Spin Transport in Two Dimensional Hopping Systems

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A two dimensional hopping system with Rashba spin-orbit interaction is considered. Our main interest is concerned with the evolution of the spin degree of freedom of the electrons. We derive the rate equations governing the evolution of the charge density and spin polarization of this system in the Markovian limit in one-particle approximation. If only two-site hopping events are taken into account, the evolution of the charge density and of the spin polarization is found to be decoupled. A critical electric field is found, above which oscillations are superimposed on the temporal decay of the total polarization. A coupling between charge density and spin polarization occurs on the level of three-site hopping events. The coupling terms are identified as the anomalous Hall effect and the recently proposed spin Hall effect. Thus, an unpolarized charge current through a sheet of finite width leads to a transversal spin accumulation in our model system.

I. INTRODUCTION

The emerging field of spintronics tries to put the spin degree of freedom of electrons to use in a fashion akin to electronics, where the charge of the electrons is utilized. One of the advantages of spintronics is, that spatial inhomogeneities of the spin distribution are not burdened with an energetic penalty, quite in contrast to inhomogeneous charge distributions. On the other hand, spin is not conserved, whereas charge is. This is a disadvantage of spintronics, which means that spin polarization normally decays with time. Of special interest are techniques which influence the spin by purely electrical means, without utilizing magnetic fields or magnetic materials. Spin-orbit interaction (SOI) provides such a mechanism.

In recent years much has been done in this field for itinerant electrons, favoring very clean samples of high mobility. This investigation, on the other hand, studies the behavior of spins in a hopping system. Here, mobilities are very low, either through disorder (Anderson localization), or through strong electron-phonon interaction (polaron formation). Transport is thermally activated and incoherent. In the absence of effective spin scattering mechanisms, the low mobility might lead to long spin coherence times for a given spin coherence length, which is one motivation for this study, apart from the intrinsic scientific interest of the question of spin behavior in hopping systems.

Previous studies of SOI in hopping systems centered on the influence of the spin dynamics on charge transport (e.g. magneto-conductance), not on the spin dynamics itself. Furthermore, the effective spin coupling between hopping sites has normally been taken to be random, which is appropriate for spin scattering on charged impurities, but not for SOI due to intrinsic or external electric fields which are constant over length scales of several hopping lengths. But such a mechanism would be required if one has the intent of affecting the spins in a systematic way, i.e. realize spintronics.

To be specific, we consider a system where the spin dynamics is solely determined by spin-orbit interaction through the Rashba-mechanism, and no other spin scattering occurs (e.g. magnetooconductance, which is not on the spin dynamics itself). Furthermore, the effective spin coupling between hopping sites has normally been taken to be random, which is appropriate for spin scattering on charged impurities, but not for SOI due to intrinsic or external electric fields which are constant over length scales of several hopping lengths. But such a mechanism would be required if one has the intent of affecting the spins in a systematic way, i.e. realize spintronics.

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Two prominent examples of the interplay between charge and spin transport are the anomalous Hall effect and the spin Hall effect: The observation that a spin polarized charge current leads to a transversal Hall voltage, even without an external magnetic field, is called the anomalous Hall effect (see e.g. Ref. and references therein). The inverse effect, that, in materials showing the anomalous Hall effect, an unpolarized charge current leads to a transversal spin (but not charge!) current has been proposed by Hirsch and is called the spin Hall effect. Both of these effects will in the following be identified for our model system.

This paper is organized in the following way: Section II is concerned with the question of how to include the Rashba SOI into the hopping formalism. In Section III the rate equations governing the evolution of the (1-particle) density matrix are derived. This is done by calculating the diagrams of second and third order (two-site hopping and three-site hopping) in the Konstantinov-Perel diagram technique in 1-particle approximation and applying the Markovian limit. The rate equations for the density matrix are transformed into rate equations for the particle density and the spin orientation, which is an equivalent representation, but much more lucid physically. It is found that two-site hopping
II. RASHBA SPIN-ORBIT INTERACTION IN HOPPING SYSTEMS

The first question which arises, is how to include the spin-orbit interaction (SOI) into the formalism of hopping transport. The Rashba Hamiltonian reads

\[ H = \frac{\mathbf{p}^2}{2m} - \frac{\hbar}{m} \mathbf{\sigma} \cdot (\mathbf{K} \times \mathbf{p}) + V(r), \]

where we introduce the quantity \( \mathbf{K} = m \alpha \mathbf{e}_z / \hbar^2 \), which (i) has the dimension of an inverse length, (ii) is perpendicular to the two-dimensional plane (unit vector \( \mathbf{e}_z \)), and (iii) the length of which signifies the Rashba SOI strength \( \alpha \). The same expression Eq. (1) can be used for the generic SOI due to a spatially constant field \( \mathbf{E} \), in which case \( \mathbf{K} = \frac{\mathbf{e}_z}{4mc} \mathbf{E} \).

The symbol \( \mathbf{\sigma} \) denotes the vector of Pauli spin matrices.

Eq. (1) can be transformed to

\[ H = \frac{1}{2m} (\mathbf{p} - \hbar \mathbf{\sigma} \times \mathbf{K})^2 + V(r), \]

while ignoring an irrelevant constant energy offset. Thus, in principle, the Rashba SOI can be dealt with as a SU(2) gauge potential. Since the gauge potential is a constant, this would be quite trivial, were it not for the fact that SU(2) is non-Abelian. If the gauge were Abelian, a wave function \( \Psi(\mathbf{r}) \) would be studded with the factor \( \exp(i \mathbf{\sigma} \cdot (\mathbf{K} \times \mathbf{r}) ) \) in order to include SOI. Due to the non-Abelian nature, there are additional higher order contributions in \( \mathbf{K} \). Those can be neglected, provided \( K \) is sufficiently small.

The Hamiltonian which we consider reads

\[ H = \sum_{m \sigma} \epsilon_m a_m^{\dagger} a_{m \sigma} + \sum_{m,m',\sigma,\sigma'} J_{m'm}^{\sigma \sigma'} a_{m' \sigma'}^{\dagger} a_{m \sigma} + H_{e-ph} + H_{ph}, \]

where \( H_{e-ph} \) denotes the electron-phonon interaction and \( H_{ph} \) is the Hamiltonian of the phonon system. Here, \( a_{m \sigma}^{\dagger} (a_{m \sigma}) \) is the creation (annihilation) operator of an electron at site \( m \) in spin state \( \sigma \), \( \epsilon_m \) is the site energy, and \( J_{m'm}^{\sigma \sigma'} \) is the resonance integral between the states \( m \sigma \) and \( m' \sigma' \). Without SOI, the resonance integral is diagonal in spin space and will be denoted as \( J_{m'm} \) in the following. Note, that the usual spin splitting due to Rashba SOI is not manifest here, since Kramer’s degeneracy demands, that the two spin states of a localized eigenstate have to be degenerate.

