Weak localization in transition metal dichalcogenide monolayers and their heterostructures with graphene

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We calculate the interference correction to the conductivity of doped transition metal dichalcogenide monolayers (TMDC). Because of the interplay between valley structure and intrinsic spin-orbit coupling (SOC), these materials exhibit a rich weak localization (WL) behavior that is qualitatively different from conventional metals or similar two-dimensional materials such as graphene. Our results can also be used to describe graphene/TMDC heterostructures, where the SOC is induced in the graphene sheet. We discuss new parameter regimes that go beyond existing theories, and can be used to interpret recent experiments in order to assess the strength of SOC and disorder. Furthermore, we show that an in-plane Zeeman field can be used to distinguish the contributions of different kinds of SOC to the WL magnetoresistance.

I. INTRODUCTION

Transition metal dichalcogenide monolayers (TMDC) are a class of two-dimensional semiconductors of the form MX$_2$, where M is a transition metal and X is a chalcogen. Similarly to graphene, TMDCs have a hexagonal lattice structure, and a number of them (M=Mo, W; X=S, Se, Te) have minima/maxima of the conduction/valence band at the two corners (valleys) $\pm K$ of the Brillouin zone. Unlike graphene, however, TMDCs have two inequivalent lattice sites and no inversion symmetry, which allows for a large band gap in their spectrum.

Because of the heavy constituent atoms, these materials also host strong intrinsic spin-orbit coupling (SOC), which acts as an effective out-of-plane Zeeman field with opposite orientation in the two valleys. This valley-dependent SOC enables a variety of applications of TMDCs in optoelectronics and so-called valleytronics, as electrons from different valleys can be excited selectively with circularly polarized light. When sufficiently doped, several TMDCs become superconducting, with an important role, as it causes unconventional “Ising pairing” of the Cooper pairs and a great enhancement of the in-plane upper critical field.

The possibility of inducing SOC in a graphene sheet by coupling it to TMDCs in heterostructures has recently sparked scientific interest, as it can lead to phenomena such as edge states and the spin Hall effect. The induced SOC originates from hybridization of the transition metal and carbon orbitals. It has two contributions: Kane-Mele SOC, which can open a topological gap at the Dirac points $\pm K$, and so-called valley-Zeeman SOC, which breaks the inversion symmetry of graphene and causes spin-splitting in the band structure.

Transport measurements in highly doped TMDCs and graphene/TMDC heterostructures can give information about the amplitude and mechanism of SOC by studying the quantum correction to the conductance, due to weak localization (WL) and/or antilocalization (WAL) of electrons. W(A)L can be probed by applying a perpendicular magnetic field $B_{\perp}$, which suppresses the quantum correction by breaking time reversal symmetry. By measuring the resulting magnetoconductance as a function of $B_{\perp}$ and fitting it to theoretical models, one can extract parameters such as scattering and spin relaxation rates.

So far, the experiments have been interpreted using the so-called Hikami-Larkin-Nagaoka (HLN) formula (for TMDC experiments) or a similar formula provided by the McCann-Fal’ko (MF) theory in the regime of strong intervalley scattering (for graphene/TMDC experiments). HLN theory holds for two-dimensional single-band systems in the presence of SOC. If SOC is weak, constructive electron interference along time-reversed trajectories gives rise to a decrease in conductance (WL). Strong SOC leads to a phase shift due to the spin precession, which results in destructive interference and an increase in conductance (WAL). In Dirac materials, such as TMDCs and graphene, the physical picture becomes more complex. Here, the quantum correction is sensitive to the sublattice degree of freedom, or so-called lattice isospin. Due to the associated Berry phase, it can introduce phase shifts similarly to the spin physics. Furthermore, the multivalley nature of these materials and intervalley scattering also influence the quantum correction. MF theory takes these effects into account for the case of graphene, and gives a full description of WL and WAL with any disorder that satisfies time-reversal symmetry. In the presence of spin-orbit impurities and in the regime of strong intervalley scattering, such that the valley physics is suppressed, it reduces to the HLN formula.

However, the applicability of MF and HLN theories to TMDC and graphene/TMDC is limited, since they were both developed to describe spin-degenerate systems and do not capture spin-splitting caused by the presence of valley-Zeeman SOC. A theory for TMDCs that takes it into account was given by Ochoa et al. in the regime close to the bottom/top of the conduction/valence band, $|\mu| \approx E_g$, where $\mu$ is the chemical potential and $2E_g$ is the band-gap. This parameter regime, however, does not fully describe graphene/TMDC heterostructures and highly doped TMDCs, where $|\mu| \gg E_g$.

In this work, we present a general theory of the interfer-
ence correction for a massive Dirac material with valley-Zeeman SOC. Furthermore, we account for the effect of an in-plane Zeeman field. Our formula can be applied to TMDC and graphene/TMDC heterostructures. Namely, we generalize Ref. [28] to any chemical potential \( \mu \), and we show that several contributions to the interference-induced magnetoresistance are sensitive to the magnitude of doping, and are modified or suppressed as the doping increases. We discuss in detail the regime where intervalley scattering dominates over any spin-dependent scattering, which is the most commonly invoked regime when interpreting the experimental data. We find that the interplay between valley-Zeeman SOC \( \Delta V_Z \) and intervalley scattering, parameterized by the scattering time \( \tau_{iv} \), leads to new regimes of WL and WAL. In the limit \( \tau_{iv}^{-1} \gg \Delta V_Z \), MF still holds and HLN is valid if \( \tau_{iv}^{-1} \gg \tau_{o}^{-1} \), where \( \tau_{o} \) accounts for inelastic dephasing of electrons. However, we find new behavior not captured by these formulas if \( \Delta V_Z \gg \tau_{iv}^{-1} \). Since both TMDCs and graphene/TMDCs are expected to have substantial valley-Zeeman SOC, our newfound regimes are experimentally relevant and can be used to extract parameters from the interference-induced magnetoresistance in both systems.

This article is organized in the following way: In Sec. \[\text{I}\] we introduce the model Hamiltonian for disordered TMDC and graphene/TMDC heterostructures. In Sec. \[\text{II}\] we calculate the interference correction for these materials using the standard diagrammatic technique for disordered systems. We discuss our results in Sec. \[\text{IV}\].

\[\text{II. THE MODEL}\]

The low-energy Hamiltonian describing TMDC monolayers and graphene/TMDC heterostructures in the vicinity of the \( \pm K \) points, and in the presence of a parallel magnetic field is given by [22]

\[ H_0 = H_0 + H_{SOC} + H_W + H_{||}, \]

where

\[ H_0 = v(q_x \sigma_x \eta_z + q_y \sigma_y) + E_g \sigma_z, \]

\[ H_{SOC} = \Delta_{KM} \sigma_z s_z \eta_z + \Delta V_Z s_z \eta_z + \lambda (\sigma_x s_y \eta_z - \sigma_y s_x) + \zeta (q_x \sigma_x s_z + q_y \sigma_y s_z), \]

\[ H_W = \kappa (q_x^2 - q_y^2) \sigma_x - 2 \kappa q_x q_y \sigma_y \eta_z, \]

\[ H_{||} = \hbar s_x. \]

(1)

Here, we use units where \( \hbar = k_B = 1 \). The two Dirac cones are described by \( H_0 \), where \( \mathbf{q} = (q_x, q_y) = q(\cos \theta, \sin \theta) \) is a small momentum displacement measured from \( \pm K \), \( v \) is the velocity associated with the linearized kinetic dispersion, and \( E_g \) is the difference in on-site energy responsible for opening the band gap. Spin-orbit coupling is described by \( H_{SOC} \), where \( \Delta_{KM} \) and \( \Delta V_Z \) characterize Kane-Mele and valley-Zeeman SOC, respectively. Rashba SOC, which is related to a mirror symmetry breaking due to the substrate or external fields, is described by \( \lambda \). The spin-dependence of the velocity is accounted for by \( \zeta \). \( H_W \) describes the so-called trigonal warping. Finally, \( H_{||} \) is the in-plane Zeeman field, where the Zeeman energy \( h = \frac{1}{2} g \mu B_{||} \) is determined by the amplitude of the in-plane magnetic field and the \( g \)-factor, which is expected to take the value \( g \approx 2 \) in these materials. We introduce Pauli matrices \( \sigma_x, \sigma_y, \sigma_z \) and \( \eta_z, \eta_y \) acting in sublattice, spin, and valley space, respectively. The Hamiltonian \( H_0 \) contains all terms up to the first order in \( \mathbf{q} \) allowed by the symmetries of the system, as well as \( H_W \) and \( H_{||} \), which break rotational and time-reversal symmetry, respectively.

