Spin Hall-effect 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.

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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.[1,2] 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.[3] 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., magnetoconductance[4–10]), not on the spin dynamics itself. Furthermore, the effective spin coupling between hopping sites has normally been taken to be random,[8,9,11–14] 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[15–18] and no other spin scattering occurs (e.g., no magnetic impurities or spin scattering on charged impurities). The electronic system is two-dimensional (2D) and—in order to calculate explicit expressions—assumed to be ordered (small polaronic system). The disordered system is expected to behave qualitatively similar, but its investigation must be delegated to future publications.

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. 19 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[20–22] 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 Sec. III the rate equations governing the evolution of the (one-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 one-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 does not introduce a coupling between the equations for the particle (charge) density and the equations for the spin po-

larization. Three-site hopping processes introduce such a coupling and indeed lead to the anomalous Hall-effect and the spin Hall-effect for this hopping system.

Sections IV and V give solutions of the rate equations for an ordered hopping system (i.e., a system of small polarons). First, bulk properties (i.e., no boundaries) are considered. A short account of the results of Sec. IV has been published in Ref. 23. Then, in Sec. V, a strip of finite width is considered, which introduces boundary condition at the transversal edges. The stationary state with an unpolarized charge current shows spin accumulation at the boundaries, which is an expression of the spin Hall-effect.

The Appendixes primarily deal with mathematical details. Appendix C considers the magnetic field due to spin accumulation as a possible means of detection of spin accumulation.

II. RASHBA SPIN-ORBIT INTERACTION IN HOPPING SYSTEMS

The first question which arises is how to include the SOI into the formalism of hopping transport. The Rashba Hamiltonian reads

$$H=\frac{\mathbf{p}^2}{2m}-\frac{\hbar}{m}\boldsymbol{\sigma}\cdot(\mathbf{K}\times\mathbf{p})+V(\mathbf{r}), \tag{1}$$

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 α. The same expression, Eq. (1), can be used for the generic SOI due to a spatially constant electric field $\mathbf{E}$, in which case $\mathbf{K}=(e/4mc^2)\mathbf{E}$. The symbol $\boldsymbol{\sigma}$ denotes the vector of Pauli spin matrices. The quantity $\mathbf{p}$ denotes the momentum, m the (effective) electron mass, e the electron charge, and $V(\mathbf{r})$ the (spatially varying) potential.

Equation (1) can be transformed to

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

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 $\exp[i\boldsymbol{\sigma}\cdot(\mathbf{K}\times\mathbf{r})]$ 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

$$H=\sum_{m\sigma}\epsilon_m a^\dagger_{m\sigma}a_{m\sigma}+\sum_{mm'\sigma\sigma'}J^{\sigma'\sigma}_{m'm}a^\dagger_{m'\sigma'}a_{m\sigma}+H_{e-ph}+H_{ph}, \tag{3}$$

where H_{e-ph} denotes the electron-phonon interaction and H_{ph} is the Hamiltonian of the phonon system. Here, $a^\dagger_{m\sigma}$ ($a_{m\sigma}$) is the creation (annihilation) operator of an electron at site m in spin state σ, ϵ_m is the site energy, and $J^{\sigma'\sigma}_{m'm}$ 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 $J^{\sigma'\sigma}_{m'm}$. The four numbers belonging to each pair of sites $m'm$ are collected into a 2×2 matrix in spin space $\hat{J}_{m'm}$. Clearly $\hat{J}_{m'm}\to J_{m'm}\hat{I}_2$ for $\mathbf{K}\to\mathbf{0}$, 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,[8,9,11,17,24–27] $\hat{J}_{m'm}=\exp(-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m'm})J_{m'm}$, 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 $-\mathrm{i}\boldsymbol{\sigma}\cdot(\mathbf{K}\times\mathbf{R}_{m'm})$, 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,

$$\hat{J}_{m'm}=e^{-\mathrm{i}\boldsymbol{\sigma}\cdot(\mathbf{K}\times\mathbf{R}_{m'm})}J_{m'm}. \tag{4}$$

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 $\mathbf{K}\times\mathbf{R}_{m'm}\ll1$ 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,[28] 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 following 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 (one-electron) density matrix $\langle a^\dagger_{m'\sigma'}a_{m\sigma}\rangle$ 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 decohere (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 prob-

ability $\rho_m=\langle a_m^\dagger a_m\rangle$ becomes a 2×2 matrix $\hat{\rho}_m|_{\sigma'\sigma}=\langle a_{m\sigma'}^\dagger a_{m\sigma}\rangle$ 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 nondiagonal 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 $\hat{J}_{m'm}$ (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

$$\frac{d}{dt}\hat{\rho}_m=\sum_{m_1}\{e^{-i\boldsymbol{\sigma}\cdot(\mathbf{K}\times\mathbf{R}_{m_1m})}\hat{\rho}_{m_1}e^{i\boldsymbol{\sigma}\cdot(\mathbf{K}\times\mathbf{R}_{m_1m})}W_{m_1m}-\hat{\rho}_mW_{mm_1}\},\tag{5}$$

where the transition rates $W_{m'm}$ are the same as are obtained without SOI. An explicit expression is given in Eq. (B1).

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 third-order terms in matrix representation are given in Appendix B.

