduction in terms of irreducible representations of \( D_{3h}'' \) is inferred from:

\[
(E_2', E_1') \times (E_2', E_1') \sim 2A_1' + 2A_2' + 2E' + E_1' + E_2' + 2E_3'
\]

This space of electronic operators can be constructed from two commuting Pauli algebras \( \Sigma_i, \Lambda_i \). The definitions are summarized in Tab. III. The basis is \( \{ \psi_{c,v} \} \), where \( \psi_{c,v} \) represents the wave function of the conduction or valence state at \( K_\pm \) points, in such a way that time reversal operation (including spin) reads \( i \sigma_y \Lambda_y \Sigma_y K \). The operators \( \Lambda_i, \Sigma_i \) and all their combinations are \( 4 \times 4 \) matrices, which in this basis can be written as

\[
\Sigma_{x,y,z} = \tau_0 \otimes \sigma_{x,y,z},
\]

\[
\Lambda_{x,y,z} = \tau_{x,y,z} \otimes \sigma_0,
\]

where \( \tau_i \) and \( \sigma_i \) are Pauli matrices which act in valley and conduction/valence subspaces.

The Hamiltonian up to second order in \( \mathbf{p} \) reads

\[
\mathcal{H} = \gamma \mathbf{p} \cdot \Sigma + \frac{\Delta}{2} \Lambda_z \Sigma_z + \frac{\alpha + \beta}{2} I |\mathbf{p}|^2 + \frac{\alpha - \beta}{2} \Lambda_z \Sigma_z |\mathbf{p}|^2 + \kappa \left[ (p_x^2 - p_y^2) \Lambda_z \Sigma_x - 2p_x p_y \Lambda_z \Sigma_y \right],
\]

which corresponds to the Hamiltonian in Eqs. (2a)-(2d) of Ref. 2. Microscopically, the linear term in \( \mathbf{p} \) comes from the strong hybridization between conduction and valence band states away from \( K_\pm \) points, both dominated by orbitals localized in the metal transition atoms. Such hybridization is responsible for the non-zero Berry curvature of the bands [3],

\[
\Omega_{c,v}^\tau (\mathbf{p}) \approx \mp \frac{2 \gamma^2 \left[ \Delta - (\alpha - \beta) |\mathbf{p}|^2 \right]}{\left[ \Delta + (\alpha - \beta)^2 |\mathbf{p}|^2 \right] + 4 \gamma^2 |\mathbf{p}|^2}^{3/2}.
\]

The different orbital composition of conduction and valence bands introduce certain electron-hole asymmetry, and it is also responsible for the distinct strengths of the intrinsic spin-orbit splitting of the bands. We also include trigonal warping effects in the bands through the last term of the Hamiltonian. The isoenergy contours around \( K_\pm \) points deduced from this model are shown in Fig. 2. By projecting this Hamiltonian onto one of the bands we obtain the Hamiltonian in Eq. (1a) of the main text with

\[
m_{c,v}^\tau = \frac{1}{2 \left( \alpha + \beta + \frac{\Delta}{\Delta} \right)},
\]

\[
\mu = \frac{2 \gamma \kappa}{\Delta},
\]

The spin-orbit coupling terms can be incorporated by introducing another set of Pauli matrices for spin. With all these elements we can construct phenomenologically the disorder potentials.

| \( D_{3h}'' \) | \( E \) | \( 2T \) | \( \sigma_0 \) | \( 2T \sigma_0 \) | \( 2C_3 \) | \( 2TC_3 \) | \( 2TC_3^2 \) | \( 2S_3 \) | \( 2TS_3 \) | \( 9TC_3^2 \) | \( 9T \sigma_v \) |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| \( A_1' \) | 1 | 1 | -1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| \( A_2' \) | 1 | 1 | -1 | 1 | 1 | 1 | -1 | -1 | -1 | 1 | 1 |
| \( A_1'' \) | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 | 1 |
| \( A_2'' \) | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 | 1 | 1 |
| \( E' \) | 2 | 2 | -2 | -2 | -1 | -1 | -1 | 1 | 1 | 0 | 0 | 0 |
| \( E'' \) | 2 | -1 | 2 | -2 | -1 | -1 | -1 | 2 | -1 | 0 | 0 | 0 |
| \( E_3' \) | 2 | -1 | 2 | -1 | -1 | 2 | -1 | 2 | -1 | 0 | 0 | 0 |
| \( E_2' \) | 2 | -1 | 2 | -1 | -1 | 2 | -1 | 2 | -1 | 0 | 0 | 0 |
| \( E_3'' \) | 2 | -1 | 2 | -1 | -1 | 2 | -1 | 2 | -1 | 0 | 0 | 0 |

Table I: Character table of \( D_{3h}'' \).
Table II: Classification of the Bloch wave functions at \( K \) according to the irreps of \( D_{3h}^{\text{odd}} \). The sign \( \pm \) corresponds to combinations of orbitals at \( K \) points, and \( w = e^{\frac{2\pi}{3}} \).