The central question for the inclusion of SOI into the hopping Hamiltonian now consists in determining the spin structure of \( J_{m'm}^{\sigma \sigma'} \). The four numbers belonging to each pair of sites \( m'm \) are collected into a \( 2 \times 2 \) matrix in spin space \( \hat{J}_{m'm} \). Clearly \( \hat{J}_{m'm} \rightarrow J_{m'm} \hat{I}_2 \) for \( \mathbf{K} \rightarrow 0 \), where \( \hat{I}_2 \) denotes the two-dimensional unit matrix. Since the Hamiltonian has furthermore to be Hermitic and invariant under time-reversal symmetry, the spin structure is given by an SU(2) matrix \( 8,9,16,17,24,35,36,37 \). Thus, \( \hat{J}_{m'm} = \exp(-i \mathbf{\sigma} \cdot \mathbf{A}_{m'm}) J_{m'm}, \) where all components of the vector \( \mathbf{A} \) have to be real numbers and the condition \( \mathbf{A}_{m'm} = -\mathbf{A}_{mm'} \) must be obeyed. The arguments after Eq. (2) show that the term linear in \( \mathbf{K} \) reads \(-i \mathbf{\sigma} \cdot (\mathbf{K} \times \mathbf{R}_{m'm}) \), where \( \mathbf{R}_{m'm} = \mathbf{R}_{m'} - \mathbf{R}_m \) is the distance vector between the sites, and \( \mathbf{R}_m \) is the coordinate vector of site \( m \). Thus,

\[ \hat{J}_{m'm} = e^{-i \mathbf{\sigma} \cdot (\mathbf{K} \times \mathbf{R}_{m'm})} J_{m'm}, \]

For this expression for \( \hat{J} \) to be valid, \( \mathbf{K} \) has to be sufficiently small, as explained in the paragraph after Eq. (2). In this case, this means, that the condition \( \mathbf{K} \times \mathbf{R}_{m'm} \ll 1 \) must be valid for the distance vectors \( \mathbf{R}_{m'm} \), which are relevant to the case at hand (e.g. the typical hopping length or the lattice constant). The same expression, but applied to the Green’s function of a hopping system, has been derived in Ref. 4.
In some sense, this is equivalent to the Holstein transformation, where the influence of a magnetic field on a hopping system is taken into account through a phase factor, and where higher order (in the magnetic field) corrections are neglected.

We are now prepared to derive rate equations governing the hopping system with the inclusion of Rashba SOI in the next section.

### III. RATE EQUATIONS

We apply the Konstantinov-Perel diagram technique in order to obtain rate equations for the density matrix. The off-diagonal elements of the (1-electron) density matrix \( \langle a_{m\sigma}^\dagger a_{m\sigma} \rangle \) can usually be neglected in a hopping system (otherwise, the transport mechanism would not be hopping). Here, we have to keep in mind, that the correlations between different spin states on the same site contain information regarding the (expectation value of the) spin orientation. Furthermore, the model which we consider, aims at systems where the spin degrees of freedom do not de-cohere (lose their phase memory) while the electron stays on a site. Thus, we must retain the off-diagonal elements in spin space on the same site (i.e. diagonal in the site index) of the density matrix. In this way, by including the SOI the occupation probability \( \rho_m = \langle a_{m\sigma}^\dagger a_{m\sigma} \rangle \) becomes a \( 2 \times 2 \)-matrix \( \hat{\rho}_m | \sigma \rangle \langle \sigma | = \langle a_{m\sigma}^\dagger a_{m\sigma} \rangle \) in spin space.

In order to adapt the Konstantinov-Perel diagram technique to the SOI case, each site index can be thought of as additionally containing the spin index. The summations run over all sites and also the two spin states. The electron-phonon interaction is unaffected by the spin state. Thus, the extension of the formalism reduces to (i) studding each site index with a spin index (and extending the corresponding sums) and (ii) allowing expectation values which are non-diagonal in spin space. The number of terms in a given diagram proliferates quite rapidly with the order of the diagram and makes its computation tedious. The calculations are greatly simplified, if one replaces the explicit summation over the spin indices by matrix multiplication in spin space. This can be achieved by collecting the interaction matrix elements \( J \) (which depend on two-site and two spin indices) into appropriate matrices in spin space \( \hat{J}_{m\sigma m} \) (which only depend on two site indices) and doing likewise with the density matrix elements.

The second order diagrams (two-site hopping) yield in one-particle approximation and in the Markovian limit the rate equations

\[
\frac{d}{dt} \hat{\rho}_m = \sum_{m_1} \left\{ e^{-i\mathbf{\sigma} \cdot (\mathbf{K} \times \mathbf{R}_{m_1 m})} \hat{\rho}_{m_1} e^{i\mathbf{\sigma} \cdot (\mathbf{K} \times \mathbf{R}_{m_1 m})} W_{m_1 m} - \hat{\rho}_m W_{mm_1} \right\},
\]

where the transition rates \( W_{m' m} \) are the same as are obtained without SOI.

The physical meaning of Eq. 5 is easier to assess, if the following transformation is applied: Representing the \( 2 \times 2 \)-density matrix at site \( m \) by \( \hat{\rho}_m = \frac{1}{2} \rho_m \mathbf{I}_2 + \frac{1}{2} \rho_m \mathbf{\sigma} \) where \( \mathbf{I}_2 \) is the two-dimensional unit matrix, the occupation probability \( \rho_m = \text{Tr}(\hat{\rho}_m) \) and the (expectation value of the) spin orientation \( \rho_m = \text{Tr}(\mathbf{\sigma} \hat{\rho}_m) \) are introduced. Please note, that in the following we will use the wording “spin orientation” without emphasizing each time, that its calculation and makes its computation tedious. The calculations are greatly simplified, if one replaces the explicit summation over the spin indices by matrix multiplication in spin space. This can be achieved by collecting the interaction matrix elements \( J \) (which depend on two-site and two spin indices) into appropriate matrices in spin space \( \hat{J}_{m\sigma m} \) (which only depend on two site indices) and doing likewise with the density matrix elements.

The factors (matrices in spin space) surrounding \( \hat{\rho}_m \) in Eq. 5 are inverses of each other. Thus, by taking the trace (in spin space) of Eq. 5 these factors disappear and one obtains

\[
\frac{d}{dt} \rho_m = \sum_{m_1} \left\{ \rho_{m_1} W_{m_1 m} - \rho_m W_{mm_1} \right\}.
\]

On the other hand, multiplying Eq. 5 by \( \mathbf{\sigma} \) and then taking the trace, one obtains the rate equation for the spin orientation (see Appendix A)

\[
\frac{d}{dt} \rho_m = \sum_{m_1} \left\{ \hat{D}_{m_1 m} : \rho_{m_1} W_{m_1 m} - \rho_m W_{mm_1} \right\},
\]

where the quantity \( \hat{D} \) is a \( 3 \times 3 \)-matrix describing a rotation about the axis \( \mathbf{A}_{m_1 m} = \mathbf{K} \times \mathbf{R}_{m_1 m} \). The Eqs. 6 and 7 are the sought for rate equations which replace Eq. 5.

One can see, that in two-site approximation the equations for the occupation number and the spin orientation decouple. Note, that the terms of order \( \mathbf{K}^2 \) are retained in Eq. 6, in addition to the terms of order \( \mathbf{K} \), since the third-order terms, to be derived next, give contributions only to second order. The behavior of an ordered (polaronic) hopping system obeying Eqs. 6 and 7 is considered in Section IV

Next, the three-site probabilities (third order diagrams) are calculated. These contributions yield higher order corrections to the two-site probabilities, as well as some terms, which go beyond the physics of the two-site expressions.
Only the latter type of third order terms will be retained in the following calculations. The products of spin matrices occurring in the third order terms are calculated in Appendix B. The rate equations up to terms of order $\mathbf{K}^2$ and neglecting superfluous terms as mentioned above read

\[
\frac{d}{dt}\rho_m = \sum_{m_1} \left\{ W_{m_1m}\rho_{m_1} - W_{mm_1}\rho_m \right\} + \sum_{m_1m_2} \mathbf{K} \cdot (\mathbf{R}_{m_1m} \times \mathbf{R}_{m_2m}) \cdot \mathbf{K} \cdot \left\{ W_{m_1m_2m}^R\rho_{m_1} - W_{mm_1m_2}^R\rho_m \right\}
\]