We assume that the Dirac Hamiltonian \( H_0 \) gives the dominant contribution to the energy of the system. This includes the assumption \( E_q \gg \Delta_{KM} \), which is the case in both TMDC and graphene/TMDC heterostructures according to first-principle calculations [23]. \( H_0 \) is diagonalized by a unitary transformation \( U_q = e^{-i \eta_y a_q^{\dagger} e^{i q_y^\eta y} e^{i q_y^\eta y} e^{i q_y^\eta y}} \), where \( \tan(2 \alpha_q) = q_y / q_x \) and \( \tan(2 \beta_q) = q_y / q_x \). It has a simple spectrum, \( \pm E_q = \pm \sqrt{q^2 v^2 + E^2_g} \). After projecting \( U_q H_0 U_q^{\dagger} \) onto the conduction band, we obtain the effective Hamiltonian

\[ H_q = \xi_q + \Delta_{so} s_z \eta_z + \frac{\sqrt{\mu q_F \hbar}}{\mu} (s_y \cos \theta - s_x \sin \theta) + \kappa \frac{vq_F^3}{\mu} \cos 3 \theta \eta_z + \hbar s_x. \]

(2)

Here, the energy is measured from the chemical potential, \( \xi_q = E_q - \mu \). Furthermore, we have introduced the Fermi momentum \( q_F = \sqrt{\mu^2 - E^2_g} / v \) and \( \Delta_{so} = \Delta_{KM} E_g / \mu + \Delta V_Z + \zeta v q_F^2 / \mu \). The chemical potential \( \mu \) is assumed to be sufficiently above the band gap \( E_g \), so that it is the dominant energy scale, \( |\mu - E_q| \gg \Delta_{so}, \lambda, h, \kappa q^2 \). A Hamiltonian of a similar form can be found in the valence band after the substitution \( \xi_q \rightarrow -\xi_q, \mu \rightarrow -\mu \). Although, in the remainder of the text, we will focus only on the conduction band for simplicity, our results also hold in the valence band as long as both spin-split band are occupied. This is readily achieved in graphene/TMDC heterostructures, while a very high doping is required in TMDCs, due to the large spin-splitting caused by the intrinsic SOC in the valence band [24].

The effect of impurities can be modeled by introducing a random potential disorder, \( H_{QQ}^{D_0} = U^0_{\mathbf{q}} \mathbf{q} \cdot \mathbf{q}^\eta + \sum_{i=x,y} \mathbf{q} \cdot \mathbf{q}^\eta \eta_i \), which has intra- and inter-valley components, and is diagonal in sublattice and spin space. Upon rotating \( U_q H_{QQ}^{D_0} U_q^{\dagger} \) and projecting to the conduction band, a variety of other scattering processes will be generated as combinations of the band structure and potential scattering parameters.

For simplicity, we will take all these processes into account phenomenologically by independent scattering potentials. To do so, we supplement \( H_{QQ}^{D_0} \) with all the other disorder terms allowed by the time-reversal symmetry [28], as was done previously in similar studies of weak localization [27,29]. The disorder Hamiltonian is
then given as \( H_{qq}^D = H_{qq}^{D0} + \delta H_{qq}^D \), where

\[
\delta H_{qq}^D = \sum_{i=x,y,z} U_i^q q \cdot \Sigma_i + \sum_{i=0,x,y,z} \sum_{j=x,y,z} A^q_i q \cdot \Sigma_j \delta q_i \eta_j \\
+ \sum_{j=x,y} \left[ \sum_{i=0,x,z} V_{ij}^q q \cdot \sigma_i \eta_j + \sum_{i=x,z} M_{ij}^q q \cdot \sigma_j \delta q_i \eta_j \right].
\]

(3)

Here \( \Sigma_{q,z,x} = \sigma_{q,z} \) and \( \Sigma_y = \sigma_y \eta_y \). We characterize the random disorder potentials by Gaussian correlators and assume that different kinds of disorder are uncorrelated:

\[
\langle U_i^q U_j^q \rangle = U_i^2 \delta_{ij} \delta_{q_i q_j}, \\
\langle X_{ij}^q X_{kl}^q \rangle = X_{ij}^2 \delta_{ij} \delta_{q_i q_j}.
\]

(4)

Here, the brackets \( \langle ... \rangle \) represent disorder averaging and \( X = A, V, M \). Furthermore, we use the abbreviation \( \bar{q} = -q \). The first line in Eq. (3) describes intravalley disorder. The second line describes interinterval disorder, which is due to short-range impurities, such as atomic defects. In both lines, the first and second terms account for spin-independent and spin-dependent contributions, respectively.

We provide estimates of the phenomenological parameters in Eq. (4) in the right-hand side of Table I. We do so by comparing the disorder terms generated by \( H_{qq}^D \), after rotation and projection onto the conduction band with the terms generated by \( H_{qq}^{D0} \) only, but taking into account corrections up to order \( 1/\mu \). In this way, we can relate the phenomenological disorder parameters with the main Hamiltonian (I) and the magnitude of the potential disorder.

We proceed by writing the rotated phenomenological disorder potential, \( U_q H_{qq}^D U_q^\dagger \), in the projected basis

\[
H_{qq}^D = \sum_{i=0,x,y,z} \left[ U_i^q q \cdot f_{i,\theta,\theta'} + \sum_{j=x,y,z} A^q_{ij} q \cdot g_{j,\theta,\theta'} \delta q_i \eta_j \right] \\
+ \sum_{j=x,y} \left[ \sum_{i=0,x,z} V_{ij}^q q \cdot g_{j,\theta,\theta'} \eta_j + \sum_{i=x,z} M_{ij}^q q \cdot g_{j,\theta,\theta'} \delta q_i \eta_j \right].
\]

(5)

where the functions \( f_{i,\theta,\theta'} \) and \( g_{i,\theta,\theta'} \) capture the anisotropy of the projected disorder potential, which is due to the momentum dependence of the unitary transformation \( U_q \). In particular, \( f_{i,\theta,\theta'} = 1 + e^{-i \eta_z (\theta - \theta')} + \frac{E}{\mu} (1 - e^{-i \eta_z (\theta - \theta')}) \) and \( f_{i,\theta,\theta'} = \frac{\nu q v}{\mu} (e^{-i \eta_{\theta,\theta'} + e^{i \eta_{\theta,\theta'}}) \eta_z \). Furthermore, \( f_{i,\theta,\theta'} = i f_{i,\theta,\theta'} \eta_z \), \( f_{i,\theta,\theta'} = f_{i,\theta',\theta}, \) \( g_{i,\theta,\theta'} = g_{i,\theta',\theta}, \) \( g_{i,\theta,\theta'} = f_{i,\theta,\theta'} \eta_z \), \( g_{i,\theta,\theta'} = f_{i,\theta,\theta'} \eta_z \), \( g_{i,\theta,\theta'} = f_{i,\theta,\theta'} \eta_z \), \( g_{i,\theta,\theta'} = f_{i,\theta,\theta'} \eta_z \). Here, we used the notation \( \bar{\theta} = \theta + \pi \). In simple metals, anisotropic disorder usually only leads to the renormalization of the diffusion constant and the transport time. It has more profound physical consequences in our system, as it captures the sublattice isospin physics and the effect of the Berry curvature.