The physical meaning of Eq. (5) and its third-order generalization is easier to assess, if the following transformation is applied: Representing the 2×2-density matrix at site m by $\hat{\rho}_m=\frac{1}{2}\rho_m\hat{I}_2+\frac{1}{2}\boldsymbol{\rho}_m\cdot\hat{\boldsymbol{\sigma}}$, where $\hat{I}_2$ is the two-dimensional unit matrix, the occupation probability $\rho_m=\mathrm{Tr}(\hat{\rho}_m)$ and the (expectation value of the) spin orientation $\boldsymbol{\rho}_m=\mathrm{Tr}(\boldsymbol{\sigma}\hat{\rho}_m)$ are introduced. Please note that in the following we will use the wording ''spin orientation'' without emphasizing each time that its expectation value is meant. Of course, a spin-1/2 particle does not have a classical spin orientation.

Taking the appropriate trace (see Appendix A) yields the rate equations governing the evolution of these quantities

$$\frac{d}{dt}\rho_m=\sum_{m_1}\{W_{m_1m}\rho_{m_1}-W_{mm_1}\rho_m\}+\sum_{m_1m_2}\mathbf{K}\cdot(\mathbf{R}_{mm_1}\times\mathbf{R}_{mm_2})\circ\mathbf{K}\cdot\{W^R_{m_1m_2m}\boldsymbol{\rho}_{m_1}-W^R_{mm_1m_2}\boldsymbol{\rho}_m\},\tag{6}$$

$$\frac{d}{dt}\boldsymbol{\rho}_m=\sum_{m_1}\{\hat{D}_{m_1m}\cdot\boldsymbol{\rho}_{m_1}W_{m_1m}-\boldsymbol{\rho}_mW_{mm_1}\}+\sum_{m_1m_2}\mathbf{K}\cdot(\mathbf{R}_{mm_1}\times\mathbf{R}_{mm_2})\circ\mathbf{K}\{W^R_{m_1m_2m}\boldsymbol{\rho}_{m_1}-W^R_{mm_1m_2}\boldsymbol{\rho}_m\}-\sum_{m_1m_2}\mathbf{K}\cdot(\mathbf{R}_{mm_1}\times\mathbf{R}_{mm_2})\circ\mathbf{K}\times\{W^I_{m_1m_2m}\boldsymbol{\rho}_{m_1}-W^I_{mm_1m_2}\boldsymbol{\rho}_m\},\tag{7}$$

where only terms up to order $\mathbf{K}^2$ have been retained and superfluous correction terms of higher order (as mentioned above) have been neglected. Some details of the calculations of the traces in spin space can be found in Appendix A. The quantity $\hat{D}$ is a 3×3 matrix describing a rotation about the axis $\mathbf{A}_{m_1m}=\mathbf{K}\times\mathbf{R}_{m_1m}$.

Equations (6) and (7) are the generic hopping rate equations for the model considered here (only Rashba SOI affects spin). The transition rates $W_{m'm}$, $W^R_{m_1m_2m}$, and $W^I_{m_1m_2m}$ 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. (6) and (7) would also be the starting point for an investigation of a disordered system. Summing Eq. (6) over all sites m yields $(d/dt)\Sigma_m\rho_m=0$, thus, the derived rate equation for the particle density obeys particle (and charge) conservation.

The first term on the right-hand side of Eqs. (6) and (7), respectively, gives the contribution from two-site hopping processes. The remaining terms arise from three-site hopping processes. One can see that in two-site approximation the equations for the occupation number and the spin orientation decouple.

Whereas the second-order transition rates W_{m_1m} are those of a system without SOI, the third-order transition rates $W^{R\text{ or }I}_{mm_1m_2}$ differ from the corresponding quantities without SOI. Without SOI, the third-order transition rates (let us call them $W^{(3)}$ summarily) are important for the Hall-effect. $W^{(3)}$ are divided into parts which are symmetric in the magnetic field and parts which are antisymmetric. Only the latter are important for the Hall-effect, thus the symmetric parts are normally neglected. Here, since the magnetic field is zero, the antisymmetric 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

$$\frac{d}{dt}\rho(\mathbf{q}) = [W(\mathbf{q}) - W(\mathbf{0})]\rho(\mathbf{q}) + [\mathbf{W}^R(\mathbf{q}) - \mathbf{W}^R(\mathbf{0})]\cdot\boldsymbol{\rho}(\mathbf{q}) \tag{8}$$

and

$$\begin{aligned}\frac{d}{dt}\boldsymbol{\rho}(\mathbf{q}) = {} & [W(\mathbf{q}) - W(\mathbf{0})]\boldsymbol{\rho}(\mathbf{q}) - 2\hat{W}(\mathbf{q})\cdot\boldsymbol{\rho}(\mathbf{q}) \\ & - 2[\mathbf{K}\times\mathbf{W}(\mathbf{q})]\times\boldsymbol{\rho}(\mathbf{q}) + [\mathbf{W}^R(\mathbf{q}) - \mathbf{W}^R(\mathbf{0})] \\ & \times\rho(\mathbf{q}) - [\mathbf{W}^I(\mathbf{q}) - \mathbf{W}^I(\mathbf{0})]\times\boldsymbol{\rho}(\mathbf{q}).\end{aligned} \tag{9}$$

Here,

$$\mathbf{W}(\mathbf{q}) = \frac{1}{i}\frac{\partial}{\partial\mathbf{q}}W(\mathbf{q}), \tag{10}$$

$$\hat{W}(\mathbf{q}) = -\left(\mathbf{K}^2\frac{\partial}{\partial\mathbf{q}}\circ\frac{\partial}{\partial\mathbf{q}} + \mathbf{K}\circ\mathbf{K}\frac{\partial}{\partial\mathbf{q}}\cdot\frac{\partial}{\partial\mathbf{q}}\right)W(\mathbf{q}), \tag{11}$$

$$\mathbf{W}^{RI}(\mathbf{q}) = \mathbf{K}\circ\mathbf{K}\cdot\left(\frac{\partial}{\partial\mathbf{q}}\times\frac{\partial}{\partial\mathbf{q}_1}\right)W^{RI}(\mathbf{q}\mathbf{q}_1)|_{\mathbf{q}_1=0}, \tag{12}$$

where the last equation is to be understood as applying to the superscripts R and I, respectively.