(8)

\[
\frac{d}{dt}\rho_m = \sum_{m_1} \left\{ \hat{D}_{m_1m}\cdot\rho_{m_1} W_{m_1m} - \rho_m W_{mm_1} \right\} + \sum_{m_1m_2} \mathbf{K} \cdot (\mathbf{R}_{m_1m} \times \mathbf{R}_{m_2m}) \cdot \mathbf{K} \left\{ W_{m_1m_2m}^R\rho_{m_1} - W_{mm_1m_2}^R\rho_m \right\} - \sum_{m_1m_2} \mathbf{K} \cdot (\mathbf{R}_{m_1m} \times \mathbf{R}_{m_2m}) \cdot \mathbf{K} \times \left\{ W_{m_1m_2m}^I\rho_{m_1} - W_{mm_1m_2}^I\rho_m \right\}.
\]

(9)

Eqs. (8) and (9) are the generic hopping rate equations for the model considered here (only Rashba SOI affects spin). The transition rates $W_{m'm'}$, $W_{m_1m_2m}$, and $W_{m_1m_2}^I$ are independent of spin and are determined by the type of hopping considered (e.g. small polaron hopping or hopping between impurities). In the remaining part of the paper, we focus on an ordered (polaronic) system, but Eqs. (8) and (9) would also be the starting point for an investigation of a disordered system. Summing Eq. (8) over all sites $m$ yields $\frac{d}{dt} \sum_m \rho_m = 0$, thus, the derived rate equation for the particle density obeys particle (and charge) conservation.

Whereas the second order transition rates $W_{m_1m}$ are those of a system without SOI, the third order transition rates $W_{m_1m_2m}^R$ or $W_{m_1m_2}^I$ differ from the corresponding quantities without SOI. Without SOI, the third order transition rates (let us call them $W^{(3)}$ sumamry) are important for the Hall effect. The $W^{(3)}$ are divided into parts which are symmetric in the magnetic field and parts which are anti-symmetric. Only the latter are important for the Hall effect, thus the symmetric parts are normally neglected. Here, since the magnetic field is zero, the anti-symmetric part vanishes. Thus, we have to calculate the usually neglected symmetric parts of $W^{(3)}$. Furthermore, both, real ($W^R$) and imaginary ($W^I$) part of $W^{(3)}$ find entry in the formalism, whereas only the real part of the second order $W$ occurs. Nevertheless, $W^R$ is connected with the Hall mobility of a hopping system. The calculations are shown in Appendix B.

If the system is ordered (i.e. polaronic), it is advantageous to transform the equations into wave-vector space. Note that, since the spatial vectors are two-dimensional, the wave-vectors $\mathbf{q}$ will also be two-dimensional. This transformation leads to the rate equations

\[
\frac{d}{dt}\rho(\mathbf{q}) = [W(\mathbf{q}) - W(0)] \cdot \rho(\mathbf{q}) + [W^R(\mathbf{q}) - W^R(0)] \cdot \rho(\mathbf{q})
\]

(10)

and

\[
\frac{d}{dt}\rho(\mathbf{q}) = (W(\mathbf{q}) - W(0))\rho(\mathbf{q}) - 2\hat{W}(\mathbf{q}) \cdot \rho(\mathbf{q}) - 2(\mathbf{K} \times W(\mathbf{q})) \times \rho(\mathbf{q})
\]

\[
+ (W^R(\mathbf{q}) - W^R(0))\rho(\mathbf{q}) - (W^I(\mathbf{q}) - W^I(0)) \times \rho(\mathbf{q})
\]

(11)

Here,

\[
W(\mathbf{q}) = \frac{1}{i} \frac{\partial}{\partial \mathbf{q}} W(\mathbf{q})
\]

(12)

\[
\hat{W}(\mathbf{q}) = - \left( \mathbf{K}^2 \frac{\partial}{\partial \mathbf{q}} \cdot \frac{\partial}{\partial \mathbf{q}} + \mathbf{K} \cdot \mathbf{K} \frac{\partial}{\partial \mathbf{q}} \cdot \frac{\partial}{\partial \mathbf{q}} \right) W(\mathbf{q})
\]

(13)

\[
W^{RI}(\mathbf{q}) = \mathbf{K} \cdot \mathbf{K} \cdot \left( \frac{\partial}{\partial \mathbf{q} \cdot \frac{\partial}{\partial \mathbf{q}}} \right) W^{RI}(\mathbf{qq})
\]

(14)

where the last equation is to be understood as applying to the superscripts $R$ and $I$, respectively.
The basic transition rates are

\[ W(q) = \sum_m e^{i q R_m} W_{0m} \tag{15} \]

\[ W^{RI}(qq_1) = \sum_{m,m_1} e^{i q R_m} e^{i q_1 R_{m_1}} W^{RI}_{0m_1m} \tag{16} \]

In an isotropic system, taking the long wavelength limit, they read

\[ W(q) = W(0) - Dq^2 - i\mu q \cdot E \tag{17} \]

and

\[ W^{RI}(q) = i K \circ q \cdot (E \times K) W^{RI}, \tag{18} \]

the latter being calculated for a triangular lattice (see Appendix B). Here, \( D \) is the diffusion constant, \( \mu \) the mobility, and the quantities \( W^R \) and \( W^I \) are constants defined through Eq. (B8).

The rate equations thus take the shape

\[ \frac{d}{dt} \rho(q) = -i q \cdot j(q) \tag{19} \]

with the particle current density (proportional to the charge current density \( \epsilon_j \))

\[ j(q) = \mu E \rho(q) - iD q \rho(q) + W^R K \times E \circ K \cdot \rho(q) \tag{20} \]

and

\[ \frac{d}{dt} \rho(q) = -i q \cdot \dot{J}(q) + Q(q) \tag{21} \]

with the (tensorial) spin current density

\[ \dot{J}(q) = \mu E \circ \rho(q) - iD q \circ \rho(q) + 4D \dot{J}_z K \cdot \rho(q) - 4D \rho(q) \circ K + W^R K \times E \circ K \times \rho(q) \tag{22} \]

and the spin source density

\[ Q(q) = -4D K^2 \rho(q) - 4D K \circ K \cdot \rho(q) + 2\mu (K \times E) \times \rho(q) \tag{23} \]

Eq. (19) is the continuity equation for the particle (charge) density. Eq. (21) contains a source term in addition to the divergence of the current, since there is no conservation law for spin. The first two terms contributing to the charge current (20) are the drift term in the electrical field and the diffusion. The third term only occurs, when there is a finite \( z \)-component of the polarization (i.e. a magnetization \( M_z \)). The resulting current is directed perpendicular to the electric field. Thus, this term corresponds to the anomalous Hall effect. The corresponding mobility is seen to be \( \mu_{yx} = W^R K^2 \). The quantity \( \mu_{yx}/\mu \) is related to the Hall mobility (see Appendix B).

The spin current Eq. (22) mainly consists of the drift term and some diffusion terms. But the most interesting contribution is the fifth term on the right-hand side, since it is also present for vanishing spin polarization \( \rho = 0 \). This term describes a current of \( z \)-spins into the direction perpendicular to the electric field \( (K \times E) \). Thus, it is an expression of the spin Hall effect. The co-efficient \( W^R \) is the same, as the one responsible for the anomalous Hall effect.