In order to describe quantum transport in our system, we will employ standard diagrammatic technique for disordered systems. In particular, we introduce disorder-averaged, zero-temperature retarded (\( R \)) and advanced (\( A \)) Green’s functions as

\[
G_{qvw}^{RA} = \left( \omega - \mathcal{H}_q \mp i \frac{v}{2\tau} \right)^{-1}.
\]

(6)

Here, the self-energy \( \pm i/(2\tau) \) is calculated from the self-consistent Born approximation, \( \omega \) is the frequency, and the inverse scattering time \( \tau^{-1} \) is given by

\[
\tau^{-1} = \tau_0^{-1} + \tau_z^{-1} + \tau_{iv}^{-1} + \sum_{i=x,y,z} \sum_{l=x,y,z} \tau_{il}^{-1}.
\]

(7)

The individual contributions to Eq. (7) are defined in the left column of Table I, where we introduced the Fermi velocity \( v_F = v^2 q_F / \mu \) and the density of states per valley and per spin at the Fermi level \( \nu = \mu / (2\pi v_F) \). Furthermore, we will assume that the diagonal disorder rate \( \tau_0^{-1} \) is the dominant one, i.e., \( \tau^{-1} \approx \tau_0^{-1} \), and we will use the diffusive approximation \( \mid \mu - E_g \mid \gg \tau_0^{-1} \gg \Delta_{so}, \hbar, \lambda, q q^2 \).

The current operator in the projected basis is given by \( J_{xq} = v_F \cos \theta \). Due to the anisotropy of the disorder potential, the current vertex is renormalized, as illustrated in diagrammatic form in Fig. 1(a). Here, the bare vertex is dressed by a series of ladder diagrams, known as diffusons. The renormalized vertex is then given as

\[
\tilde{J}_{xq} = \frac{\tau_{tr}}{\tau_0} J_{xq} \quad \text{with} \quad \tau_{tr} = \left( 1 + \frac{v^2 q_F^2}{4 E_g^2 + v^2 q_F^2} \right) \tau_0.
\]

(8)

Here, we have introduced the transport time \( \tau_{tr} \), which takes the value \( \tau_0 \) at the bottom of the conduction band \( \mu \approx E_g \), where the spectrum is parabolic (similarly to conventional metals), and \( 2 \tau_0 \) deep in the conduction band \( \mu \geq E_g \), where the spectrum is linear (as in graphene). The Drude conductivity is then given as

\[
\sigma = \frac{e^2}{2\pi} \int \frac{d^2 p}{(2\pi)^2} Tr \left[ \tilde{J}_{xq} G_{qvw} \tilde{J}_{xq} G_{qvw} \right] \bigg|_{\omega=0} = 4e^2 v_D D.
\]

(9)

where \( D = \frac{1}{2} v_F^2 \tau_{tr} \) is the diffusion constant, and the factor \( 4 \) originates from spin and valley degeneracy. The corresponding diagram is shown in Fig. 1(b).

FIG. 1. (a) Vertex renormalization. (b) Drude conductivity diagram. Solid arrows represent Green’s functions, while the dashed lines represent disorder. The upper (lower) branch of the diagrams corresponds to retarded (advanced) Green’s functions.

III. INTERFERENCE CORRECTION

The interference correction to the Drude conductivity (4) can be expressed in terms of Cooperons, \( C_{\alpha \beta, \alpha' \beta'} \).
which represent disorder averages of two Green’s functions and correspond to maximally crossed diagrams. The Greek indices in the subscript (Latin indices in the superscript) correspond to the spin (valley) degree of freedom and take values ±1. The Cooperons are determined from a system of coupled Bethe-Salpeter equations, as shown in diagrammatic form in Fig. 2a). Namely,

\[
C_{ab, a'b'}(\theta, \theta'; \mathbf{Q}) = W_{ab, a'b'}(\theta, \theta') + \int_0^{2\pi} \frac{d\theta''}{2\pi} W_{ab, a'b'}(\theta, \theta'') \Pi_{\alpha_1\beta_1, \alpha_2\beta_2}(\theta'', \theta') C_{\alpha_1\beta_1 \alpha_2 \beta_2, a'b'}(\theta'', \theta'; \mathbf{Q}). \tag{10}
\]

Here, summation over repeated indices is assumed, and we have introduced the disorder correlator \(W\) and the polarization operator \(\Pi\) as

\[
W_{ab, a'b'}(\theta, \theta') = \langle[H^D_{\mathbf{Q} \mathbf{Q}''}]_{ab} a_{a'}(\mathbf{Q}) b'_{a''}(\mathbf{Q}'') \rangle \quad \text{and} \quad \Pi_{\alpha_1\beta_1, \alpha_2\beta_2}(\theta'; \mathbf{Q}) = \nu \int d\xi_q [G^R_{\mathbf{Q} + \omega' \alpha_1 \alpha_2} G^A_{\mathbf{Q} - \omega' \beta_1 \beta_2}]. \tag{11}
\]

Note that the Green’s functions are diagonal in valley space, so the polarization operator only depends on two valley indices. The weak localization correction \(\delta\sigma\) can now be expressed in terms of Cooperons as

\[
\delta\sigma = \frac{e^2}{2\pi} \int d^2\mathbf{Q} \left[ \int_0^{2\pi} \frac{d\theta d\theta'}{2\pi} 4\pi \nu \tau_0^3 \left[ 2\pi\delta(\theta - \theta') - 2\pi\nu \tau_0 W^{ab, ab}_{\alpha\beta, \alpha\beta}(\theta, \theta') \right] \tilde{J}_{x\mathbf{Q}} \tilde{J}_{x\mathbf{Q}} C_{\alpha\beta, \alpha\beta}(\theta, \theta'; \mathbf{Q}) \right]. \tag{12}
\]

Here, the first contribution in the square bracket comes from the bare Hikami box \([\text{shown in Fig. 2b}]\), while the second one comes from two Hikami boxes dressed by an intravalley impurity line [shown in Fig. 2c]).

In order to resolve the angular structure of the Cooperons, we proceed by solving Eq. (10) in the presence of the dominant diagonal scattering, \(\tau_0^{-1}\), only. The other types of scattering will not affect this structure, but only introduce additional Cooperon gaps. We proceed with this calculation in the same spirit as in Ref. [33]. First, we expand the Cooperons and the disorder correlator in harmonics,

\[
C_{ab, a'b'}(\theta, \theta'; \mathbf{Q}) = \sum_{n=\pm \infty} C_{ab, a'b'}^n(\mathbf{Q}) e^{-in(\theta - \theta')},
\]

\[
W^{ab, a'b'}_{\alpha\beta, \alpha\beta}(\theta, \theta') = \sum_{n=\pm \infty} W_{ab, a'b'}^n e^{-in(\theta - \theta')}, \tag{13}
\]

Since there is no spin-dependent scattering, the Cooperons do not have spin structure, so we can omit the spin indices. Furthermore, \(a = a'\) and \(b = b'\) in the absence

| Scattering rate | Estimates |
|-----------------|-----------|
| \(\tau_0^{-1} = \pi \nu U_0^2 (1 + \frac{E_z^2}{\mu^2})\) | / |
| \(\tau_{iv}^{-1} = \pi \nu (U_{i}^2 + U_{e}^2)\) | / |
| \(\tau_{i}^{-1} = \pi \nu (A_{i}^2 + A_{e}^2)\) | / |
| \(\tau_{zo}^{-1} = \pi \nu (A_{z_i}^2 + A_{z_e}^2)\) | / |
| \(\tau_{zo}^{-1} = \pi \nu (A_{z_i}^2 + A_{z_e}^2)\) | / |
| \(\tau_{zo}^{-1} = \pi \nu (A_{z_i}^2 + A_{z_e}^2)\) | / |

\[\text{TABLE I. Left: Dominant diagonal scattering rate, } \tau_0^{-1}, \text{ and other } 11 \text{ independent scattering rates originating from the disorder Hamiltonian. The notation for the scattering rates was taken and adapted from Ref. [27]. The index } z \text{ indicates that the related disorder potential is sublattice dependent. } \tau_{iv}^{-1} \text{ and } \tau_{zo}^{-1} \text{ indicate coupling to the valley matrices } \eta_z, \text{ and } \eta_z, \text{ respectively. Indices } e \text{ and } o \text{ indicate coupling to the spin matrices } s_z, \text{ and } s_{z,y}, \text{ respectively. Spin-independent disorder is represented by the rates } \tau_{iv}^{-1}, \tau_{zo}^{-1} \text{ and } \tau_{iv}^{-1} \text{, which describe diagonal, intervally, and sublattice-dependent intravalley disorder. Spin-dependent disorder is represented by the rates } \tau_{i}^{-1} \text{ and } \tau_{zo}^{-1} \text{, which describes intra- } (i = z, x, v), \text{ and intervalley } (i = v, x) \text{, and spin-preserving } (j = e) \text{ or spin-flipping } (j = o) \text{ disorder. Right: Estimates of the parameters of the phenomenological disorder potential, making use of the procedure introduced in Sec. I}].\]
of intervalley scattering. The only Cooperon that enters the interference correction (12) is the intravalley one, $C_{aa,aa}^a(\theta, \theta')$. From Eqs. (10) and (13), we get a system of coupled equations for its harmonics, whose solution yields

$$C_{aa,aa}^a(\theta, \theta'; Q) = C_{aa,aa}^0(\theta) + C_{aa,aa}^a(Q)e^{-i\theta(\theta - \theta')}$$

with

$$C_{aa,aa}^0(\theta) = \frac{1}{2\pi n v_F D} |D(\theta)|^2 - i\omega + \tau_\phi + \Gamma_i \equiv \frac{1}{\tau_0}$$