The basic transition rates are

$$W(\mathbf{q}) = \sum_m e^{i\mathbf{q}\cdot\mathbf{R}_m}W_{0m}, \tag{13}$$

$$W^{RI}(\mathbf{q}\mathbf{q}_1) = \sum_{m_1 m} e^{i\mathbf{q}\cdot\mathbf{R}_m}e^{i\mathbf{q}_1\cdot\mathbf{R}_{m_1}}W^{RI}_{0m_1 m}. \tag{14}$$

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

$$W(\mathbf{q}) = W(\mathbf{0}) - D\mathbf{q}^2 - i\mu\mathbf{q}\cdot\mathbf{E} \tag{15}$$

and

$$\mathbf{W}^{RI}(\mathbf{q}) = \mathrm{i}\mathbf{K}\circ\mathbf{q}\cdot(\mathbf{E}\times\mathbf{K})W^{RI}, \tag{16}$$

the latter being calculated for a triangular lattice (see Appendix B). Here, D is the diffusion constant, μ the mobility, and the quantities W^R and W^I are constants defined through Eq. (B10).

The rate equations thus take the shape

$$\frac{d}{dt}\rho(\mathbf{q}) = -i\mathbf{q}\cdot\mathbf{j}(\mathbf{q}), \tag{17}$$

with the particle current density (proportional to the charge current density $e\mathbf{j}$)

$$\mathbf{j}(\mathbf{q}) = \mu\mathbf{E}\rho(\mathbf{q}) - iD\mathbf{q}\rho(\mathbf{q}) + W^R\mathbf{K}\times\mathbf{E}\circ\mathbf{K}\cdot\boldsymbol{\rho}(\mathbf{q}), \tag{18}$$

and

$$\frac{d}{dt}\boldsymbol{\rho}(\mathbf{q}) = -\mathrm{i}\mathbf{q}\cdot\hat{J}(\mathbf{q}) + \mathbf{Q}(\mathbf{q}), \tag{19}$$

with the (tensorial) spin current density

$$\begin{aligned}\hat{J}(\mathbf{q}) = {} & \mu\mathbf{E}\circ\boldsymbol{\rho}(\mathbf{q}) - iD\mathbf{q}\circ\boldsymbol{\rho}(\mathbf{q}) + 4D\hat{I}_3\mathbf{K}\cdot\boldsymbol{\rho}(\mathbf{q}) - 4D\boldsymbol{\rho}(\mathbf{q})\circ\mathbf{K} \\ & + W^R\mathbf{K}\times\mathbf{E}\circ\mathbf{K}\rho(\mathbf{q}) - W^I\mathbf{K}\times\mathbf{E}\circ\mathbf{K}\times\boldsymbol{\rho}(\mathbf{q})\end{aligned} \tag{20}$$

and the spin source density

$$\mathbf{Q}(\mathbf{q}) = -4D\mathbf{K}^2\boldsymbol{\rho}(\mathbf{q}) - 4D\mathbf{K}\circ\mathbf{K}\cdot\boldsymbol{\rho}(\mathbf{q}) + 2\mu(\mathbf{K}\times\mathbf{E})\times\boldsymbol{\rho}(\mathbf{q}). \tag{21}$$

Equation (17) is the continuity equation for the particle (charge) density. Equation (19) 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 (18) 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 μ_{yx}/μ is related to the Hall mobility (see Appendix B).

The spin current, Eq. (20), 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 $\boldsymbol{\rho}=\mathbf{0}$. This term describes a current of z spins into the direction perpendicular to the electric field ($\mathbf{K}\times\mathbf{E}$). Thus, it is an expression of the spin Hall-effect. The coefficient 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 $\mathbf{x}=K\mathbf{r}$, wave vector $\boldsymbol{\xi} = \mathbf{q}/K$, time $\tau = DK^2t$, and electric field $\boldsymbol{\epsilon} = \mu\mathbf{E}/(DK)$. The transformed third order probabilities are denoted as $\epsilon_R = (KE/D)W^R$ and $\epsilon_I = (KE/D)W^I$. Note that ϵ_R can be expressed as $\mu_{yx}\epsilon/\mu$. Thus, ϵ_R is an analog of the Hall mobility multiplied by the electrical field. Furthermore, the coordinate system is fixed such that $\mathbf{e}_z\propto\mathbf{K}$, $\mathbf{e}_x\propto\mathbf{E}$, and $\mathbf{e}_y\propto\mathbf{K}\times\mathbf{E}$. Then $\mathbf{K}=K\mathbf{e}_z$ and $\mathbf{E}=E\mathbf{e}_x$. This transforms the rate equations (17) and (19) to