In order to simplify notation, dimensionless quantities are introduced: dimensionless space \( x = K r \), wave vector \( \xi = q/K \), time \( \tau = DK^2 t \) and electric field \( \epsilon = \mu E/(DK) \). The transformed third order probabilities are denoted as \( \epsilon_R = \frac{KE}{D} W^R \) and \( \epsilon_I = \frac{KE}{D} W^I \). Note, that \( \epsilon_R \) can be expressed as \( \mu_{yx}/\epsilon/\mu \). Thus, \( \epsilon_R \) is an analog of the Hall mobility multiplied by the electrical field. Furthermore, the co-ordinate system is fixed such, that \( e_z \propto K \), \( e_x \propto E \), and \( e_y \propto K \times E \). Then \( K = K e_z \) and \( E = E e_x \). This transforms the rate equations (19) and (21) to

\[ \frac{d}{d\tau} \rho(\xi, \tau) = -i (\xi^2 + i \xi x \epsilon) \rho(\xi, \tau) - i \epsilon_R \xi y \rho_z(\xi, \tau) \tag{24} \]
and

\[
\frac{d}{d\tau}\rho(\xi, \tau) = -\left(\xi^2 + i\xi \varepsilon\rho - 4i(e_z \times \xi) \times \rho - i\varepsilon_R\xi_y e_z \rho + i\varepsilon_I \xi_y \times \rho\right) - 4\rho - 4e_z \rho_z + 2e \varepsilon_y \times \rho
\]

(25)

The three terms on the right-hand side of Eq. (24) are the diffusion contribution, the drift in the electric field and the anomalous Hall effect. The first terms on the right-hand side of Eq. (25) are: diffusion, drift (Ohmic current), a precession term for diffusing spins, the spin Hall effect, and a precession of the spin about the \(z\)-axis. The last three terms contribute to the spin decay. The first two of those can be expanded as \( -4e_z \rho_z - 4e_y \rho_y - 8e_z \rho_z \), thus the decay rate for the \(z\)-component is twice as large compared with the in-plane components.

**IV. BULK SYSTEM**

By setting the wave vector \(\xi\) to zero, the evolution equations for the quantities integrated over the whole system (total charge and total spin polarization, e.g. \(\rho(\xi = 0, \tau) = \int d^2x \rho(x, \tau)\)) are obtained

\[
\frac{d}{d\tau} \rho(0, \tau) = 0 \quad \quad (26)
\]

\[
\frac{d}{d\tau} \rho(0, \tau) = -4\rho - 4e_z \rho_z + 2e \varepsilon_y \times \rho. \quad \quad (27)
\]

Eq. (26) is an expression of charge conservation. It is to be seen, that the evolution of the space integrated quantities does not depend on the third-order parameters \(\epsilon_R\) and \(\epsilon_I\).

The three components of Eq. (27) read

\[
\frac{d}{d\tau}\rho_x = -4\rho_x + 2\varepsilon\rho_z \quad \quad (28a)
\]

\[
\frac{d}{d\tau}\rho_y = -4\rho_y \quad \quad (28b)
\]

\[
\frac{d}{d\tau}\rho_z = -8\rho_z - 2\varepsilon\rho_x, \quad \quad (28c)
\]

the solution of which is

\[
\rho_x(\tau) = e^{-6\tau} \left[ \rho_x(0) \cosh(2\tau \sqrt{1 - \varepsilon^2}) + \frac{\rho_x(0) + \varepsilon \rho_z(0)}{\sqrt{1 - \varepsilon^2}} \sinh(2\tau \sqrt{1 - \varepsilon^2}) \right] \quad \quad (29a)
\]

\[
\rho_y(\tau) = e^{-4\tau} \rho_y(0) \quad \quad (29b)
\]

\[
\rho_z(\tau) = e^{-6\tau} \left[ \rho_z(0) \cosh(2\tau \sqrt{1 - \varepsilon^2}) - \frac{\varepsilon \rho_x(0) + \rho_z(0)}{\sqrt{1 - \varepsilon^2}} \sinh(2\tau \sqrt{1 - \varepsilon^2}) \right] \quad \quad (29c)
\]

\(\rho_x(0), \rho_y(0),\) and \(\rho_z(0)\) are the initial conditions. Note, that there is a critical electrical field strength \(\varepsilon_c = 1\). In smaller fields the total spin polarization decays exponentially with time, but in larger fields, it additionally rotates with time. This critical electric field \(E_c = DK/\mu\) can also be expressed as \(E_c = k_B TK/\epsilon\), provided the Einstein relation between \(D\) and \(\mu\) is valid. Furthermore, without electric field, the \(z\)-component of the total spin polarization decays twice as fast as the other two components.

Taking for definiteness the initial condition \(\rho(0) = e_z\), one obtains

\[
\rho_x(\tau) = e^{-6\tau} \frac{\epsilon}{\sqrt{1 - \varepsilon^2}} \sinh(2\tau \sqrt{1 - \varepsilon^2}) \quad \quad (30a)
\]

\[
\rho_y(\tau) = 0 \quad \quad (30b)
\]

\[
\rho_z(\tau) = e^{-6\tau} \left[ \cosh(2\tau \sqrt{1 - \varepsilon^2}) - \frac{1}{\sqrt{1 - \varepsilon^2}} \sinh(2\tau \sqrt{1 - \varepsilon^2}) \right] \quad \quad (30c)
\]

for \(\epsilon < 1\), whereas for \(\epsilon > 1\) the hyperbolic functions become trigonometric functions. Expressed differently, for \(\epsilon > 1\) the eigen-values of the set of equations (28) become complex, which means that its eigen-modes become oscillatory.
Thus,

\[ \rho_x(\tau) = e^{-6\tau} \frac{\epsilon}{\sqrt{\epsilon^2 - 1}} \sin(2\tau \sqrt{\epsilon^2 - 1}) \]  
\[ \rho_y(\tau) = 0 \]  
\[ \rho_z(\tau) = e^{-6\tau} \frac{\epsilon}{\sqrt{\epsilon^2 - 1}} \cos(2\tau \sqrt{\epsilon^2 - 1} + \phi), \]

with \( \sin \phi = 1/\epsilon \). Note, that the frequency of the polarization oscillation \( 2\sqrt{\epsilon^2 - 1} \) increases with the electric field \( \epsilon \). Apart from the decay factor \( e^{-6\tau} \), the polarization \( \rho(\tau) \) describes a slanted ellipse in the \( x\)-\( z \)-plane, i.e. the plane spanned by the Rashba field \( \mathbf{K} \) and the electric field \( \mathbf{E} \). The co-ordinates \( x = \rho_x e^{6\tau} \sqrt{\epsilon^2 - 1}/\epsilon \) and \( z = \rho_z e^{6\tau} \sqrt{\epsilon^2 - 1}/\epsilon \) determine the ellipse \( x^2 + 2xz \sin \phi + z^2 = \cos^2 \phi \). The inclination of this ellipse (angle between \( z \)-axis and the main diagonal) increases with electric field. For \( \epsilon \rightarrow 1 \) the angle \( \phi \rightarrow \pi/2 \), i.e. the ellipse degenerates to a line with an inclination of \( 45^\circ \) to the perpendicular direction. In the limit of strong electric field \( \epsilon \rightarrow \infty \), the angle \( \phi \) vanishes, and the ellipse becomes a circle. In order to observe these oscillations, the corresponding frequency should be larger or of the order of the inverse decay time constant, which leads in this case to the approximate condition \( \epsilon \gtrsim 10 \).

Let us consider next the case of an inhomogeneous initial condition. We take a \( z \)-spin starting at the origin \( \rho(x, \tau = 0) = \delta(x)e_z \). The total spin polarization is still described by Eqs. (29). In order to obtain the local spin orientation, one has to solve Eqs. (29) and (22). This is done by solving these equations in Laplace-space and the following back-transformation to time \( \tau \) and wave-vector space \( \xi \) to \( x \).