(14)

Here, $a = \pm 1$, $\Gamma_0 = \frac{\mu E_g}{\tau_0 (\mu + E_g)^2}$ and $\Gamma_a = \frac{2E_g^2}{\rho_0 (\mu + E_g)}$ are the relevant Cooperon gaps, and $D_0 = \frac{8\pi^2 v_F^2}{\rho_0 (3 + E_g^2/\rho_0^2)}$ and $D_a = v_F^2 \frac{(E_g^2 + \mu^2)^2}{\rho_0 (3 + E_g^2/\rho_0^2)}$ are diffusion constants. Furthermore, we introduced the inelastic dephasing rate, $\tau_\phi^{-1}$.

We see that, in general, both $C_0$ and $C_a$ will have a large gap of the order $\tau_0^{-1}$ and, thus, will be suppressed in the diffusive limit, except in two special cases. Firstly, $\Gamma_0$ vanishes at $\mu = E_g$. Close to the band bottom, for $\mu / E_g \sim 2\sqrt{\tau_0 / \tau_\phi}$, one finds $\Gamma_0 \lesssim \tau_\phi^{-1}$. Thus, in this regime, the Cooperon $C_0$ is not suppressed. Secondly, $\Gamma_a$ vanishes for $\mu \to \infty$. Thus, deep in the band, at $\mu / E_g \gtrsim \sqrt{2\tau_0 / \tau_\phi}$, one finds $\Gamma_a \lesssim \tau_\phi^{-1}$, and the Cooperon $C_a$ is not suppressed. Higher-order harmonics, although non-zero, will always have a non-vanishing gap of the order $\tau_0^{-1}$ and will be neglected. We can therefore write

$$C_{aa,aa}^a(\theta, \theta'; Q) = \frac{\Xi}{2\pi n v_F D} |D(\theta)|^2 - i\omega + \tau_\phi^{-1} + \Gamma_\Xi,$$

where

$$\Xi = \begin{cases} 
1, & \frac{\mu}{E_g} - 1 \lesssim \sqrt{\frac{\tau_\phi}{\tau_0}}, \\
0, & \sqrt{\frac{\tau_\phi}{\tau_0}} \ll \frac{\mu}{E_g} - 1 \ll \sqrt{\frac{\tau_\phi}{\tau_0}}, \\
-1, & \frac{\mu}{E_g} \gtrsim \sqrt{\frac{\tau_\phi}{\tau_0}},
\end{cases}$$

(15)

and $\Gamma_1 = \frac{\tau_0^{-1} |v q_F/(2\mu)|^4}{2\tau_0^{-1} (E_g/\mu)^2}$. Note that the diffusion constants $D_0$ and $D_a$ reduce to $D$, introduced in Eq. (2), in the relevant limits.

Upon inserting Eq. (15) into Eq. (12), we obtain the quantum correction for massive Dirac fermion systems in the presence of smooth disorder, consistent with Ref. [33]. Its behavior is governed by the doping-dependent coefficient $\Xi$: for a high Dirac mass ($\Xi = 1$) we get WL, whereas in the massless system ($\Xi = -1$), we get WAL. The quantum correction vanishes in the intermediate mass regime. This can be reinterpreted in terms of the Berry phase of a massive Dirac material given as $\varphi_B = \pi (1 - E_g/\mu)$, which introduces no phase shift to the electron interference in the large mass limit (leading to WL), and a shift of $\pi$ for massless systems (leading to WAL).

Next, we will find the intervalley Cooperon $C_{s,s}^{s,s}(\theta, \theta'; Q)$. Note that it does not enter the quantum correction (12), but it is useful to resolve its angular structure for later use. We find that the only harmonic that is not gapped is $C_0$, and we can write

$$C_{s,s}^{s,s}(\theta, \theta'; Q) = C_{s,s}^0(\theta) + C_{s,s}^s(Q)e^{-i\theta(\theta - \theta')}$$

(16)

Finally, we proceed to solve the Cooperon equation in the presence of all disorder terms. Additional intervalley Cooperons of the form $C_{s,s}^{s,s}$ can now exist. Since they are coupled to $C_{s,s}^{s,s}$ via intervalley scattering, which does not introduce additional angular dependence, they will also be angularly-independent. Using Eqs. (15) and (16), we can write for all Cooperons

$$C_{ab,a'b'}^{s,s}(\Xi; Q) = [C_{0}^{s,s}(\theta)\delta_{\Xi,1} + C_{a}^{s,s}(Q)\delta_{\Xi,-1}] \times \delta_{aa'}\delta_{bb'} + C_{0}^{s,s}(Q)\delta_{aa'}\delta_{bb'}$$

$$W_{ab,a'b'}^{s,s}(\Xi; Q) = [W_{0}^{s,s}(\Xi)\delta_{\Xi,1} + W_{a}^{s,s}(\Xi)\delta_{\Xi,-1}] \times \delta_{aa'}\delta_{bb'}$$

(19)

Then, Eq. (10) can be written in a simpler, angularly-independent form,

$$C_{ab,a'b'}^{s,s}(\Xi; Q) = W_{ab,a'b'}^{s,s}(\Xi)$$

$$+ W_{aa,bb}(\Xi)\Pi_{aa',\beta_1}(\Xi)C_{a'b',\beta_1}(\Xi)$$

(19)

Next, we employ a transformation to the singlet-triplet basis in spin and valley space,

$$A_{s'a'}^{l,l'} = \frac{1}{4}[s_y s_x \alpha \beta [\eta_\alpha \eta_\beta]^{-1} \sigma_{aa'}^{b,b'}[s_y s_x \beta \alpha'] [\eta_\alpha' \eta_\beta']^{-1} \sigma_{aa'}^{b,b'}]$$

(19)

where indices $s, s' = x, y, z$ and $l, l' = x, y, z$ correspond to spin- and valley-singlet Cooperon modes, respectively, while $s, s' = x, y, z$ and $l, l' = x, y, z$ correspond to spin- and valley-triplet modes. Here, the operator $A$ can stand for a Cooperon ($C$), disorder-correlator ($W$), or a polarization operator ($\Pi$). The disorder correlator is diagonal.
in the singlet-triplet space, $W_{s's'}^{\text{cl}}(\Xi) = W_s^{\text{cl}}(\Xi) \delta_{ss'} \delta_{ll'}$, and the Cooperon equation Eq. (18) after the transformation becomes

$$C_{s's'}^{\text{cl}}(\Xi; Q) = W_s^{\text{cl}}(\Xi) \delta_{ss'} \delta_{ll'} + W_s^{\text{cl}}(\Xi) \Pi_{s'l}(Q) C_{s'l'}^{\text{cl}}(\Xi; Q). \tag{20}$$

The quantum correction involves only the diagonal Cooperons $C^{\text{cl}}_{ss} = C_s^{\text{cl}}$. Note that triplets modes $C^s$ and $C^y$ are related to the intravalley Cooperons, while the valley-singlet $C^0$ and triplet $C^z$ are related to intervalley ones. We obtain

$$\delta \sigma = -\frac{e^2 D}{\pi} \frac{1}{2\pi \nu \tau_0^2} \int \frac{d^2 Q}{(2\pi)^2} \times \sum_s c_s \left[ \sum_{l=0,z} c_l C_s^{\text{cl}}(\Xi; Q) + \Xi \sum_{l=x,y} c_l C_s^{\text{cl}}(\Xi; Q) \right], \tag{21}$$

where $c_s = -1,1,1,1$ and $c_l = 1,1,-1$ for $s,l = 0,x,y,z$. Eq. (21) generalizes similar expressions from Refs. [27] and [28] which are valid at $\Xi = -1$ and $\Xi = 1$, respectively.