$$\frac{d}{d\tau}\rho(\boldsymbol{\xi},\tau) = -(\boldsymbol{\xi}^2 + i\xi_x\epsilon)\rho(\boldsymbol{\xi},\tau) - i\epsilon_R\xi_y\rho_z(\boldsymbol{\xi},\tau) \tag{22}$$

and

$$\begin{aligned}\frac{d}{d\tau}\boldsymbol{\rho}(\boldsymbol{\xi},\tau) = {} & -(\boldsymbol{\xi}^2 + \mathrm{i}\xi_x\epsilon)\boldsymbol{\rho} - 4i(\mathbf{e}_z\times\boldsymbol{\xi})\times\boldsymbol{\rho} - i\epsilon_R\xi_y\mathbf{e}_z\rho \\ & + i\epsilon_I\xi_y\mathbf{e}_z\times\boldsymbol{\rho} - 4\boldsymbol{\rho} - 4\mathbf{e}_z\rho_z + 2\epsilon\mathbf{e}_y\times\boldsymbol{\rho}.\end{aligned} \tag{23}$$

The three terms on the right-hand side of Eq. (22) 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. (23) 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 $-4\mathbf{e}_x\rho_x - 4\mathbf{e}_y\rho_y - 8\mathbf{e}_z\rho_z$, 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 $\boldsymbol{\xi}$ to zero, the evolution equations for the quantities integrated over the whole system [total charge and total spin polarization, e.g., $\rho(\boldsymbol{\xi}=\mathbf{0},\tau)=\int d^2\mathbf{x}\rho(\mathbf{x},\tau)$] are obtained

$$\frac{d}{d\tau}\rho(\mathbf{0},\tau)=0, \tag{24}$$

$$\frac{d}{d\tau}\boldsymbol{\rho}(\mathbf{0},\tau)=-4\boldsymbol{\rho}-4\mathbf{e}_z\rho_z+2\epsilon\mathbf{e}_y\times\boldsymbol{\rho}. \tag{25}$$

Equation (24) 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 ϵ_R and ϵ_I.

The solution of Eq. (25) reads

$$\rho_x(\tau)=e^{-6\tau}\left[\rho_x(0)\cosh(2\tau\sqrt{1-\epsilon^2})+\frac{\rho_x(0)+\epsilon\rho_z(0)}{\sqrt{1-\epsilon^2}}\sinh(2\tau\sqrt{1-\epsilon^2})\right], \tag{26a}$$

$$\rho_y(\tau)=e^{-4\tau}\rho_y(0), \tag{26b}$$

$$\rho_z(\tau)=e^{-6\tau}\left[\rho_z(0)\cosh(2\tau\sqrt{1-\epsilon^2})-\frac{\epsilon\rho_x(0)+\rho_z(0)}{\sqrt{1-\epsilon^2}}\sinh(2\tau\sqrt{1-\epsilon^2})\right], \tag{26c}$$

where $\rho_x(0)$, $\rho_y(0)$, and $\rho_z(0)$ are the initial conditions. Note that there is a critical electrical-field strength $\epsilon_c=1$. In smaller fields the total spin polarization decays exponentially with time, but in larger fields, it additionally rotates with time. Expressed differently, for $\epsilon>1$ the eigenvalues of the set of equations (25) become complex, which means that its eigenmodes become oscillatory. This critical electric field $E_c=DK/\mu$ can also be expressed as $E_c=k_BTK/e$, provided the Einstein relation between D and μ is valid. Furthermore, without electric field, the z component of the total spin polarization decays twice as fast as the other two components.[23,29]

Taking for definiteness the initial condition $\boldsymbol{\rho}(0)=\mathbf{e}_z$, one obtains

$$\rho_x(\tau)=e^{-6\tau}\frac{\epsilon}{\sqrt{\epsilon^2-1}}\sin(2\tau\sqrt{\epsilon^2-1}), \tag{27a}$$

$$\rho_y(\tau)=0, \tag{27b}$$

$$\rho_z(\tau)=e^{-6\tau}\frac{\epsilon}{\sqrt{\epsilon^2-1}}\cos(2\tau\sqrt{\epsilon^2-1}+\phi), \tag{27c}$$

with $\sin\phi=1/\epsilon$. This expression is appropriate for $\epsilon>1$, whereas for $\epsilon<1$ the trigonometric functions become hyperbolic functions.

Note that the frequency of the polarization oscillation $2\sqrt{\epsilon^2-1}$ increases with the electric field ϵ. Apart from the decay factor $e^{-6\tau}$, the polarization $\boldsymbol{\rho}(\tau)$ 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 coordinates $x=\rho_x e^{6\tau}\sqrt{\epsilon^2-1}/\epsilon$ 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) does not depend on the electric field. For $\epsilon\to1$ the angle $\phi\to\pi/2$, i.e., the ellipse degenerates to a line with an inclination of 45° to the perpendicular direction. In the limit of strong electric field $\epsilon\to\infty$, the angle ϕ 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 $\epsilon\gtrsim10$.

Let us consider next the case of an inhomogeneous initial condition. We take a z-spin starting at the origin $\boldsymbol{\rho}(\mathbf{x},\tau=0)=\delta(\mathbf{x})\mathbf{e}_z$. The total spin polarization is still described by Eqs. (26). In order to obtain the local spin orientation, one has to solve Eqs. (22) and (23). This is done by solving these equations in Laplace-space and the following back transformation from Laplace space s to time τ and wave-vector space $\boldsymbol{\xi}$ to $\mathbf{x}$.