The asymptotic behavior of the local spin polarization for large times \( \tau \rightarrow \infty \) and small distances \( |x| \ll 2\sqrt{\tau} \) (Large distances will not be relevant here, since they are strongly suppressed by the “diffusion factor” \( \exp(-x^2/4\tau) \)) is

\[ \rho_z(x, \tau) = \exp \left\{ -\frac{(x + \epsilon \tau)^2}{4\tau} - \frac{7}{4} \right\} \frac{3}{8\sqrt{\pi\tau}} J_0 \left( \frac{\sqrt{15}}{2} |x| \right) \]  

Note, that in this approximation (long times and short distances), the sign of the polarization — determined by the argument of the Bessel function \( J_0 \) — only depends on the distance to the origin, and is furthermore not time dependent. This spatial oscillation is due to the precession terms in the rate equations. The exponential factor exhibits a decay term with (dimensionless) time constant \( 4/7 \) and a drift-diffusion term with drift velocity \( -\epsilon \) and diffusion constant 1.

V. STRIP OF FINITE WIDTH

The distinguishing feature of a strip of finite width is, that there is no current (neither charge, nor spin) across the transversal boundaries. Thus, the spin-Hall current must be compensated by a diffusion current, i.e. a finite spin density can be expected to occur near the boundary. Indeed, the following will show, that a transversal spin accumulation will occur in this situation. For a broad strip, the non-zero spin density is mainly constricted to near the boundaries.

The strip is oriented, so that the \( x \)-direction is along the length of the strip (the direction of the current flow), the \( y \)-direction is along the width of the strip and the \( z \)-direction is perpendicular to the 2D strip (see Fig. 11). The strip extends from \( y = -b \) to \( y = b \), thus, its width is \( 2b \). Going from wave-vector space back to \( x \)-space and assuming that \( \rho(x) \) and \( \rho(x) = (\rho_x, \rho_y, \rho_z) \) depend only on the \( y \)-coordinate, the following set of differential equations determine the stationary state

\[ \rho''_x + \epsilon R \rho'_x = 0 \]  
\[ \rho'_z - \epsilon \rho''_y + 4\rho_y = 0 \]  
\[ \rho'_y + \epsilon R \rho'_y + 4\rho_x = 0 \]  
\[ \rho'''_z - \epsilon \rho'_y - 4\rho_z - 8\rho_y = 0 \]

where the prime denotes the derivation with respect to \( y \). The boundary conditions at \( y = \pm b \) are obtained by equating the normal component of the currents \( \rho_x \) and \( \rho_y \) at the boundary to zero. This yields

\[ (\rho'_x + \epsilon R \rho_x)_{y=\pm b} = 0 \]  
\[ (\rho'_z + \epsilon \rho'_y)_{y=\pm b} = 0 \]  
\[ (\rho'_y - \epsilon \rho_x + 4\rho_z)_{y=\pm b} = 0 \]  
\[ (\rho'_z + \epsilon R \rho - 4\rho_y)_{y=\pm b} = 0. \]
One has to keep in mind, that we want the solution to lowest order in $K$. The zero-th order solution of Eqs. (33a) to (33d) is obtained by removing all terms at least linear in $K$, i.e. setting $\epsilon_I = 0$ and $\epsilon_R = 0$. This immediately yields the solution $\rho(y) = \text{const.}$ and $\rho(y) = 0$. This solution is inserted into the terms containing $\epsilon_R$ and $\epsilon_I$, which yields the equations for the first order solution

\[ \rho'' = 0 \]  
\[ \rho''_z + 2\epsilon \rho_z - 4 \rho_x = 0 \]  
\[ \rho''_y + 4 \rho'_y - 4 \rho_y = 0 \]  
\[ \rho''_z - 4 \rho'_y - 2 \epsilon \rho_x - 8 \rho_z = 0 \]

with the boundary conditions

\[ (\rho')_{|y=\pm b} = 0 \]
\[ (\rho')_{|y=\pm b} = 0 \]
\[ (\rho'_y + 4 \rho_z)_{|y=\pm b} = 0 \]
\[ (\rho'_z - 4 \rho_y)_{|y=\pm b} = \epsilon_R \rho. \]

The solution of this set of equations can easily be constructed, since the only difference to the equations of zero-th order is the finite right-hand side in the boundary condition (36d). Again, $\rho(y) = \text{const.}$, and the 3 vectorial $\rho$-components are weighted sums of functions $\sinh(\lambda y)$ and $\cosh(\lambda y)$ where $\lambda$ takes on the three values: $\lambda_1 = 2$, $\lambda_2 = \sqrt{2 + 2i\epsilon^2 + 7} = \sqrt{8 + \epsilon^2 - 1 + i\sqrt{8 + \epsilon^2}} + 1$ and $\lambda_3 = \sqrt{2 - 2i\epsilon^2 + 7} = \lambda_2^2$. Thus, to lowest order in $K$,

\[ \frac{\rho_z(y)}{\epsilon_R \rho} = -\frac{16\epsilon}{\alpha} \lambda_2 c_2 s_3 \sinh(2y) + \frac{2\epsilon}{\alpha} \left( 16 c_1 s_3 + \frac{\epsilon^2}{2} \lambda_3 s_1 c_3 \right) \sinh(\lambda_2 y) + \text{c.c.} \]  
\[ \frac{\rho_y(y)}{\epsilon_R \rho} = \frac{4\epsilon^2}{\alpha} \lambda_2 c_2 c_3 \cosh(2y) + \frac{4\lambda_2}{\alpha} \left( 16 c_1 s_3 + \frac{\epsilon^2}{2} \lambda_3 s_1 c_3 \right) \cosh(\lambda_2 y) + \text{c.c.} \]  
\[ \frac{\rho_x(y)}{\epsilon_R \rho} = -\frac{\lambda_2^2 - 4}{\alpha} \left( 16 c_1 s_3 + \frac{\epsilon^2}{2} \lambda_3 s_1 c_3 \right) \sinh(\lambda_2 y) + \text{c.c.} \]

with the abbreviations

\[ \alpha = \lambda_2 c_2 \left[ \frac{\epsilon^2}{2} |\lambda_2|^2 \lambda_2 s_1 c_3 + 16 (\lambda_2^2 + 12 + \epsilon^2) c_1 s_3 \right] - \text{c.c.} \]

and

\[ c_i = \cosh(\lambda_i b), \quad s_i = \sinh(\lambda_i b) \quad (i = 1, 2, 3). \]

One can see, that the electron density $\rho$ and the spin Hall co-efficient $\epsilon_R$ only influence the amplitude of the polarization. They do not affect the spatial dependence of $\rho(y)$. The $x$- and $z$-component of the polarization are anti-symmetric with respect to a sign change of $y$, whereas the $y$-component is symmetric.

For a large electric field $\epsilon \gg 1$

\[ \rho_z(y) \approx -\text{sgn}(y) \frac{\epsilon_R \rho}{\sqrt{2\epsilon}} \sin\left( \sqrt{\epsilon}(b - |y|) + \frac{\pi}{4} \right) e^{-\sqrt{\epsilon}(b - |y|)} \]  
\[ \rho_y(y) \approx -\frac{\epsilon_R \rho}{\epsilon} \sin\left( \sqrt{\epsilon}(b - |y|) \right) e^{-\sqrt{\epsilon}(b - |y|)} \]  
\[ \rho_z(y) \approx -\text{sgn}(y) \frac{\epsilon_R \rho}{\sqrt{2\epsilon}} \cos\left( \sqrt{\epsilon}(b - |y|) + \frac{\pi}{4} \right) e^{-\sqrt{\epsilon}(b - |y|)} \]

The main effects of increasing the electric field $\epsilon$ consists in a sharper concentration of the polarization near the boundary (due to the exponential term) and an increase of the amplitude of the $x$- and $z$-component of the polarization (because $\epsilon_R / \sqrt{\epsilon} = \sqrt{\epsilon \mu_{yx}} / \mu \propto \sqrt{\epsilon}$).