Table III: Definitions of the electronic operators in the two bands effective model at \( K \) points.

Figure 2: Isoenergy contours around \( K \) points deduced from Eq. (1) for conduction (left) and valence (right) bands. We take \( \gamma = 3.82 \text{ eV} \cdot \text{Å}, \alpha = 1.72 \text{ eV} \cdot \text{Å}^2, \beta = -0.13 \text{ eV} \cdot \text{Å}^2, \) and \( \kappa = -1.02 \text{ eV} \cdot \text{Å}^2 \). [2] The spin-orbit splitting is neglected.
Intra-valley disorder enters as scalar, mass, and gauge potentials,
\[ \delta H (r) = U (r) I + M (r) \Lambda_z \Sigma_z + \Lambda_z \Sigma \cdot A (r). \]  
(4)

When we project these terms onto a single band we obtain
\[ \delta H_{c,v} = U_{c,v} (r) \pm \frac{\gamma}{\Delta} \{ p, A (r) \} \tau_z, \]  
(5)

with \( U_{c,v} (r) = U (r) \pm M (r) + \frac{\gamma}{\Delta} [\nabla \times A (r)]_z \). This corresponds to 1st and 3rd terms of Eq. (1b) of the main text with
\[ u_0 (r) = U (r) \pm M (r) + \frac{\gamma}{\Delta} [\nabla \times A (r)]_z, \]
\[ a_j (r) = \pm \frac{\gamma}{\Delta} A (r). \]  
(6)

Inter-valley disorder can be incorporated following the same procedure. Within the two-bands model we have in general
\[ V^{int} (r) = \sum_{n=x,y,z} \sum_{l=x,y} V_{nt} (r) \Sigma_n \Lambda_l. \]  
(7)

We can write down the spin-dependent disorder potentials in the same fashion, distinguishing even and odd terms under the reflection symmetry \( z \rightarrow -z \) defined by the layer of transition metal atoms,
\[ V^e (r) = s_z \left[ \sum_{n=x,y,z} U_n^e (r) \Sigma_n + \sum_{l=x,y,z} V_{nl}^e (r) \Lambda_l \right], \]
\[ V^o (r) = \sum_{j=x,y} s_j \left[ \sum_{n=x,y,z} U_j^o (r) \Sigma_n + \sum_{l=x,y,z} V_{jl}^o (r) \Lambda_l \right]. \]  
(8)

Even terms conserve z-spin, whereas odd terms induce spin-flip. After projecting these terms onto a single band we obtain for inter-valley disorder potentials, Eq. (7),
\[ V_{c,v}^{int} (r) = V_{c,v} (r) \cdot \tau, \]  
with
\[ V_{c,v}^x (r) = V_{yy} + V_{xx} - \frac{\gamma}{\Delta} (\partial_y V_{yx} \mp \partial_x V_{yy}), \]
\[ V_{c,v}^y (r) = -V_{yx} + V_{xx} - \frac{\gamma}{\Delta} (\partial_y V_{yx} \pm \partial_x V_{xx}). \]  
(9)

Similarly, for even and odd spin-dependent disorder potentials we arrive at
\[ V_{c,v}^e (r) = (V_{c,v}^e \pm U_{c,v}^e) \tau_z s_z + \frac{\gamma}{\Delta} s_z \left[ \pm \{ p, U_{c,v}^e \} + [\nabla \times U_{c,v}^e]_z \tau_z + (\pm \{ p_y, V_{c,v}^o \} - \{ p_x, V_{c,v}^o \}) \tau_x - (\{ p_x, V_{c,v}^o \} \pm \{ p_y, V_{c,v}^o \}) \tau_y \right], \]
\[ V_{c,v}^o (r) = \sum_{j=x,y} s_j \left[ (V_{c,v}^o \pm U_{c,v}^o) \tau_z + \frac{\gamma}{\Delta} \left[ \pm \{ p, U_{c,v}^o \} + [\nabla \times U_{c,v}^o]_z \tau_z + (\pm \{ p_y, V_{c,v}^o \} - \{ p_x, V_{c,v}^o \}) \tau_x - (\{ p_x, V_{c,v}^o \} \pm \{ p_y, V_{c,v}^o \}) \tau_y \right] \right]. \]  
(10)
From Eqs. (9)-(10) we identify the rest of parameters in Eq. (1b) of the main text:

\[
\begin{align*}
    u_z (r) &= V_z^e \pm \epsilon U_z^e + \frac{\gamma}{\Delta} \left( \nabla \times U^2 \right)_z, \\
    a_{yz} &= \frac{\gamma}{\Delta} U_y^e, \\
    u_{sz}^f &= V_{sz}^o \pm \epsilon U_{sz}^o + \frac{\gamma}{\Delta} \left( \nabla \times U^o \right)_z, \\
    w_{z\alpha} &= \frac{\gamma}{\Delta} U_{z\alpha}^o, \\
    u_{z f} &= V_{c,v}, \\
    w_{x z} &= \frac{\gamma}{\Delta} (-V_{x}^o, \pm V_{y}^o), \\
    w_{y z} &= \frac{\gamma}{\Delta} (-V_{y}^o, \mp V_{x}^o), \\
    w_{\alpha x} &= \frac{\gamma}{\Delta} (-V_{\alpha}^o, \pm V_{\alpha y}^o), \\
    w_{\alpha y} &= \frac{\gamma}{\Delta} (-V_{\alpha y}^o, \mp V_{\alpha x}^o).
\end{align*}
\]

Quantum transport regimes

**Regime (A)**

We consider first the situation when only one subband with opposite spin polarization at each valley is crossed by the Fermi level. We introduce a set of generators of U(2), \(\sigma_{0,x,y,z}\), with \(\sigma_0\) the identity and \(\sigma_{x,y,z}\) Pauli matrices
acting on the Hilbert space span by the doublet \((K_+, \uparrow), (K_-, \downarrow)\). With this choice time inversion is implemented by the anti-unitary operator \(T = i\sigma_y K\), where \(K\) is complex conjugation.

The semi-classical DC conductivity is just \(g_{ij} = 2e^2\nu D\delta_{ij}\), where \(\nu = m^* / (2\pi\hbar^2)\) is the density of states per fermionic species, and \(D = D^2 / (2\pi\hbar\tau)\) is the diffusion coefficient. The corrections due to quantum interference are expressed in terms of particle-particle correlation functions known as Cooperons, whose dynamics are governed by the Bethe-Salpeter equation, diagrammatically depicted in Fig. 3. First, we decompose the disorder correlators introduced in the main text (Fig. 3 a)) and Cooperons (Fig. 3 b)) in singlet \((l, s = 0)\) and triplet \((l, s = x, y, z)\) modes as

\[
C_{ss'} \equiv \frac{1}{2} [\sigma_y \sigma_{s''}]_{\alpha\beta} C_{\alpha\beta\alpha'\beta'} [\sigma_y \sigma_y]_{\beta\beta'},
\]

\[
W_{ss'} \equiv \frac{1}{2} [\sigma_y \sigma_{s''}]_{\alpha\beta} W_{\alpha\beta\alpha'\beta'} [\sigma_y \sigma_y]_{\beta\beta'},
\]

where the sum in \(\alpha, \beta, \alpha', \beta'\) indices is assumed. Then, the Bethe-Salpeter equations (Fig. 3 c)) can be written in a compact way as

\[
C_{s_1s_2}(Q, \omega) = W_{s_1s_2} + \sum_{s, s'} \sum_{l, l'} W_{s_1s'} C_{s_2s_2}(Q, \omega) \Pi_{ss'}(Q, \omega),
\]

where

\[
\Pi_{ss'}(Q, \omega) = \frac{1}{2} \int \frac{d^2p}{(2\pi\hbar)^2} \text{Tr} \left[ \sigma_y \sigma_y \left( \hat{G}^R(p, \hbar\omega + \varepsilon_F) \right)^T \sigma_y \sigma_y \hat{G}^A(Q - p, \varepsilon_F) \right].
\]

The retarded/advanced Green operators are just

\[
\hat{G}^{R,A}(p, \omega) = G^{R,A}(p, \omega) \sigma_0, \text{ with } G^{R,A}(p, \omega) = \frac{1}{\hbar \omega - \varepsilon_p \pm i\frac{\hbar}{2\tau}},
\]

then

\[
\Pi_{ss'}(Q, \omega) = \int \frac{d^2p}{(2\pi\hbar)^2} G^R(p, \hbar\omega + \varepsilon_F) G^A(Q - p, \varepsilon_F) \times \delta_{ss'} \approx \frac{2\pi\nu\tau}{\hbar} \left( 1 + i\tau\omega - \tau D |Q|^2 \right) \times \delta_{ss'},
\]

where the last result corresponds to the polarization operator in the so called diffusive approximation \((\tau D |Q|^2, \tau \omega \ll 1)\).