The asymptotic behavior of the local spin polarization for large times $\tau\to\infty$ and small distances $|\mathbf{x}|\ll2\sqrt{\tau}$ [Large distances will not be relevant here, since they are strongly suppressed by the "diffusion factor" $\exp(-\mathbf{x}^2/4\tau)$.] is

$$\rho_z(\mathbf{x},\tau)=\exp\left\{-\frac{(\mathbf{x}+\boldsymbol{\epsilon}\tau)^2}{4\tau}-\frac{7}{4}\tau\right\}\frac{3}{8\sqrt{\pi\tau}}J_0\left(\frac{\sqrt{15}}{2}|\mathbf{x}|\right). \tag{28}$$

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 $-\boldsymbol{\epsilon}$ 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 nonzero spin density is mainly constricted 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. 1). The strip extends from $y=-b$ to $y=b$; thus, its width is $2b$. Going from wave-vector space back to $\mathbf{x}$ space and assuming that $\rho(\mathbf{x})$ and $\boldsymbol{\rho}(\mathbf{x})=(\rho_x,\rho_y,\rho_z)$ depend only on the y coordinate, the

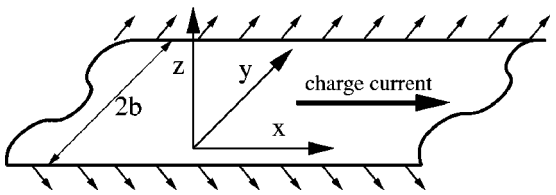

FIG. 1. The coordinate system chosen for the strip of finite width. The charge current within the strip is nonpolarized. But at the transversal boundaries $y=\pm b$, a finite spin density occurs due to ϵ_R, i.e., this situation leads to spin accumulation.

following set of differential equations determine the stationary state

$$\rho'' + \epsilon_R \rho_z' = 0, \tag{29a}$$

$$\rho_x'' + \epsilon_I \rho_y' + 2\epsilon\rho_z - 4\rho_x = 0, \tag{29b}$$

$$\rho_y'' - \epsilon_I \rho_x' + 4\rho_z' - 4\rho_y = 0, \tag{29c}$$

$$\rho_z'' + \epsilon_R \rho' - 4\rho_y' - 2\epsilon\rho_x - 8\rho_z = 0, \tag{29d}$$

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 (18) and (20) at the boundary to zero. This yields

$$(\rho' + \epsilon_R \rho_z)\big|_{y=\pm b} = 0, \tag{30a}$$

$$(\rho_x' + \epsilon_I \rho_y)\big|_{y=\pm b} = 0, \tag{30b}$$

$$(\rho_y' - \epsilon_I \rho_x + 4\rho_z)\big|_{y=\pm b} = 0, \tag{30c}$$

$$(\rho_z' + \epsilon_R \rho - 4\rho_y)\big|_{y=\pm b} = 0. \tag{30d}$$

One has to keep in mind that we want the solution to lowest order in K. The zeroth order solution of Eqs. (29a)–(30d) 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 $\boldsymbol{\rho}(y) = 0$. This solution is inserted into the terms containing ϵ_R and ϵ_I, which yield the equations for the first-order solution. Compared to the zeroth order equations, there is only one additional term: $\epsilon_R \rho$ gives a finite right-hand side in the boundary condition for the z component [corresponding to Eq. (30d)], all other terms containing ϵ_R and ϵ_I are still zero. The solution of this set of equations is easily constructed. Again, $\rho(y) = \text{const}$, and the three vectorial ρ components are weighted sums of functions $\sinh(\lambda y)$ and $\cosh(\lambda y)$, where λ takes on the three values: $\lambda_1 = 2$, $\lambda_2 = (\sqrt{8+\epsilon^2}-1)^{1/2} + i(\sqrt{8+\epsilon^2}+1)^{1/2}$ and $\lambda_3 = \lambda_2^*$. Thus, to lowest order in **K**,

$$\frac{\rho_x(y)}{\epsilon_R \rho} = -\frac{16\epsilon}{\alpha}\lambda_2 c_2 s_3 \sinh(2y) + \frac{2\epsilon}{\alpha}\left(16 c_1 s_3 + \frac{\epsilon^2}{2}\lambda_3 s_1 c_3\right)\sinh(\lambda_2 y) + \text{c.c.}, \tag{31a}$$

$$\frac{\rho_y(y)}{\epsilon_R \rho} = \frac{4\epsilon^2}{\alpha}\lambda_2 c_2 s_3 \cosh(2y) + \frac{4\lambda_2}{\alpha}\left(16 c_1 s_3 + \frac{\epsilon^2}{2}\lambda_3 s_1 c_3\right)\cosh(\lambda_2 y) + \text{c.c.}, \tag{31b}$$

$$\frac{\rho_z(y)}{\epsilon_R \rho} = -\frac{\lambda_2^2 - 4}{\alpha}\left(16 c_1 s_3 + \frac{\epsilon^2}{2}\lambda_3 s_1 c_3\right)\sinh(\lambda_2 y) + \text{c.c.}, \tag{31c}$$

with the abbreviations

$$\alpha = \lambda_2 c_2 \left[\frac{\epsilon^2}{2}|\lambda_2|^2 \lambda_2 s_1 c_3 + 16(\lambda_2^2 + 12 + \epsilon^2) c_1 s_3\right] - \text{c.c.} \tag{32}$$

and

$$c_i = \cosh(\lambda_i b), \quad s_i = \sinh(\lambda_i b) \quad (i = 1,2,3). \tag{33}$$

One can see that the electron density ρ and the spin Hall coefficient ϵ_R only influence the amplitude of the polarization. They do not affect the spatial dependence of $\boldsymbol{\rho}(y)$. The x and z component of the polarization are antisymmetric with respect to a sign change of y, whereas the y component is symmetric.