For $b \gg 1$ (i.e. in natural units: width $\gg K^{-1}$) the spin polarization is significant only near the boundaries due to the hyperbolic functions. This suggests that there is a “spin diffusion length” governing the spatial extent of non-zero $\rho$ near the borders. This suggestion can be fleshed out in the following way: We consider the half plane $y \geq 0$, set the
electric field $\epsilon$ to zero and apply the boundary condition $\rho(y = 0) = \rho_0$. The differential equations for the stationary state (and homogeneous in $x$) are

$$\rho_{zz}'' - 4\rho_{zz} = 0, \quad \rho_{yy}'' + 4\rho_{yy} - 4\rho_{yy} = 0, \quad \rho_{zz}'' - 4\rho_{zz}'' - 8\rho_{zz} = 0,$$

which conceptually corresponds to an equation with the structure $D\Delta \rho - \rho/\tau = 0$, only that here the decay rate $1/\tau$ depends on the direction (thus, it is a tensor), and there is an additional “torque” term. Since in Eq. (41) all co-efficients are numbers (in dimensionless units) the resulting “spin diffusion length” $\sqrt{D/\tau}$ is also a number of the order of one (in the present case: $1/2$ for the $x$-component and $1/\sqrt{8 - 1} \approx 0.74$ for the other two components, corresponding to the real parts of $\lambda_1$, $\lambda_2$ and $\lambda_3$ at $\epsilon = 0$). Thus, expressed in natural units, this length is $K^{-1}$ times a constant of order one, i.e. this spin diffusion does not introduce a new length scale in addition to the Rashba length scale $K^{-1}$.

The spin current of a non-polarized electrical current in an infinitely extended plane consists of $z$-spins being transported perpendicularly to the electrical field $E$ (see Eq. (22)). Here, this spin current is “transformed” into spin accumulation by applying boundary conditions. Seen in this light, it is perhaps somewhat surprising that the resulting spin polarization has finite $x$- and $y$-components, in addition to the $z$-component. But this can be explained by the following observation: The calculated spin polarization $\rho(y)$ is — though stationary — not static. It represents an equilibrium between the “spin supply” by the spin Hall effect on the one hand, and other contributions of the spin current as well as the spin decay, on the other hand. Even though the “supply” only yields $z$-spins, the tensorial nature of the current leads to spin precession, such that in the equilibrium state all components occur.

Due to the spin polarization (magnetization) a magnetic field $H_M$ is generated, which may in principle allow to detect this polarization. In order to actually measure this magnetic field, one has to take into account, that there is also a magnetic field $H_I$ due to the electric current through the strip. These fields are calculated in Appendix C.

In principle, the magnetic field $H_M + H_I$ interacts with the spin degrees of freedom through the Zeeman energy and also applies a torque to the spins. These effects have been neglected in this paper.

The (in-)significance of the back-reaction of the magnetic field due to the spins on the spins can be estimated in the following way: Using the magnetic susceptibility $\chi$ and the Bohr magneton $\mu_B$, the spin polarization due to the back reaction can be expressed as $\rho_{xx} = \chi H/\mu_B \approx \chi M/\mu_B = \chi \rho$. Thus, the influence of the magnetic field on the spins can be neglected, provided the condition $\chi \ll 1$ is fulfilled.

VI. DISCUSSION

We have studied the spin dynamics of a hopping model where Rashba SOI is the sole spin scattering mechanism. Rate equations have been derived in the one-particle approximation and the Markovian limit, including two-site and three-site hopping processes. Further calculations are performed for the case of polaron hopping, where one can work in wave-vector space.

As expected, an initial spin polarization has been found to decay exponentially with time, if the electric field is low. But, there is a critical electric field, above which the total spin polarization shows oscillations (rotations) overlaying the decay. This can be understood as follows:

The rotation of a spin initially at a certain site $m_1$ during a single hop to another site $m_2$ depends only on the difference vector $R_{m_2m_1}$. The spin rotates in the plane spanned by the vectors $K$ and $R_{m_2m_1}$. Let us consider a spin starting at the origin and being orientated along the $z$-direction at $t = 0$. The motion of the electron in the radial directions leads to concentric “waves” around the origin of spins having the same $z$- and radial component. But, due to the diffusive motion, the electron does not only take the straight path radially outwards, but explores an increasingly entangled trajectory, thereby randomizing the spin orientation. The random motion only affects a decrease of the magnitude of the polarization (it neither creates polarization, nor does it favor any specific orientation). Thus, the preferred orientation given by the radial motion is preserved, but its magnitude diminished.

An electric field does affect the charge transport, but in two-site hopping approximation it does not affect the elementary processes responsible for the transport of spin orientation. Thus, in this case, the spin polarization is simply the product of particle density and spin orientation, which has a constant magnitude itself (quite in contrast to the situation with three-site hopping processes). In this way, one can see, that the electric field does not change the spatial distribution of the spin orientation (e.g. the sign of the $z$-component), but only changes the temporal evolution of the spatial charge distribution (the “weight” of the local spin orientation). This explains the time independence of the argument of the Bessel function in Eq. (42).

On the other hand, in a very large electric field an electron follows preferably a straight trajectory along the field (large drift component in comparison to the diffusion). The importance of diffusion about this trajectory is reduced, thereby also reducing the randomization of the spin. This explains, why it is possible for the electric field to become
so strong, that the spatial oscillations of the spin orientation survive the averaging over the whole volume, so that they appear as temporal oscillations.

Without an electric field, the decay of an initial spin orientation is found to behave anisotropic: The 3-component (perpendicular to the plane) decays twice as fast as the in-plane components.

The inclusion of three-site hopping terms leads to the occurrence of a transport co-efficient ($\epsilon^R$ or $\mu_{yx}$) which provides a coupling between charge and spin transport. A spin current produces a transversal charge current (anomalous Hall effect), and a charge current produces a transversal spin current (spin Hall effect). In a two-dimensional plane of finite width, this transversal spin current manifests itself as a spin accumulation at the boundaries of the strip.

Finally, some remarks about the experimental relevance are in order here. The Rashba SOI strength is widely given as being of the order $\alpha \approx 10^{-9}$ eV cm. It is possible to change this value by applying a gate voltage to the two-dimensional plane, where a variation by at least 50% has been shown to be realizable. This might be conceptually favorable for the implementation of spintronics devices, where electric means to control spins are sought.

Using the value of $\alpha$ mentioned above, one obtains $K \approx 1/(76 \text{ A})$, assuming that the effective electron mass is equal to its elementary mass. Thus, the condition $K \times R_{m,m} \ll 1$ for the validity of our theory demands in this case, that the typical hopping length is shorter than 76 A. This value is conveniently large, so that the range of polaronic nearest neighbor hopping is well within the validity range. But impurity hopping or variable range hopping are also not out of the question. Furthermore, for a smaller Rashba co-efficient, the permitted length increases and it is furthermore modified by the effective electron mass. If the Einstein relation between diffusion co-efficient and the mobility is assumed to be valid, the critical electric field strength $E_c = k_B T K/e$ for the oscillatory behavior of the total spin polarization is estimated to be about $10^4$ V/cm at a temperature of 100 K.