The diagonal Cooperon modes $C_s^{\text{cl}}$, necessary to compute $\delta \sigma$, are determined by solving Eq. (20). Due to the spin-splitting described by $\Delta_{ss}$ and $\hbar$, the polarization operator $\Pi_{s's'}^{\text{cl}}(Q)$ is not diagonal in the singlet-triplet space. As a consequence, some Cooperon modes are coupled, as will be discussed in the further text.

First, we solve the Cooperons that are not coupled by the valley-Zeeman SOC or the in-plane field, with the indices $(s,l) = (y,x),(y,y),(z,0),(z,z)$. They are given by

$$C_s^{\text{cl}} = \frac{1}{2\pi \nu \tau_0} \frac{1}{P_s^{(0)}}. \tag{22}$$

Here, we have introduced $P_s^{(0)} = D|Q|^2 - i\omega + \tau_0^{-1} + \Gamma_s^\prime$. The Cooperon gaps $\Gamma_s^\prime$ are specified in Table I. Because the intravalley Cooperons have different angular dependence in the two extreme limits of Eq. (15), their gaps $\Gamma_x^\prime$ and $\Gamma_y^\prime$ will also depend on the relevant limit (right-hand side of Table I). Intervalley Cooperons, on the other hand, do not depend on angles and chemical potential and have the same gaps for any $\mu$ (left-hand side of Table I).

The Cooperon gaps contain the scattering rates originating from the phenomenological disorder potential $\delta$. Their estimates, listed in Table I, are inversely proportional to the scattering times $\tau_0$ and $\tau_{iv}$. These rates are therefore induced and reinforced by disorder, and behave similarly to the Eliot-Yaffet spin relaxation mechanism [34,35]. Additionally, scattering rates that are proportional to the potential scattering time $\tau_0$ also enter the gaps:

$$\tau_{BB}^{-1} = 2 \left( \frac{\lambda v q_{eF}}{\mu} \right)^2 \tau_{tr}, \quad \tau_{VV}^{-1} = 2 \Delta_{ss}^2 \tau_0,$$

and

$$\tau_{WW}^{-1} = 2 \left( \frac{\kappa v q_{eF}}{\mu} \right)^2 \tau_0. \tag{23}$$

They are related with Rashba SOC, valley-Zeeman SOC, and trigonal warping, respectively. These rates appear since electrons, due to the details of the band structure, acquire an additional phase upon propagation in-between two scattering events. Disorder suppresses this effect, similarly to the Dyakonov-Pereira spin relaxation mechanism.

Next, we address the coupled Cooperon modes. The effect of the in-plane Zeeman field $\hbar$ applied along the $x$-direction is such that it couples the spin-singlet $C_0$ and spin-triplet $C_z$, as discussed for conventional metals [37]. Intrinsic SOC behaves similarly to an effective Zeeman field in $z$-direction, but acts differently from the true Zeeman field as it does not break the time-reversal symmetry, and therefore does not affect the spin- and valley-singlet $C_0^0$, which is protected by this symmetry. It couples the Cooperons $C_x^{(0)}$ with $C_y^{(0)}$, and $C_0^{(0)}$ with $C_y^{(0)}$, as discussed in Ref. [28]. The equations for all the coupled Cooperon modes can be compactly written in a matrix form

$$\begin{bmatrix} P_0^{(y)} & \mp 2\Delta_{ss} - 2i\hbar \\ \pm 2\Delta_{ss} & P_0^{(x)} & 0 \\ -2i\hbar & 0 & P_0^{(y)} \end{bmatrix} \begin{bmatrix} C_{zz}(yy) & C_{xy}(zy) & C_{yz}(yz) \\ C_{zz}(xz) & C_{xy}(yz) & C_{yz}(zx) \\ C_{zz}(zy) & C_{xy}(zy) & C_{yz}(xz) \end{bmatrix} = \frac{1}{2\pi \nu \tau_0^2} \begin{bmatrix} \tau_0^{(0)} - 2\Delta_{ss} - 2i\hbar \\ 2\Delta_{ss} & P_0^{(y)} & 0 \\ -2i\hbar & 0 & P_0^{(y)} \end{bmatrix} \begin{bmatrix} C_{00}^{(z)} & C_{0z}^{(z)} & C_{0z}^{(z)} \\ C_{x0}^{(z)} & C_{xy}^{(z)} & C_{xz}^{(z)} \\ C_{z0}^{(z)} & C_{zy}^{(z)} & C_{zz}^{(z)} \end{bmatrix}. \tag{24}$$

Eq. (24) summarizes 4 matrix equations, each involving 3 coupled modes. Since the Green’s functions are diagonal in valley space, the equations for intra- and intervalley Cooperons are decoupled. This can be seen in Eq. (24), where the left-hand (right-hand) side describes matrix equations for intravalley (intervalley) Cooperon modes.

Finally, after inverting the matrices in Eq. (24), we obtain all Cooperon modes. Combining them with Eq. (21), and introducing the conductance quantum $\sigma_0 = e^2/(2\pi^2\hbar)$, we arrive at the expression for the interference correction
Relaxation gaps for $C^0$ and $C^ς$

| Gap $\Gamma_0$ | Gap $\Gamma^\parallel$ | Gap $\Gamma^\perp$ |
|----------------|------------------------|-------------------|
| $\Gamma_0 = 0$ | $\Gamma^\parallel = 2\tau_{v,e} - 2\tau_{v,o} + 2\tau_{\bar{v},e} + 2\tau_{\bar{v},o} + \tau_{\bar{v},e} + \tau_{\bar{v},o}$ |
| $\Gamma^\parallel = 0$ | $\Gamma^\parallel = 2\tau_{v,e} - 2\tau_{v,o} + 2\tau_{\bar{v},e} + 2\tau_{\bar{v},o} + \tau_{\bar{v},e} + \tau_{\bar{v},o}$ |
| $\Gamma^\perp = 0$ | $\Gamma^\perp = 2\tau_{v,e} - 2\tau_{v,o} + 2\tau_{\bar{v},e} + 2\tau_{\bar{v},o} + \tau_{\bar{v},e} + \tau_{\bar{v},o}$ |

Relaxation gaps for $C^x$ and $C^ς$ at $\Xi = -1$.

| Gap $\Gamma_x$ | Gap $\Gamma^\parallel$ | Gap $\Gamma^\perp$ |
|----------------|------------------------|-------------------|
| $\Gamma_x = 0$ | $\Gamma^\parallel = 2\tau_{v,e} - 2\tau_{v,o} + 2\tau_{\bar{v},e} + 2\tau_{\bar{v},o} + \tau_{\bar{v},e} + \tau_{\bar{v},o}$ |
| $\Gamma^\parallel = 0$ | $\Gamma^\parallel = 2\tau_{v,e} - 2\tau_{v,o} + 2\tau_{\bar{v},e} + 2\tau_{\bar{v},o} + \tau_{\bar{v},e} + \tau_{\bar{v},o}$ |
| $\Gamma^\perp = 0$ | $\Gamma^\perp = 2\tau_{v,e} - 2\tau_{v,o} + 2\tau_{\bar{v},e} + 2\tau_{\bar{v},o} + \tau_{\bar{v},e} + \tau_{\bar{v},o}$ |

Relaxation gaps for $C^x$ and $C^ς$ at $\Xi = 1$.