The weak localization correction reads in general

\[
\delta g_{ii} = \frac{e^2\hbar}{2\pi m^*} \sum_{s_1, s_2} \int \frac{d^2p}{(2\pi\hbar)^2} \text{Tr} \left[ \hat{G}^R(p, \varepsilon_F) \sigma_y \sigma_{s_1}^T \left( \hat{G}^A(-p, \varepsilon_F) \right)^T \sigma_y \sigma_{s_2} \hat{G}^A(p, \varepsilon_F) \right] \int \frac{d^2Q}{(2\pi)^2} C_{s_1s_2}(Q).
\]

Using the matrix structure of the Green operators, noting that

\[
\text{Tr} \left[ \sigma_y \sigma_{s_1}^T \sigma_y \sigma_{s_2} \right] = \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & -2 \end{bmatrix}_{s_1, s_2},
\]

we can write the weak localization correction to conductivity as the contribution of 4 Cooperon modes (1 singlet \(s = 0\) and 3 triplet \(s = x, y, z\), with \(\hat{C}_s \equiv 2ie\tau/\hbar C_{ss}\)),

\[
\delta g_{ii} = -\frac{2e^2D}{\pi\hbar} \int \frac{d^2Q}{(2\pi)^2} \left[ \hat{C}_x(Q) + \hat{C}_y(Q) + \hat{C}_z(Q) - \hat{C}_0(Q) \right],
\]

which are fundamental solutions of diffusion-relaxation kernels

\[
[-D\nabla^2 - i\omega + \Gamma_x] \hat{C}_s(r - r', \omega) = \delta(r - r').
\]
### Table IV: Relation between Cooperon relaxation gaps and scattering rates in the regime (A).

| Relaxation gaps | Relaxation rates |
|----------------|------------------|
| $\Gamma_0 = 0$ | $\frac{1}{\tau} = \frac{1}{\tau} + \frac{1}{\tau}$ |
| $\Gamma_x = \Gamma_y = \frac{1}{\tau^2} + \frac{1}{\tau}$ |
| $\Gamma_z = 2\frac{1}{\tau^2} + \frac{15\hbar^2 p^2}{4\ell^2}$ |

This is deduced from the Bethe-Salpeter, Eq. (13), assuming the low frequency and momentum expansion for the polarization operator, Eq. (16), and also that diagonal scattering dominate over the rest, $\tau / \tau_0 \sim 1$ [4].

In such diffusive approximation, the integration in Eq. (19) has a natural ultraviolet cut-off imposed by the inverse of the mean free path $\ell = \sqrt{D\tau}$, whereas the infrared cut-off is imposed by the decoherence length $\ell_\varphi = \sqrt{D\tau_\varphi}$. Then, the weak localization correction to conductivity reads just as

$$
\delta g_{ii} = -\frac{2e^2 D}{\pi \hbar} \int \frac{d^2Q}{(2\pi)^2} \left[ \frac{1}{DQ^2 + \Gamma_x} + \frac{1}{DQ^2 + \Gamma_y} + \frac{1}{DQ^2 + \Gamma_z} - \frac{1}{DQ^2 + \Gamma_0} \right].
$$

(21)

The relations between the relaxation gaps, $\Gamma_x$, and the rates associated to different scattering mechanisms introduced in the main text are summarized in Tab. IV. After performing the integration in $Q$ and assuming $\tau^{-1} \gg \Gamma_x$ we obtain Eq. (5a) of the main text.

In the presence of an out-of-plane magnetic field, $B$, $|Q|^2$ in Eq. (21) is quantized into $Q^2_n = (n + 1/2) \ell_B^{-2}$, with the magnetic length defined as $\ell_B = \sqrt{\hbar/4eB}$. For $\ell_B \gg \ell$ the diffusive approximation is still valid, and the weak localization correction to conductivity reads

$$
\delta g_{ii} (B) = -\frac{e^2 D \ell_B^{-2}}{\pi \hbar} \sum_s \sum_{n=0}^{n_{max}} \frac{c_s \ell_B^{-2} (n + \frac{1}{2}) + \Gamma_s + \tau^{-1}}{\ell_B^{-2} (n + \frac{1}{2}) + \Gamma_s + \tau^{-1}},
$$