The calculations in Appendix B show a close connection between Hall mobility and the co-efficient for the spin Hall effect. There, the conductivity and the Hall mobility of the hexaboride compounds $\text{Eu}_x\text{Ca}_9\text{B}_6$ are measured, and the authors conclude, that the transport mechanism is polaron hopping (in a certain range of concentrations $x$ and for high temperatures). The reported Hall mobility in the polaronic hopping regime is of the order of 100 cm$^2$/Vs. Using this value, Eq. (B12) gives the estimate $\mu_{yx}/\mu \approx 0.23$, i.e. the transversal mobility for the spin Hall effect is about a fourth of the longitudinal mobility. Taking Eq. (B25) into account, this gives a relative spin polarization (3-component) at the boundary of a two-dimensional strip $|\rho_z(b)/\rho|$ of about 5% at the critical electric field strength $\epsilon = 1$.

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APPENDIX A: CALCULATION OF THE SPIN MATRICES

Applying the identity $(\sigma \cdot A)(\sigma \cdot B) = (A \cdot B) + i\sigma \cdot (A \times B)$, valid for any vectors $A$ and $B$, to the series expansion of the exponential function, one easily obtains the relation

$$e^{i\sigma \cdot A} = \cos |A| + i\sigma \cdot A \frac{\sin |A|}{|A|}, \quad (A1)$$

which is valid for any vector $A$.

The quantity $\text{Tr} (e^{-i\sigma A_{m,m}} \hat{\rho}_{m} e^{i\sigma A_{m,m}})$ occurs in the calculation of the contribution of two site diagrams to the rate equations. It can be transformed to $\text{Tr} (e^{i\sigma A_{m,m}} \sigma e^{-i\sigma A_{m,m}} \hat{\rho}_{m})$. With the help of Eq. (A1), the spin factors in the trace can be calculated to be

$$e^{i\sigma A_{m,m}} = e^{i\sigma A_{m,m}} e^{-i\sigma A_{m,m}} \approx \hat{D}_{m,m} \sigma, \quad (A2)$$

where the quantity $\hat{D}$ is a 3 $\times$ 3-matrix describing a rotation about the axis $A_{m,m} = K \times R_{m,m}$ and through the angle $2|A_{m,m}|$. This is valid to quadratic order in $A$. Explicitly,

$$\hat{D}_{m,m} = e_z \times e_R \times e_R + \sin |2A|(e_R \circ e_z - e_z \circ e_R) + \cos |2A|(e_z \circ e_z + e_R \circ e_R). \quad (A3)$$

The symbol “$\circ$” denotes the dyadic product and the orthogonal unit vectors are $e_z = K/K$ and $e_R = R_{m,m}/|R_{m,m}|$. Here, it is used that $K$ is perpendicular to the plane, i.e. $K \cdot R = 0$ for all vectors $R$ within the plane. Retaining in
this expression only terms of up to second order in $K$ (since $A \ll 1$), one obtains

$$\hat{D}_{m_1m} = \hat{I}_3 + 2|\hat{A}||\hat{e}_R \circ \hat{e}_z - \hat{e}_z \circ \hat{e}_R| - 2|\hat{A}|^2(\hat{e}_z \circ \hat{e}_z + \hat{e}_R \circ \hat{e}_R),$$

(A4)

where $\hat{I}_3$ is the identity matrix in three dimensions. Note that $\det(\hat{D}) = 1 + O(A^4)$, where $O(x)$ is Landau’s big-O notation, i.e. that the length of the vector $\rho$ does not change (up to $O(A^4)$) due to the application of the operator $\hat{D}$. Omitting the $A^2$-term, the length of the vector would change in second order of $A$; then, $\hat{D}$ would not represent a rotation.

The products of spin matrices in the three-site diagrams are calculated using the following scheme: After rotating the operators within the trace, so that $\rho$ is the last operator, the spin factors preceding $\rho$ in the trace are calculated in order to obtain an expression of the form $f + g\sigma$. Here, $f$ and $g$ are scalars in spin space. Thus, taking the trace yields $\text{Tr}((f + g\sigma)\rho) = f\rho + g\rho$, an expression where the spin operators have disappeared and are replaced by the particle density and the spin orientation. Using the operator identity $e^{A}e^{B} = e^{A + B}e^{[A,B]/2}$, where the error is of third and higher order in the operators $A$ and $B$, one obtains

$$e^{-i\sigma A_{m_2m}e^{-i\sigma A_{m_2m_1}}} \approx e^{-i\sigma A_{m_2m}}e^{i\sigma(A_{m_2m_1} \times A_{m_2m})}$$

(A5)

and

$$e^{-i\sigma A_{m_2m}e^{-i\sigma A_{m_2m_1}}} \approx e^{i\sigma(A_{m_2m_1} \times A_{m_2m})}.$$ (A6)

Using Eqs. (A2), (A3), and (A6), which are all valid to second order in $A$ (i.e. also in $K$), and Eq. (A1), the spin structure of the three-site terms can be calculated, e.g.

$$\text{Tr} \left(e^{-i\sigma A_{m_2m}e^{-i\sigma A_{m_2m_1}}} e^{-i\sigma A_{m_2m_1}} \hat{\rho} \right) \approx \cos |A_2| \rho + i \frac{\sin |A_2|}{|A_2|} A_2 \cdot \rho$$

$$\approx \rho + i A_2 \cdot \rho,$$

(A7)

$$\text{Tr} \left(e^{-i\sigma A_{m_2m}e^{-i\sigma A_{m_2m_1}}} e^{-i\sigma A_{m_2m_1}} \hat{\rho} \right) \approx \hat{D}_{m_2m_1} \cdot \left[\cos |A_2| \rho + i \frac{\sin |A_2|}{|A_2|} A_2 \rho - \frac{\sin |A_2|}{|A_2|} A_2 \times \rho\right]$$

$$\approx \hat{D}_{m_2m_1} \cdot \rho + i A_2 \rho - A_2 \times \rho,$$

(A8)

where the abbreviation $A_2 = A_{m_2m_1} \times A_{m_2m_2}$ is used, and the second approximation for each relation is the truncation to second order in $K$.

The expressions (A7) and (A8) occur together with the (complex) third order transition rate $W^{(3)}$. Adding the corresponding complex conjugate diagram, one obtains terms which contain the real part $W^{R} = 2\text{Re}(W^{(3)})$ and some which contain the imaginary part $W^{I} = 2\text{Im}(W^{(3)})$. Without SOI, only the real part is relevant, since there is no complex pre-factor in this case.

**APPENDIX B: THIRD ORDER TRANSITION PROBABILITY FOR SMALL POLARONS**

The third order diagrams (three-site hopping) give the additional contribution to the right-hand side of the rate equation (5)

$$\sum_{m_1m_2} \left\{ - e^{-i\sigma A_{m_2m}e^{-i\sigma A_{m_2m_1}}} \hat{\rho}_{m_1} e^{-i\sigma A_{m_1m}} W^{(3)}_{m_1m_2m} 
+ e^{-i\sigma A_{m_1m_1}^*} \hat{\rho}_{m_1} e^{-i\sigma A_{m_2m}^*} W^{(3)*}_{m_1m_2m} 
- \hat{\rho}_{m_1} e^{-i\sigma A_{m_1m_1}^*} e^{-i\sigma A_{m_2m}^*} W^{(3)*}_{m_1m_2m} 
+ e^{-i\sigma A_{m_2m}^*} e^{-i\sigma A_{m_2m_1}^*} \hat{\rho}_{m_1} W^{(3)*}_{m_1m_2m} \right\}. \ (B1)$$