| Gap $\Gamma_x$ | Gap $\Gamma^\parallel$ | Gap $\Gamma^\perp$ |
|----------------|------------------------|-------------------|
| $\Gamma_x = 0$ | $\Gamma^\parallel = 2\tau_{v,e} - 2\tau_{v,o} + 2\tau_{\bar{v},e} + 2\tau_{\bar{v},o} + \tau_{\bar{v},e} + \tau_{\bar{v},o}$ |
| $\Gamma^\parallel = 0$ | $\Gamma^\parallel = 2\tau_{v,e} - 2\tau_{v,o} + 2\tau_{\bar{v},e} + 2\tau_{\bar{v},o} + \tau_{\bar{v},e} + \tau_{\bar{v},o}$ |
| $\Gamma^\perp = 0$ | $\Gamma^\perp = 2\tau_{v,e} - 2\tau_{v,o} + 2\tau_{\bar{v},e} + 2\tau_{\bar{v},o} + \tau_{\bar{v},e} + \tau_{\bar{v},o}$ |

Quantum interference is very sensitive to a magnetic field $B_\perp$ perpendicular to the monolayer, as it breaks the coherence of time reversed paths of electrons, responsible for WL and WAL. This is used as a probe of W(A)L in experiments, which measure the magnetococonductance as a function of $B_\perp$. The perpendicular field couples to the momentum of the electrons, unlike the parallel field $B_\parallel$, which only couples to spin via the Zeeman effect. It leads to a quantization of momenta $|Q| \rightarrow Q_n = (n + 1/2)|l_{B_\perp}|$, where $n = 0, 1, 2, \ldots$ denotes the Landau levels and $l_{B_\perp} = \sqrt{\hbar/4eB_\perp}$ is the magnetic length. We assume $l_B \gg l$, such that the diffusive limit is not violated, which imposes a constraint on the maximum field $B_\perp \ll \hbar/(4eD\tau_0)$. We evaluate the magnetococonductance $\Delta\sigma = \delta\sigma(B_\perp) - \delta\sigma(0)$ as
Here, we have introduced

\[
F(z) = \ln(z) + \psi \left( \frac{1}{2} + \frac{1}{z} \right) \approx \left\{ \begin{array}{ll}
\frac{z^2}{24}, & z \ll 1, \\
\ln z, & z \gg 1,
\end{array} \right.
\]

where \( \psi(z) \) is the digamma function, and \( B_i^J = \hbar \Gamma_i^J / (4eD) \) and \( B_{so} = \Delta_{so} / (eD) \) are effective magnetic fields associated with the scattering rates and spin-orbit coupling.

Eq. (28) acquires a simple form if the decoherence rate \( \tau_\phi^{-1} \) is either the dominant or the smallest scattering rate. For very long \( \tau_\phi \), such that \( \tau_\phi^{-1} \ll \Gamma_i^J \), all the gapped Cooperons can be neglected, and only the third term in Eq. (28) remains. Then, we have \( \Delta \sigma / \sigma_0 = -1/2F(B_i^J / B_\phi) \), as in conventional metal with strong SO disorder. For short decoherence times, \( \tau_\phi^{-1} \gg \Gamma_i^J \), all the Coperon gaps can be neglected. Different contributions to Eq. (28) then cancel pairwise, and we obtain \( \Delta \sigma / \sigma_0 = 2\Xi F(B_i^J / B_\phi) \). This exhibits WL, WAL or a vanishing quantum correction for \( \Xi = 1, -1, 0 \) respectively, similarly to a Dirac material in a smooth disorder potential.

The magnetoconductance formula Eq. (28) captures the rich localization behavior of TMDCs and graphene/TMD. Due to the large number of parameters it is difficult to apply it directly to experiments. In the next section, we will present and discuss several realistic regimes in which this result significantly simplifies, and compare them to the existing theories.

\[
\frac{\Delta \sigma}{\sigma_0} = 2\Xi F \left( \frac{B_i^J}{B_\phi + B_{iv}} \right) + \frac{1}{2} F \left( \frac{B_i^J}{B_\phi + 2B_{asy}} \right) - \frac{1}{2} F \left( \frac{B_i^J}{B_\phi} \right) - \gamma_{iv} \sum_{\pm} \pm F \left( \frac{B_i^J}{B_\phi + B_{iv} (1 \pm \frac{1}{\tau_{iv}}) + B_s} \right).
\]

Here \( \tau_s^{-1} = \tau_{sym}^{-1} + \tau_{asy}^{-1} \), and \( B_i = \hbar / (4eDR_i) \). We see that the magnetoconductance is determined by the combination of valley and spin physics, described by the intervalley scattering rate \( \tau_{iv}^{-1} \), and spin scattering rates \( \tau_{sym}^{-1} \) and \( \tau_{asy}^{-1} \). The interplay between intervalley scattering and valley-Zeeman SOC is captured by the coefficient \( \gamma_{iv} \). We will proceed by analyzing this interplay in two limits: \( \tau_{iv}^{-1} \gg \Delta_{so} \) and \( \Delta_{so} \gg \tau_{iv}^{-1} \).

Within these two limits, we can readily address 3 regimes of the decoherence rate: (i) \( \tau_\phi^{-1} \ll \tau_s^{-1} \), (ii) \( \tau_s^{-1} \ll \tau_\phi^{-1} \ll \tau_{iv}^{-1} \), and (iii) \( \tau_{iv}^{-1} \ll \tau_\phi^{-1} \), where the quantum correction acquires a simple form. The cases (i) and (iii), where the decoherence rate is the dominant or the smallest one, respectively, were previously discussed in the general context of Eq. (28). The intermediate regime (ii) is not universal. In the limit \( \tau_{iv}^{-1} \gg \Delta_{so} \), it yields \( \Delta \sigma / \sigma_0 = F(B_i / B_\phi) \). This is analogous to con-

IV. DISCUSSION

We will proceed by analyzing the magnetoresistance formula (28) in the regimes of strong (Sec. IV A) and weak short-range disorder (Sec. IV B). We will also address the effect of an in-plane Zeeman field (Sec. IV C).

A. Strong short-range disorder

The regime where intervalley scattering dominates over all spin-dependent scattering rates, \( \tau_{iv}^{-1} \gg \tau_{ij}^{-1} \), with \( i = z, zv, iv \) and \( j = z, o \), is the most commonly used regime when interpreting the measurements of the quantum correction. In this case, the effect of spin-dependent disorder can be captured with only two scattering rates, \( \tau_{asy}^{-1} \) and \( \tau_{iv}^{-1} = \tau_{iv,z,v}^{-1} + \tau_{iv,z,o}^{-1} + \tau_{BR}^{-1} \).

Here \( \tau_{sym}^{-1} \) contains all the spin-dependent scattering processes that satisfy mirror (\( z \to -z \)) symmetry and thus preserve the electron spin. On the other hand, \( \tau_{asy}^{-1} \) contains spin-flip processes that break this symmetry. In this regime, \( \Gamma_{iv}^{-1} \approx \Gamma_{iv}^{zv} \approx \Gamma_{iv}^{z,o} \), and \( \gamma_{iv} \approx 1/\sqrt{1 - 4\Delta_{so} \tau_{iv}^{-1}} \). Furthermore, we will assume that the effect of trigonal warping captured in \( \tau_{asy}^{-1} \) and \( \tau_{iv}^{-1} \) for intravalley Cooperons (see the bottom of Table II) is small compared to intervalley scattering. In this case we have \( \tau_{iv}^{-1} \approx \tau_{iv,z,v}^{-1} \approx \tau_{iv,z,o}^{-1} \), and the magnetoconductance (28) becomes

\[
\frac{\Delta \sigma}{\sigma_0} = 2\Xi F \left( \frac{B_i^J}{B_\phi + B_{iv}} \right) + \frac{1}{2} F \left( \frac{B_i^J}{B_\phi + 2B_{asy}} \right) - \frac{1}{2} F \left( \frac{B_i^J}{B_\phi} \right) - \gamma_{iv} \sum_{\pm} \pm F \left( \frac{B_i^J}{B_\phi + B_{iv} (1 \pm \frac{1}{\tau_{iv}}) + B_s} \right).
\]
ventional metal without SO impurities, and represents a sum of three spin-triplets $C_{0}^{i} (i = x, y, z)$, which contribute as $3/2F(B_{z}/B_{\phi})$, and a spin-singlet $C_{0}^{y}$, which contributes as $-1/2F(B_{z}/B_{\phi})$. For $\Delta_{so} \gg \tau_{iv}^{-1}$, the two triplets $C_{0}^{x}$ and $C_{0}^{y}$ are suppressed by the SOC, and the quantum correction vanishes.