(22)

with $c_{0,x,y,z} = -1, +1, +1, +1$. Thanks to the property of the digamma function,

$$
\psi (x + n_{max} + 1) - \psi (x) = \sum_{n=0}^{n_{max}} \frac{1}{x + n},
$$

(23)

we can perform the summation, leading to

$$
\delta g_{ii} (B) = -\frac{e^2 D \ell_B^{-2}}{\pi \hbar} \sum_s c_s \left[ \ln \left( \frac{h\tau^{-1}}{4eDB} \right) - \psi \left( \frac{1}{2} + \frac{B_x + B_z}{B} \right) \right],
$$

(24)

with $B_s = \frac{\hbar \Gamma_s}{4eD}$. Note that we have taken the limit $n_{max} \to \infty$,

$$
\psi \left( x + n_{max} + \frac{3}{2} \right) \to \ln (n_{max}) \approx \ln \left( \frac{h\tau^{-1}}{4eDB} \right).
$$

(25)

Substrating the zero field correction, the magnetoresistance defined as $\Delta \rho (B) = \rho (B) - \rho (0) = -\Delta g (B) / \rho^2$ can be written as Eq. (5b) of the main text.

### Regime (B)

In this case we must account for valley and spin separately. In terms of the Pauli algebras introduced in the main text we can write the weak localization correction to conductivity as

$$
\delta g_{ii} = \frac{e^2 \hbar^3}{2\pi m^2} \sum_{s_1, s_2} \int \frac{d^2p}{(2\pi)^2} T \text{Tr} \left[ \hat{G}^R (p, \varepsilon_F) \left( \tau_x \tau_{l_1}^T \right) \otimes \left( \sigma_y \sigma_{s_2}^T \right) \left( \hat{G}^A (-p, \varepsilon_F) \right)^T \right] \times \int \frac{d^2Q}{(2\pi)^2} C_{s_1 s_2} (Q),
$$

(26)
As before, we decompose the Cooperon and disorder correlators in singlet and triplet modes of valley (l) and spin (s):

\[ C^{ll'}_{ss'} = \frac{1}{4} \left[ s_y s_y \right]_{\alpha \beta} \left[ \tau_x \tau_l \right]^{ab} C^{\alpha \beta \alpha' \beta'} \left[ s_y s_y \right]_{\beta' \alpha'} \left[ \tau_l' \tau_x \right]^{b' a'} , \]

\[ W^{ll'}_{ss'} = \frac{1}{4} \left[ s_y s_y \right]_{\alpha \beta} \left[ \tau_x \tau_l \right]^{ab} W^{\alpha \beta \alpha' \beta'} \left[ s_y s_y \right]_{\beta' \alpha'} \left[ \tau_l' \tau_x \right]^{b' a'} . \] (28)

Then, the Bethe-Salpeter equations (Fig. 3 c)) can be written in a compact way as

\[ C^{l_1 l_2}_{s_1 s_2}(Q,\omega) = W^{l_1 l_2}_{s_1 s_2} + \sum_{s,s'} \sum_{l,l'} W^{l_1 l'_2}_{s s'} C^{l_2}_{s s'}(Q,\omega) \Pi^{l'_2}_{s s'}(Q,\omega) , \]

where

\[ \Pi^{l'_2}_{s s'}(Q,\omega) = \frac{1}{4} \left[ \frac{d^2 p}{(2\pi)^2} \right] Tr \left[ (\tau_l \tau_x) \otimes (s_y s_y) \left( \hat{G}^{ll'}(p,\hbar \omega + \varepsilon_F) \right)^T (\tau_l' \tau_x) \otimes (s_y s_y) \hat{G}^A(Q - p,\varepsilon_F) \right] . \] (30)

Hence, the weak localization correction to conductivity are given by 16 Cooperon modes \( \tilde{C}^{l}_{s} = \frac{2\pi e^2}{h} C^{ll'}_{ss'} \),

\[ \delta g_{ii} = -2e^2 D \int \frac{d^2 Q}{(2\pi)^2} \sum_{s,l} c^{l l'}_{s l} \tilde{C}^{l}_{s} (Q) , \]

with

\[ c^{0}_{0,0,0} = -1, +1, +1, +1 , \]

\[ c^{1}_{0,0,0} = +1, +1, +1, -1 . \] (31)