The third order transition rates are $W^{R}_{m_1m_2m} = W^{(3)}_{m_1m_2m} + W^{(3)*}_{m_1m_2m} = 2\text{Re}(W^{(3)}_{m_1m_2m})$ and $W^{I}_{m_1m_2m} = -i(W^{(3)}_{m_1m_2m} - W^{(3)*}_{m_1m_2m}) = 2\text{Im}(W^{(3)}_{m_1m_2m})$, derived from the quantity

$$W^{(3)}_{m_1m_2m} = \frac{1}{\hbar^2} J_{m_2m} J_{m_2m_1} J_{m_1m} I.$$

(B2)
where the symbol \( I \) denotes the integral

\[
I(E) = e^{-3ST} \int_{-\infty}^{\infty} dt_1 \int_{0}^{\infty} dt_2 \left( \exp \left\{ \sum_{q} \frac{\Gamma_q}{2} \sinh(h\omega_q\beta/2) \right\} \right.
\times \left[ \cos \omega_q(t_1 + i\hbar\beta/2) + \cos \omega_q(t_2 + i\hbar\beta/2) + \cos \omega_q(t_1 - t_2 + i\hbar\beta/2) \right] - 1 \bigg) - 1 \bigg) \right)
\times \exp \left\{ \frac{i\hbar}{e} E \cdot R_{mm_1} t_1 - \frac{i\hbar}{e} E \cdot R_{mm_2} t_2 \right\} \tag{B3}
\]

with the abbreviations

\[
\Gamma_q = \frac{|\gamma(q)|^2 (1 - \cos q \cdot g)}{N} \tag{B4}
\]

and

\[
S_T = \sum_q \frac{\Gamma_q}{2} \coth(h\omega_q\beta/2). \tag{B5}
\]

The sums runs over the phonon wave-vectors \( q \). \( \gamma(q) \) is the electron-phonon interaction constant, \( \omega_q \) the phonon frequency, \( N \) the number of phonon states, \( \beta = 1/(k_B T) \), and \( g \) is a vector connecting two nearest-neighbor sites. Note, that the integral is independent of the direction of \( g \). Thus, the resulting expression is isotropic.

Taking two times the real part, the integral over \( t_2 \) would extend from \(-\infty \) to \( \infty \). This would be the expression to be calculated for the small polaron Hall effect. Here, we cannot take this step, because we also need to calculate the imaginary part of the expression \( \tag{B3} \).

The three-site rate obeys the principle of detailed balance

\[
W^{(3)}_{mm_2m_1} = W^{(3)}_{m_1m_2m} e^{-\beta E \cdot R_{mm_1}} \tag{B6}
\]

and has the further symmetry

\[
W^{(3)}_{m_1mm_2} = W^{(3)}_{m_1m_2m}. \tag{B7}
\]

Using these symmetries, the long wave-length limit of the third order term Eq. \( \tag{14} \) for a triangular lattice (hexagonal crystal symmetry) can be calculated as

\[
W^R(q) = iK \circ q \cdot (E \times K)^3 e^{-\frac{i\hbar}{e} E \cdot K} Re(W^{(3)}_{012}). \tag{B8}
\]

In order to calculate \( W^I \) the imaginary part of \( W^{(3)} \) has to be used instead of the real part. The indices 0, 1 and 2 denote the sites located at the vertices of an elementary triangle of the lattice. \( W^{(3)}_{012} \) has to be calculated in zero electric field. Thus, there only remains to determine the integral \( I(0) \) in order to obtain the third order coefficients.

For a sufficiently large phonon dispersion, the main contribution to the integral \( I \) comes from a saddle point \((t_{1s}, t_{2s}) \) at \((\pm i\hbar\beta/3, i\hbar\beta/2) \). Under the condition \( \hbar\omega_q \ll k_B T \) (high temperatures compared with the Debye temperature), the exponent in the integrand can be expanded in a series in \( t_1 \) and \( t_2 \), which is truncated after the second order terms. The integral can then be calculated and one obtains

\[
I \approx \frac{\hbar^2}{E_a k_B T} \frac{2\pi}{4\sqrt{3}} e^{-\frac{4E_a}{3k_B T}} \left( 1 - i \sqrt{\frac{3k_B T}{E_a}} e^{-\frac{E_a}{k_B T}} \right), \tag{B9}
\]

where

\[
E_a = \sum_q \frac{\hbar\omega_q \Gamma_q}{4}. \tag{B10}
\]

Combining Eq. \( \tag{B9} \) with Eq. \( \tag{B8} \), the mobility \( \mu_{yx} \) connected with the anomalous Hall effect and the spin Hall effect reads

\[
W^R K^2 = \mu_{yx} = \mu_0 \frac{\sqrt{3}\pi}{4} \frac{(Ka)^3 J^3}{E_a k_B T} e^{-\frac{4E_a}{3k_B T}}, \tag{B11}
\]
where $\mu_0 = e a^2/h$ and $a$ is the distance between nearest neighbors (lattice constant). This expression can be compared with the Hall mobility $\mu_H$ for small polaron hopping\textsuperscript{22} to give the relation

$$\frac{\mu_{yx}}{\mu} = 2(Ka)^2 \mu_H \mu_0 = \frac{2\hbar K^2 \mu_H}{e}.$$ \hspace{1cm} \text{(B12)}

The effective activation energy for the $W^R$ processes (e.g. the spin Hall effect) is $4E_a/3$ [see the real part of Eq.\textsuperscript{13}], which is identical to the situation for the ordinary Hall effect. On the other hand, the activation energy for the $W^I$ processes is $E_a$, i.e. $W^I \gg W^R$ for small temperatures $k_B T \ll E_a$.

### APPENDIX C: MAGNETIC FIELDS DUE TO SPIN ACCUMULATION AND ELECTRIC CURRENT

The magnetic field generated by the spin polarization (magnetization) $\mathbf{M}(\mathbf{r}) = \mathbf{M}(y) = \mu_B \rho(y)$ in the strip reads

$$\mathbf{H}_M(y, z) = -K \nabla \int_{-b}^{b} dy' M_y(y') (y - y') + M_z(z') \frac{z}{z^2 + (y - y')^2}.$$ \hspace{1cm} \text{(C1)}

Note, that the field $\mathbf{H}_M$ has no $x$-component, even though the spin polarization has a finite $x$-component $M_x$. The magnetic field $\mathbf{H}_M$ may be exploited in order to detect the spin accumulation. In this case, one has to keep in mind, that the electrical current in $x$-direction also leads to a magnetic field $\mathbf{H}_I$\textsuperscript{28} Both fields have different symmetry. Thus, if $\mathbf{H}_M$ is not very much smaller than $\mathbf{H}_I$, a measurement of the magnetic field near the strip allows a detection of the spin accumulation.

Explicitly, the magnetic field generated by the (homogeneous) current $I = c e B_0$ within the strip reads

$$\mathbf{H}_I(y, z) = \frac{I_e y}{4\pi b} \arctan \left( \frac{2az}{y^2 + z^2 - b^2} \right) + \frac{I_e y}{8\pi b} \log \left( \frac{z^2 + (y - b)^2}{z^2 + (y + b)^2} \right).$$ \hspace{1cm} \text{(C2)}

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FIG. 1: The co-ordinate system chosen for the strip of finite width. The charge current within the strip is non-polarized. But at the transversal boundaries \( y = \pm b \), a finite spin density occurs due to \( \epsilon_R \), i.e. this situation leads to spin accumulation.

FIG. 2: The magnetic field due to the spin accumulation in the \( z-y \)-plane. The parameters are \( b = 1, \epsilon = 1 \). The horizontal line denotes the extent of the strip.

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FIG. 3: The magnetic field due to the current through the strip. The parameters are the same as in Fig. 2.