We obtain more interesting and complex behavior in the crossover regimes $\tau_{iv}^{-1} \sim \tau_{s}^{-1}$ [which includes (i) and (ii) and $\tau_{iv}^{-1} \sim \tau_{s}^{-1}$ [which includes (ii) and (iii)]. Strong intervalley scattering completely suppresses the valley structure in the first regime, so that the magnetoconductance is determined by the spin physics only. On the other hand, the valley physics dominates in the second regime, as the effect of spin-scattering is washed out by electron decoherence.

a. Limit $\tau_{iv}^{-1} \gg \Delta_{so}$: Here, Eq. (31) simplifies, as $\gamma_{iv} \approx 1$. In the crossover regime $\tau_{iv}^{-1} \tau_{s}^{-1}$, the first and the last term of Eq. (31) are suppressed by the large intervalley scattering, and we obtain

$$\frac{\Delta \sigma}{\sigma_{0}} = \frac{1}{2} F \left( \frac{B_{z}}{B_{\phi} + 2B_{asy}} \right) - \frac{1}{2} F \left( \frac{B_{z}}{B_{\phi}} \right) + \frac{1}{2} F \left( \frac{B_{z}}{B_{\phi} + B_{iv}} \right),$$

which is governed by spin-orbit scattering and is equivalent to the HLN formula. Here, we have introduced $B_{asy} = (1-\gamma_{iv})B_{s} \approx 2B_{so}/B_{iv} + B_{s} \approx B_{s} = \hbar/(4eD\tau_{s})$.

Eq. (32) exhibits WAL-WL crossover as the magnitude of the perpendicular field is increased. The effect of valley-Zeeman SOC is captured by an additional contribution to the symmetric rate $\tau_{sym}^{-1} \rightarrow \tau_{sym}^{-1} + 2\Delta_{so} \tau_{iv}$. This effect was already discussed in Refs. 25 and 38 and used to estimate $\Delta_{so}$ from the experimental data in graphene/TMD heterostructures. However, in both references, the estimated SOC is of the same order of magnitude as $\tau_{iv}^{-1}$, which is outside of the region of validity of this formula ($\tau_{iv}^{-1} \gg \Delta_{so}$). Instead, the full formula provided by Eqs. (31) should be used in order to get a more reliable estimate of the valley-Zeeman SOC.

Next, we address the crossover regime $\tau_{iv}^{-1} \sim \tau_{s}^{-1}$. The spin scattering rates can be neglected, and the second and third term of Eq. (31) cancel out, which yields

$$\frac{\Delta \sigma}{\sigma_{0}} = 2\Xi F \left( \frac{B_{z}}{B_{\phi} + B_{iv}} \right) + F \left( \frac{B_{z}}{B_{\phi}} \right) - F \left( \frac{B_{z}}{B_{\phi} + 2B_{iv}} \right),$$

In graphene ($\Xi = -1$) without SOC, it is the same result as in Ref. 31. As a function of a perpendicular field, it exhibits pure WL for $\Xi = 1$ and $\Xi = 0$, and WL-WL crossover for $\Xi = -1$. Fig. 3(a) gives a schematic representation of the different regimes in the limit $\tau_{iv}^{-1} \gg \Delta_{so}$.

b. Limit $\Delta_{so} \gg \tau_{iv}^{-1}$: Since $\gamma_{iv} \approx 0$, only the first three terms of Eq. (31) contribute to the magnetoconductance. In the crossover regime $\tau_{iv}^{-1} \approx \tau_{s}^{-1}$, we have

$$\frac{\Delta \sigma}{\sigma_{0}} = \frac{1}{2} F \left( \frac{B_{z}}{B_{\phi} + 2B_{asy}} \right) - \frac{1}{2} F \left( \frac{B_{z}}{B_{\phi}} \right),$$

which corresponds to pure WAL behavior as a function of $B_{z}$, that saturates on the scale of $B_{asy}$. This kind of saturation was noticed in several recent quantum correction measurements that exhibit flat WAL curves, such as Refs. 20, 24, and 25.

Finally, we analyze the crossover regime $\tau_{iv}^{-1} \sim \tau_{s}^{-1}$. We find

$$\frac{\Delta \sigma}{\sigma_{0}} = 2\Xi F \left( \frac{B_{z}}{B_{\phi} + B_{iv}} \right),$$

which exhibits pure WAL, pure WL, or vanishes for $\Xi = 1$, $\Xi = -1$ and $\Xi = 0$, respectively. Fig. 3(b) gives a schematic representation of the different regimes in the limit $\Delta_{so} \gg \tau_{iv}^{-1}$.

Fig. 4 illustrates the behavior of the magnetoconductance beyond the two extreme limits $\tau_{iv}^{-1} \gg \Delta_{so}$ and $\Delta_{so} \gg \tau_{iv}^{-1}$, analyzed above. Fig. 4(a) addresses the crossover from the regime described by Eq. (32) to Eq. (34) as the magnitude of valley-Zeeman SOC is increased. Similarly, Fig. 4(b) shows a crossover from Eq. (33) to Eq. (35).

B. Weak short-range disorder

In this section we analyze the regime where intervalley scattering rate is much weaker than all intravalley spin-scattering rates, $\tau_{ij}^{-1} \gg \tau_{iv}^{-1}$, where $i = z, zr$ and $j = z, o$. The intervalley spin-scattering rates are assumed to be even weaker, $\tau_{iv,z/r} \ll \tau_{iv}^{-1}$, and thus neglected. The
magnetoconductance formula is then given as

\[ \frac{\Delta \sigma}{\sigma_0} = 2\Xi F\left( \frac{B_\perp}{B_\phi + B_{\perp}^0} \right) - \frac{1}{2} F\left( \frac{B_\perp}{B_\phi} \right) + \frac{1}{2} F\left( \frac{B_\perp}{B_\phi + 2B_{\perp}^0} \right) - \Xi \gamma_s \sum_{\pm} \pm F\left( \frac{B_\perp}{B_\phi + B_{\perp}^0 \pm \frac{B_{\perp}^0}{\gamma_s}} \right). \]  

(36)

In this regime, the quantum correction is governed by the interplay between \( \Delta_{\mathrm{so}} \), and the combination of the spin-scattering rates \( \Gamma_\perp \), described by the coefficient \( \gamma_s \). Unlike the case of strong short-range disorder, the Cooperons containing \( \gamma_{\mathrm{iv}} \) cancel out in this regime, so the ratio of intervalley scattering and valley-Zeeman SOC does not affect \( \Delta \sigma \). The three intravalley Cooperon gaps \( \Gamma_\perp^x, \Gamma_\perp^z \) and \( \Gamma_\perp^0 \) that enter Eq. [36] have a similar structure, and depend on the trigonal warping \( (\tau_1^{-1}, \tau_1^z^{-1}) \) and different spin-dependent scattering rates. To simplify the further analysis, we will assume that they are of the same order of magnitude, and introduce the notation \( \tau_{s'}^{-1} = \max(\tau_1^{-1}, \tau_1^z^{-1}) \).

We proceed similarly to the previous section, and analyze the 3 extreme limits with respect to the decoherence rate. If it is the smallest, \( \tau_\phi^{-1} \ll \tau_{iv}^{-1} \), or the largest, \( \tau_\phi^{-1} \ll \tau_{s'}^{-1} \), scattering rate, the general arguments presented after Eq. [28] apply. In the intermediate limit \( \tau_{iv}^{-1} \ll \tau_\phi^{-1} \ll \tau_{s'}^{-1} \), the quantum correction vanishes.