As in the previous case, we take the low momentum and frequency expansion of the polarization operator assuming the diffusive approximation, \( \tau D |Q|^2, \tau \omega \ll 1 \). We must distinguish then between the 8 gapless modes in the absence of \( D^g_{\nu} \) symmetry-breaking disorder potentials, \( \tilde{C}^{l}_{s}, \tilde{G}^{l}_{s}, \tilde{C}^{l}_{s}^{*}, \tilde{G}^{l}_{s}^{*} \), \( \tilde{C}^{l}_{s y x y} \), which are solutions of the diffusion-relaxation kernels,

\[ -D \nabla^2 - i\omega + \Gamma^{l}_{s} \tilde{C}^{l}_{s} (r - r',\omega) = \delta (r - r') , \] (32)

and the gapful modes, which in the present regime do not contribute due to the mismatch between the Fermi surfaces corresponding to different spin polarizations at each valley. The weak localization correction to conductivity in this regime reads

\[ \delta g = \frac{e^2}{\pi h} \left[ \ln \left( \frac{\tau^{-1}}{\tau^{-1}_F} \right) + \ln \left( \frac{\tau^{-1}}{\tau^{-1}_F + \Gamma^{l}_{z}} \right) - \ln \left( \frac{\tau^{-1}}{\tau^{-1}_F + \Gamma^{l}_{0}} \right) - 4 \ln \left( \frac{\tau^{-1}}{\tau^{-1}_F + \Gamma^{l}_{z}} \right) \right] , \] (33)
where the expressions for the relaxation gaps are summarized in Tab. V. This corresponds to the first line of Eq. (8) of the main text if we neglect $\tau_{\nu}^{-1}$ and $\tau_{s}^{-1}$ in the expression for $\Gamma_{\nu}^x$, $\Gamma_{\nu}^z$, and $\Gamma_{s}^0$, which are assumed to be smaller due to their dependence on carrier concentration. Similarly for the magnetoresistance we obtain in general

$$\frac{\Delta \rho (B)}{\rho^2} = \frac{e^2}{\pi h} \left[ F \left( \frac{B}{B_{cr}} \right) + F \left( \frac{B}{B_{cr} + B_z} \right) - F \left( \frac{B}{B_{cr} + B_0^z} \right) - F \left( \frac{B}{B_{cr} + B_0^z} \right) - 4F \left( \frac{B}{B_{cr} + B_z} \right) \right],$$

(34)

where we have introduced $B_{s}^l = \frac{\lambda \tau}{4\pi D}$. This expression reduces to the second line of Eq. (8) of the main text when we expand all the $F(z)$ functions to the lowest order, $F(z) \approx z^2/24$, excepting the first term.

\[Regime \ (C)\]

In the present regime $\lambda$ represents the lowest energy scale of the problem, in particular we assume $\lambda \tau / h \ll 1$. Hence, we must take into account the contribution of the gapful modes $\tilde{C}_{0,0}^{0,0}, \tilde{C}_{0,0}^{0,z}$ that we neglected previously, which satisfy the matrix equations (for the former)

$$\begin{pmatrix} D |Q|^2 - i \omega + \Gamma_{x}^{0}(z) & -\frac{\lambda}{\hbar} \\ \frac{\lambda}{\hbar} & D |Q|^2 - i \omega + \Gamma_{y}^{0}(z) \end{pmatrix} \begin{pmatrix} \tilde{C}_{x}^{0}(z) \\ \tilde{C}_{y}^{0}(z) \end{pmatrix} = i \begin{pmatrix} \tilde{C}_{x}^{0,0}(z) \\ \tilde{C}_{y}^{0,0}(z) \end{pmatrix}$$

(35)

and for $\tilde{C}_{0,0}^{0,z}$ we have the same swapping the spin and valley indices. The relations between the relaxation gaps and the elastic scattering rates are summarized in Tab. V. After matrix inversion we have (we omit the momentum and frequency dependences and write $\Pi = D |Q|^2 - i \omega$ for simplicity)

$$\tilde{C}_{x}^{0}(z) = \frac{\Pi + \Gamma_{y}^{0}(z)}{\left( \Pi + \Gamma_{x}^{0}(z) \right) \left( \Pi + \Gamma_{y}^{0}(z) \right) + \frac{\lambda^2}{\pi^2}},$$

$$\tilde{C}_{y}^{0}(z) = \frac{\Pi + \Gamma_{x}^{0}(z)}{\left( \Pi + \Gamma_{x}^{0}(z) \right) \left( \Pi + \Gamma_{y}^{0}(z) \right) + \frac{\lambda^2}{\pi^2}},$$

(36)

and the same for $\tilde{C}_{0,0}^{0,z}$ swapping the spin and valley indices.