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

$$\rho_x(y) \approx -\operatorname{sgn}(y)\frac{\epsilon_R \rho}{\sqrt{2\epsilon}}\sin\left(\sqrt{\epsilon}(b-|y|) + \frac{\pi}{4}\right)e^{-\sqrt{\epsilon}(b-|y|)}, \tag{34a}$$

$$\rho_y(y) \approx -\frac{\epsilon_R \rho}{\epsilon}\sin[\sqrt{\epsilon}(b-|y|)]e^{-\sqrt{\epsilon}(b-|y|)}, \tag{34b}$$

$$\rho_z(y) \approx -\operatorname{sgn}(y)\frac{\epsilon_R \rho}{\sqrt{2\epsilon}}\cos\left(\sqrt{\epsilon}(b-|y|) + \frac{\pi}{4}\right)e^{-\sqrt{\epsilon}(b-|y|)}. \tag{34c}$$

The main effects of increasing the electric field ϵ 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 nonzero $\boldsymbol{\rho}$ near the borders. This suggestion can be fleshed out in the following way: We consider the half plane $y \geqslant 0$, set the electric field ϵ to zero, and apply the boundary condition $\boldsymbol{\rho}(y=0) = \boldsymbol{\rho}_0$. The differential equations for the stationary state (and homogeneous in x) are

$$\rho_x'' - 4\rho_x = 0, \quad \rho_y'' + 4\rho_z' - 4\rho_y = 0, \quad \rho_z'' - 4\rho_y' - 8\rho_z = 0, \tag{35}$$

which conceptually corresponds to an equation with the structure $D\Delta\boldsymbol{\rho} - \boldsymbol{\rho}/\tau = 0$, only that here the decay rate $1/\tau$

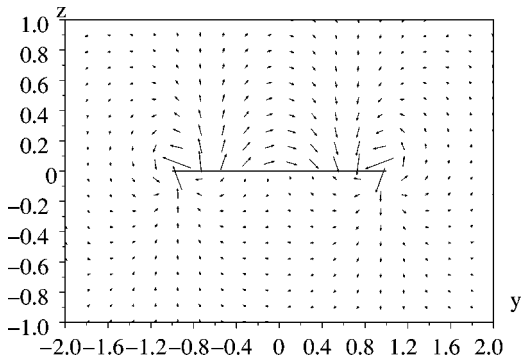

FIG. 2. The magnetic field due to the spin accumulation in the z-y plane. The parameters are $b=1$, $\epsilon=1$. The horizontal line denotes the extent of the strip.

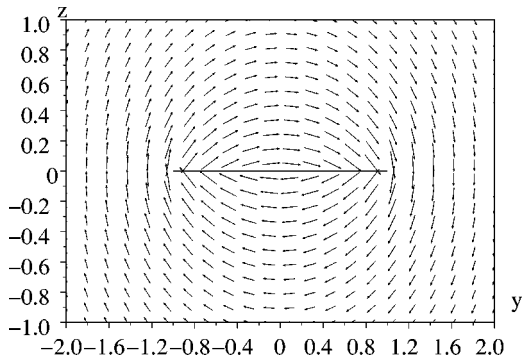

FIG. 3. The magnetic field due to the current through the strip. The parameters are the same as in Fig. 2.

depends on the direction (thus, it is a tensor), and there is an additional ''torque'' term. Since in Eq. (35) all coefficients 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 $1/(\sqrt{8}-1)^{1/2} \approx 0.74$ for the other two components, corresponding to the real parts of λ_1, λ_2, and λ_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 nonpolarized electrical current in an infinitely extended plane consists of z spins being transported perpendicularly to the electrical field $\mathbf{E}$ [see Eq. (20)]. 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 $\boldsymbol{\rho}(y)$ 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 $\mathbf{H}_M$ 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 $\mathbf{H}_I$ due to the electric current through the strip. These fields are calculated in Appendix C.

The y-z components of the magnetic field due to the spin polarization is shown in Fig. 2. For comparison, the behavior of the magnetic field due to the charge current is shown in Fig. 3. The parameters are chosen such that the dimensionless width of the strip and the dimensionless electric field are 1, respectively. One can see that the spatial behavior of the two contributions to the total magnetic field is quite different. This would, at least in principle, allow to differentiate between them.

As a last point, the magnetic field $\mathbf{H}_M+\mathbf{H}_I$ also interacts with the spin degrees of freedom through the Zeeman energy and 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 χ and the Bohr magneton μ_B, the spin polarization due to the back reaction can be expressed as $\boldsymbol{\rho}_{\mathrm{br}} = \chi\mathbf{H}/\mu_B \approx \chi\mathbf{M}/\mu_B = \chi\boldsymbol{\rho}$. 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 $\mathbf{R}_{m_2 m_1}$. The spin rotates in the plane spanned by the vectors $\mathbf{K}$ and $\mathbf{R}_{m_2 m_1}$. Let us consider a spin starting at the origin and being oriented 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. (28).