We next examine the crossover regimes. For \( \tau_\phi^{-1} \sim \tau_{iv}^{-1} \), we have

\[ \frac{\Delta \sigma}{\sigma_0} = -\frac{1}{2} F\left( \frac{B_\perp}{B_\phi} \right) + \frac{1}{2} F\left( \frac{B_\perp}{B_\phi + 2B_{\perp}^0} \right). \]  

(37)

This formula is determined by intervalley scattering only, and exhibits WAL behavior which saturates on the scale of \( B_{\perp} \). Finally, in the crossover regime \( \tau_\phi^{-1} \sim \tau_{s'}^{-1} \), we have

\[ \frac{\Delta \sigma}{\sigma_0} = 2\Xi F\left( \frac{B_\perp}{B_\phi + B_{\perp}^0} \right) - \Xi \gamma_s \sum_{\pm} \pm F\left( \frac{B_\perp}{B_\phi + B_{\perp}^0 \pm B_{\perp}^0/\gamma_s} \right). \]  

(38)

In the limit \( \Gamma_\perp \gg \Delta_{\mathrm{so}} \), one should consider all three terms in Eq. [38] since \( \gamma_s \approx 1 \). As \( \Delta_{\mathrm{so}} \) increases, the second line of Eq. [38] becomes suppressed, until it vanishes for \( \Delta_{\mathrm{so}} \gg \Gamma_\perp \), where \( \gamma_s \approx 0 \). We see that the qualitative behavior of the magnetoconductance remains the same for any \( \gamma_s \), and thus, any \( \Delta_{\mathrm{so}} \). It only depends on the doping coefficient \( \Xi \), and exhibits WL, WAL or neither for \( \Xi = 1, -1 \) and 0, respectively. These conclusions are schematically represented in Fig. 5.

In Fig. 5, the regime of weak short-range disorder, \( \tau_{s'}^{-1} \gg \tau_{iv}^{-1} \). The behavior in the crossover regions is represented in the same way as in Fig. 3.

C. Influence of the in-plane Zeeman field

One of the main difficulties when experimentally extracting the parameters from quantum magnetoresistance fits comes from the fact that there are multiple parameter combinations that can fit the same data. For example, both valley-Zeeman SOC and spin-dependent scattering can lead to pronounced WAL signals. Applying an in-plane Zeeman field can help overcome these ambiguities, as different kinds of disorder and SOC interplay differently with the field.
Note that it will always be reached if parameter regime, as will be discussed in the following. The magnitude of the in-plane Zeeman field required to reach the high-field formula (39) differs depending on the sign of the in-plane Zeeman field. If the valley-Zeeman SOC does not significantly contribute to the effective rate $\tilde{\tau}_s$, shown in Eq. (32). If the valley-Zeeman SOC and restores the Cooperons $C^0_j$ and $C^1_j$, where $i = x, y$ and $j = 0, z$, are suppressed by the strong $\Delta_{so}$ at $h = 0$. In order to reach the asymptotic formula Eq. (40), a large field $h \gg \Delta_{so}$ is needed. It negates the effect of the valley-Zeeman SOC and restores $C^0_j$ and $C^1_j$, while suppressing all $C_0$ and $C_1$. Finally, we address the limit of weak short range disorder, $\tau_s^{-1} \gg \tau_{iv}^{-1}$, described by Eq. (36) at $h = 0$. Similarly to the previously considered case, strong $h$ negates the effect of $\Delta_{so}$ and suppresses all spin-singlets and -triplets. Here, the asymptotic formula takes the form

$$\frac{\Delta \sigma}{\sigma_0} = \Xi \sum_{i=x,z} F \left( \frac{B_i}{B_0 + B_{iv}} \right) + \frac{1}{2} \left( \frac{B_i}{B_0 + 2B_{asy}} \right) - \frac{1}{2} \left( \frac{B_i}{B_0 + B_{iv}} \right).$$

Starting from the general expression (25), we will next check the magnitude of $h$ needed to reach this formula in the limits $\tau_{iv}^{-1} \gg \Delta_{so}$ and $\Delta_{so} \gg \tau_{iv}^{-1}$.

Let us consider $\tau_{iv}^{-1} \gg \Delta_{so}$ and a moderate dephasing rate $\tau_s^{-1} \sim \tilde{\tau}_s^{-1}$. In this regime, only the valley-singlets $C^0_j$ contribute to the magnetoconductance at $h = 0$, as shown in Eq. (32). If the valley-Zeeman SOC does not significantly contribute to the effective rate $\tilde{\tau}_s^{-1}$, that is, if $\tau_{iv}^{-1} \gg \Delta_{so}^2$, it is sufficient to apply the field $h \gg \tau_{iv}^{-1}$ to suppress the spin-singlet $C^0_j$ and the spin-triplet $C^1_j$, and thus reach the high-field formula Eq. (40). On the other hand, if $\Delta_{so}^2 \tau_{iv}^{-1}$, the required Zeeman field is much higher, and of the order of intervalley scattering, namely $h \gg \tau_{iv}^{-1}$. If the decoherence rate is larger, $\tau_s^{-1} \gg \tilde{\tau}_s^{-1}$, all the spin structure is suppressed by the electron decoherence, and the in-plane Zeeman field has no effect. In this case, the formula (40) is valid for any $h$ and is equivalent to Eq. (33).

Next, we consider the limit $\Delta_{so} \gg \tau_{iv}^{-1}$. In this regime, the Cooperons $C^0_j$ and $C^1_j$, where $i = x, y$ and $j = 0, z$, are suppressed by the strong $\Delta_{so}$ at $h = 0$. In order to reach the asymptotic formula Eq. (40), a large field $h \gg \Delta_{so}$ is needed. It negates the effect of the valley-Zeeman SOC and restores $C^0_j$ and $C^1_j$, while suppressing all $C_0$ and $C_1$.

Finally, we address the limit of weak short range disorder, $\tau_s^{-1} \gg \tau_{iv}^{-1}$, described by Eq. (36) at $h = 0$. Similarly to the previously considered case, strong $h$ negates the effect of $\Delta_{so}$ and suppresses all spin-singlets and -triplets. Here, the asymptotic formula takes the form

$$\frac{\Delta \sigma}{\sigma_0} = \Xi \sum_{i=x,z} F \left( \frac{B_i}{B_0 + B_{iv}^2} \right),$$

and is reached if the in-plane Zeeman field is the largest energy scale, $h \gg \tau_{iv}^{-1}, \Delta_{so}, \tau_s^{-1}$. The prefactor $\Xi$ indicates that it can exhibit WAL, WL or neither depending on the doping, similarly to Eq. (38).

To illustrate a situation where applying the in-plane field can help in the interpretation of the quantum correction, we plot two magnetoconductance curves with a similar shape, but with significantly different parameters in Fig. 6 (black line). The first curve [Fig. 6(a)] has strong spin-scattering and no valley-Zeeman SOC, while the second one has weaker spin-scattering and strong SOC [Fig. 6(b)]. The high-field saturation curve (dashed line) has a similar shape in both cases, and is described by Eq. (40). The amplitude of WL at high fields is larger in the case of strong SOC, similar to Eq. (41). Moreover, this case is more resistant to the effect of the applied field, and the crossover to WL happens at a much higher field amplitude. This is consistent with the above analysis, as the expected crossover field is $h \sim \tau_{iv}^{-1}$ for Fig. 6(a) and $h \sim \Delta_{so}$ for Fig. 6(b). Thus, apply-
ing an in-plane field helps distinguish the contributions of valley-Zeeman SOC and spin-dependent scattering to the quantum correction.

V. CONCLUSIONS

In conclusion, we have developed a theory of weak localization and magnetoconductance for TMDC monolayers and their heterostructures with graphene, using standard diagrammatic technique for disordered systems. The interplay between spin and valley physics in these materials yields a rich behavior of the quantum correction to the conductivity, which we discuss in several regimes of interest for the interpretation of recent experimental data. We generalize the HLN and MF theories and propose a formula, that can be used to extract the magnitude of valley-Zeeman and disorder from the experiments in all regimes. In some cases, interpreting the experiments is not straightforward, as different parameter combinations can explain the data equally well. An in-plane Zeeman field can be used as an additional tuning parameter to help distinguish between the contributions of different processes.

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29 Note that the time-reversal operator in this basis is $T = i s_x \eta_x K$, where $K$ is complex conjugation.
30 The fact that there are 11 distinct scattering rates, excluding the dominant $\tau_1^{-1}$, can be understood as follows. As shown in Table I in Sec. III there are 5 distinct inter-valley and 6 distinct intravalley gaps. Therefore, there should be 11 independent scattering rates to accommodate the same number of independent Cooperon channels.
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