The contribution of the gapful modes to the weak localization correction to conductivity is given by integrals of the form

$$\int \frac{d^2Q}{(2\pi)^2} \tilde{C}_{x}^{0}(Q) = \frac{1}{4\pi D} \left\{ \frac{\Gamma_0^{x} - \Gamma_0^{z}}{\sqrt{4\lambda^2/\hbar^2 - (\Gamma_0^{x} - \Gamma_0^{z})^2}} \arctan \left( \frac{2\tau_{\nu}^{-1} + \Gamma_0^{x} + \Gamma_0^{z}}{\sqrt{4\lambda^2/\hbar^2 - (\Gamma_0^{x} - \Gamma_0^{z})^2}} \right) - \arctan \left( \frac{2\tau_{\nu}^{-1} + \Gamma_0^{x} + \Gamma_0^{z}}{\sqrt{4\lambda^2/\hbar^2 - (\Gamma_0^{x} - \Gamma_0^{z})^2}} \right) \right\} + \frac{1}{2} \ln \left( \frac{(\tau_{\nu}^{-1} + \Gamma_0^{x}) (\tau_{\nu}^{-1} + \Gamma_0^{z}) + \lambda^2/\hbar^2}{(\tau_{\nu}^{-1} + \Gamma_0^{x}) (\tau_{\nu}^{-1} + \Gamma_0^{z}) + \lambda^2/\hbar^2} \right),$$

(37)

where we have employed the symmetry respect to the swapping of $x$ and $y$ indices. Note that the integral of $\tilde{C}_{x}^{0}$ yields the same result but with opposite sign in front of the arctan’s, but at the same time its contribution has opposite sign than $\tilde{C}_{x}^{0}$, therefore, only the arctan’s survive. Noting that

$$\Gamma_0^{x} - \Gamma_0^{z} = 2\tau_{\nu}^{-1},$$

$$\Gamma_0^{x} - \Gamma_0^{z} = 2\tau_{s}^{-1},$$

(38)

where the rates $\tau_{\nu}^{-1}$, $\tau_{s}^{-1}$ are introduced in the second column of Tab. V, we define

$$\gamma_{\nu} = \frac{\tau_{\nu}^{-1}}{\sqrt{\tau_{\nu}^{-2} - \frac{\lambda^2}{\pi^2}}},$$

$$\gamma_{s} = \frac{\tau_{s}^{-1}}{\sqrt{\tau_{s}^{-2} - \frac{\lambda^2}{\pi^2}}}.$$

(39)
in such a way that the weak localization correction to conductivity reads
\[
\delta g = \frac{e^2}{\pi h} \times \left\{ \ln \left( \frac{\tau^{-1}}{\tau_0^{-1} + \Gamma_0^2} \right) + \ln \left( \frac{\tau^{-1}}{\tau_0^{-1} + \Gamma_0^2} \right) - \ln \left( \frac{\tau^{-1}}{\tau_0^{-1} + \Gamma_0^2} \right) - 2 \ln \left( \frac{\tau^{-1}}{\tau_0^{-1} + \Gamma_0^2} \right) + 4 \ln \left( \frac{\tau^{-1}}{\tau_0^{-1} + \Gamma_0^2} \right) + \frac{2\gamma_v}{\pi} \ln \left( \frac{\tau_0^{-1}}{\tau_0^{-1} + \Gamma_0^2} \right) - \ln \left( \frac{\tau_0^{-1} + \Gamma_0^2}{\tau_0^{-1} + \Gamma_0^2} \right) - \ln \left( \frac{\tau_0^{-1} + \Gamma_0^2}{\tau_0^{-1} + \Gamma_0^2} \right) - \ln \left( \frac{\tau_0^{-1} + \Gamma_0^2}{\tau_0^{-1} + \Gamma_0^2} \right) + \frac{2\gamma_{sf}}{\pi} \ln \left( \frac{\tau_0^{-1}}{\tau_0^{-1} + \Gamma_0^2} \right) - \ln \left( \frac{\tau_0^{-1} + \Gamma_0^2}{\tau_0^{-1} + \Gamma_0^2} \right) - \ln \left( \frac{\tau_0^{-1} + \Gamma_0^2}{\tau_0^{-1} + \Gamma_0^2} \right) \right\}.
\]