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 anisotropically: The z 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 (ϵ^R or μ_{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 strip 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.[4,18] It is possible to change this value by applying a gate voltage to the two-dimensional plane,[30] 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 α mentioned above, one obtains $K \approx 1/(76\ \text{Å})$, assuming that the effective electron mass is equal to its elementary mass. Thus, the condition $\mathbf{K}\times\mathbf{R}_{m'm} \ll 1$ for the validity of our theory demands in this case that the typical hopping length is shorter than 76 Å. 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 coefficient, the permitted length increases and it is furthermore modified by the effective electron mass. If the Einstein relation between diffusion coefficient and mobility is assumed to be valid, the critical electric field $E_c = k_B T K/e$ 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 coefficient for the spin Hall-effect. Thus, a large Hall mobility favors also the occurrence of the spin Hall-effect. We take Ref. 31 as an example. There, the conductivity and the Hall mobility of the hexaboride compounds $Eu_{1-x}Ca_xB_6$ 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 $\text{cm}^2/(\text{Vs})$. Using this value, Eq. (B14) 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. (31c) into account, this gives a relative spin polarization (z component) at the boundary of a two-dimensional strip $|\rho_z(b)/\rho|$ of about 5% at the critical electric-field strength $\epsilon = 1$.

The present investigation can be extended in several directions. A natural generalization would be the extension to a finite electron density, which would require Pauli and/or Hubbard correlations to be taken into consideration. This also opens the possibility to investigate equilibrium properties and the behavior near equilibrium. Another line of study would be the introduction of spatial or energetic disorder. This includes disordered polaronic systems, but also hopping on impurities or Anderson localized states, and would also allow the investigation of variable range hopping in the present context. Some of these extensions are work in progress.

ACKNOWLEDGMENTS

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APPENDIX A: CALCULATION OF THE SPIN MATRICES

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

$$e^{\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}} = \cos|\mathbf{A}| + \mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}\frac{\sin|\mathbf{A}|}{|\mathbf{A}|}, \tag{A1}$$

which is valid for any vector $\mathbf{A}$.

The quantity $\mathrm{Tr}(\boldsymbol{\sigma} e^{-\mathrm{i}\boldsymbol{\sigma}\mathbf{A}_{m_1 m}}\hat{\rho}_{m_1} e^{\mathrm{i}\boldsymbol{\sigma}\mathbf{A}_{m_1 m}})$ occurs in the calculation of the contribution of two-site diagrams to the rate equations. It can be transformed to $\mathrm{Tr}(e^{\mathrm{i}\boldsymbol{\sigma}\mathbf{A}_{m_1 m}}\boldsymbol{\sigma} e^{-\mathrm{i}\boldsymbol{\sigma}\mathbf{A}_{m_1 m}}\hat{\rho}_{m_1})$. With the help of Eq. (A1), the spin factors in the trace can be calculated to be

$$e^{\mathrm{i}\boldsymbol{\sigma}\mathbf{A}_{m_1 m}}\boldsymbol{\sigma} e^{-\mathrm{i}\boldsymbol{\sigma}\mathbf{A}_{m_1 m}} \approx \hat{D}_{m_1 m}\cdot\boldsymbol{\sigma}, \tag{A2}$$

where the quantity $\hat{D}$ is a 3×3 matrix describing a rotation about the axis $\mathbf{A}_{m_1 m} = \mathbf{K}\times\mathbf{R}_{m_1 m}$ and through the angle $2|\mathbf{A}_{m_1 m}|$. This is valid to quadratic order in $\mathbf{A}$. Explicitly,

$$\hat{D}_{m_1 m} = \mathbf{e}_z\times\mathbf{e}_R\circ\mathbf{e}_z\times\mathbf{e}_R + \sin|2\mathbf{A}|(\mathbf{e}_R\circ\mathbf{e}_z - \mathbf{e}_z\circ\mathbf{e}_R) + \cos|2\mathbf{A}|(\mathbf{e}_z\circ\mathbf{e}_z + \mathbf{e}_R\circ\mathbf{e}_R). \tag{A3}$$

The symbol ''$\circ$'' denotes the dyadic product and the orthogonal unit vectors are $\mathbf{e}_z = \mathbf{K}/K$ and $\mathbf{e}_R = \mathbf{R}_{m_1 m}/|\mathbf{R}_{m_1 m}|$. Here, it is used that $\mathbf{K}$ is perpendicular to the plane, i.e.

$\mathbf{K}\cdot\mathbf{R}=0$ for all vectors $\mathbf{R}$ within the plane. Retaining in this expression only terms of up to second order in K (since $A \ll 1$), one obtains

$$\hat{D}_{m_1m}=\hat{I}_3+2|\mathbf{A}|(\mathbf{e}_R\circ\mathbf{e}_z-\mathbf{e}_z\circ\mathbf{e}_R)-2|\mathbf{A}|^2(\mathbf{e}_z\circ\mathbf{e}_z+\mathbf{e}_R\circ\mathbf{e}_R), \tag{A4}$$