This is the general expression for the weak localization correction in this regime. In order to compute the magnetoresistance we note first that
\[
\int \frac{d^2Q}{(2\pi)^2} C_0 (Q) \to 1 \quad \frac{1}{4\pi D} \sum_{n=0}^{n_{\text{max}}} \frac{n + \frac{1}{2} + \frac{B_0^2 + B_2^2 + 2B_0 B_2}{2B}}{n + \frac{1}{2} + \frac{B_0^2 + B_2^2 + 2B_0 B_2}{2B} + \frac{B_0^2}{\pi^2}} \approx
\]
\[
\approx \frac{1}{4\pi D} \left\{ \ln \left( \frac{n + \frac{1}{2} + \frac{B_0^2 + B_2^2 + 2B_0 B_2}{2B}}{n + \frac{1}{2} + \frac{B_0^2 + B_2^2 + 2B_0 B_2}{2B} + \frac{B_0^2}{\pi^2}} \right) - \frac{1}{2} \psi \left( \frac{1}{2} + \frac{B_0^2 + B_2^2 + 2B_0 B_2}{2B} + \frac{B_0 B_2}{\gamma_0 B} \right) - \frac{1}{2} \psi \left( \frac{1}{2} + \frac{B_0^2 + B_2^2 + 2B_0 B_2}{2B} - \frac{B_0 B_2}{\gamma_0 B} \right) + \frac{\gamma_v}{2} \left[ \psi \left( \frac{1}{2} + \frac{B_0^2 + B_2^2 + 2B_0 B_2}{2B} + \frac{B_0 B_2}{\gamma_0 B} \right) - \psi \left( \frac{1}{2} + \frac{B_0^2 + B_2^2 + 2B_0 B_2}{2B} - \frac{B_0 B_2}{\gamma_0 B} \right) \right] \right\}.
\]

where we have taken the limit $n_{\text{max}} \to \infty$. The sum for $C_0$ gives the same result with the opposite sign for the first 3 terms, therefore, for the same argument as before only the 2 terms in the $3^{rd}$ line survive. By applying the same argument for $C_{\delta z}$ we obtain the following general expression for the magnetoresistance:

\[
\frac{\Delta \rho (B)}{\rho^2} = \frac{e^2}{\pi h} \left[ F \left( \frac{B}{B_\phi} \right) + F \left( \frac{B}{B_\phi + B_2} \right) - F \left( \frac{B}{B_\phi} \right) - F \left( \frac{B}{B_\phi + B_2} \right) - 4F \left( \frac{B}{B_\phi + B_2} \right) + \frac{2\gamma_v G \left( \frac{B}{B_\phi + B_2} ; \frac{\gamma_0 B}{\gamma_0 B} \right)}{\gamma_0 B} \right] + 2\gamma_{sf} G \left( \frac{B}{B_\phi + B_2} ; \frac{\gamma_{sf} B}{\gamma_0 B} \right).
\]

From this expression is easy to deduce Eqs. (10) and (12) of the main text.

The former is valid in case (i), when only $\tau_{0,v,sf}^{-1}$ are taken different from 0. In this case, since only scattering rates finite at the band edge are taken into account we have $\tau_{v,sf}^{-1} = \tau_{0,v,sf}^{-1}$ and then

\[
\gamma_{v,sf} = \frac{1}{\sqrt{1 - \frac{\lambda^2 \tau_{v,sf}^{-1}}{h^2}}},
\]

As before, we expand $F(z)$ and $G(z)$ to the lowest order in $z$.

In case (ii) we only consider $\tau_{0,sf}^{-1} \neq 0$, and we assume $\tau_{v}^{-1}$ to be dominated by $\Xi_{sf}$ component, therefore $\tau_{v,sf}^{-1} \approx -\tau_{sf}^{-1}$; then we have

\[
\gamma_v = 0,
\]
\[
\gamma_{sf} = \frac{1}{\sqrt{1 - \frac{\lambda^2 \tau_{sf}^{-1}}{h^2}}},
\]

and Eq. (12) of the main text is straightforwardly deduced from Eq. (42).

[1] D. Xiao, G.-B. Liu, W. Feng, X. Xu, and W. Yao, Phys. Rev. Lett. 108, 196802 (2012).
[2] Andor Kormányos, Viktor Zólyomi, Neil D. Drummond, Péter Rakyta, Guido Burkard, and Vladimir I. Fal’ko, Phys. Rev. B 88, 045416 (2013).
[3] This is the Berry curvature deduced from the $k \cdot p$ Hamiltonian neglecting warping effects.
[4] Note that under the assumption $\tau/\tau_0 \sim 1$ the dressed Hikami box diagrams do not contribute. The velocity operators at each external vertex of these diagrams carry different momentum, and therefore they average to zero separately when evaluating the angular part of the integrals in momentum if the disorder correlator has no extra momentum dependence in order to compensate this, as it happens with diagonal disorder. This is not longer true for gauge disorder, however, given that $\tau^{-1} \propto n$, we can assume that $\tau_0^{-1} \gg \tau^{-1}$ and neglect the contribution from dressed Hikami boxes.