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 $\boldsymbol{\rho}$ 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 $\hat{\rho}$ is the last operator, the spin factors preceding $\hat{\rho}$ in the trace are calculated in order to obtain an expression of the form $f+g\boldsymbol{\sigma}$. Here, f and g are scalars in spin space. Thus, taking the trace yields $\mathrm{Tr}[(f+g\boldsymbol{\sigma})\hat{\rho}]=f\rho+g\boldsymbol{\rho}$, an expression where the spin operators have disappeared and are replaced by the particle density and the spin orientation. Using the operator identity $e^Ae^B \approx e^{A+B}e^{[A,B]/2}$, where the error is of third and higher order in the operators A and B, one obtains

$$e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{mm_2}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_2m_1}}\approx e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{mm_1}}e^{\mathrm{i}\boldsymbol{\sigma}\cdot(\mathbf{A}_{mm_1}\times\mathbf{A}_{mm_2})} \tag{A5}$$

and

$$e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{mm_2}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_2m_1}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_1m}}\approx e^{\mathrm{i}\boldsymbol{\sigma}\cdot(\mathbf{A}_{mm_1}\times\mathbf{A}_{mm_2})}. \tag{A6}$$

Using Eqs. (A2), (A5), 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.,

$$\begin{aligned}\mathrm{Tr}(&e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{mm_2}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_2m_1}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_1m}}\hat{\rho})\\ &\approx\cos|\mathbf{A}_2|\rho+\mathrm{i}\frac{\sin|\mathbf{A}_2|}{|\mathbf{A}_2|}\mathbf{A}_2\cdot\boldsymbol{\rho}\\ &\approx\rho+\mathrm{i}\mathbf{A}_2\cdot\boldsymbol{\rho},\end{aligned} \tag{A7}$$

$$\begin{aligned}\mathrm{Tr}(&e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{mm_2}}\boldsymbol{\sigma}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_2m_1}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_1m}}\hat{\rho})\\ &\approx\hat{D}_{m_2m}\cdot\left[\cos|\mathbf{A}_2|\boldsymbol{\rho}+i\frac{\sin|\mathbf{A}_2|}{|\mathbf{A}_2|}\mathbf{A}_2\rho-\frac{\sin|\mathbf{A}_2|}{|\mathbf{A}_2|}\mathbf{A}_2\times\boldsymbol{\rho}\right]\\ &\approx\hat{D}_{m_2m}\cdot\boldsymbol{\rho}+i\mathbf{A}_2\rho-\mathbf{A}_2\times\boldsymbol{\rho},\end{aligned} \tag{A8}$$

where the abbreviation $\mathbf{A}_2=\mathbf{A}_{mm_1}\times\mathbf{A}_{mm_2}$ is used, and the second approximation for each relation is the truncation to second order in $\mathbf{K}$.

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

APPENDIX B: TRANSITION PROBABILITIES FOR SMALL POLARONS

The second-order diagrams (two-site hopping) give rise to the transition rate[32]

$$\begin{aligned}W_{m_1m}=\frac{1}{\hbar^2}|J_{m_1m}|^2e^{-2S_T}\int_{-\infty}^{\infty}dt_1\Bigg(&\exp\Bigg\{\sum_{\mathbf{q}}\frac{\Gamma_q}{\sinh(\hbar\omega_q\beta/2)}\\ &\times\cos\omega_q\left(t_1+i\hbar\frac{\beta}{2}\right)\Bigg\}-1\Bigg)\exp\left\{\frac{i}{\hbar}e\mathbf{E}\cdot\mathbf{R}_{mm_1}t_1\right\},\end{aligned} \tag{B1}$$

with the abbreviations

$$\Gamma_q=\frac{|\gamma(q)|^2(1-\cos\mathbf{q}\cdot\mathbf{g})}{N} \tag{B2}$$

and

$$S_T=\sum_{\mathbf{q}}\frac{\Gamma_q}{2}\coth\left(\hbar\omega_q\frac{\beta}{2}\right). \tag{B3}$$

The sums run over the phonon wave vectors $\mathbf{q}$. $\gamma(q)$ is the electron-phonon interaction constant, ω_q the phonon frequency, N the number of phonon states, and $\beta=1/(k_BT)$. The quantity $\mathbf{g}=\mathbf{R}_{m_1m}$ can be restricted to be a vector connecting two nearest-neighbor sites, since we are interested in nearest-neighbor hopping only. Note that in this case, the integral is independent of the direction of $\mathbf{g}$. Thus, the resulting expression is isotropic in the absence of an electric field $\mathbf{E}$.

The transition rates obey the principle of detailed balance

$$\frac{W_{m_1m}}{W_{mm_1}}=e^{\beta e\mathbf{E}\cdot\mathbf{R}_{mm_1}}, \tag{B4}$$

as is easily verified using Eq. (B1).

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

$$\begin{aligned}\mathrm{i}\sum_{m_1m_2}\{&-e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{mm_2}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_2m_1}}\hat{\rho}_{m_1}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_1m}}W^{(3)}_{m_1m_2m}\\ &+e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{mm_1}}\hat{\rho}_{m_1}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_1m_2}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_2m}}W^{(3)*}_{m_1m_2m}\\ &-\hat{\rho}_me^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{mm_1}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_1m_2}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_2m}}W^{(3)*}_{mm_1m_2}\\ &+e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{mm_2}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_2m_1}}e^{-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{A}_{m_1m}}\hat{\rho}_mW^{(3)}_{mm_1m_2}\}.\end{aligned} \tag{B5}$$

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

$$W^{(3)}_{m_1m_2m}=\frac{1}{\hbar^3}J_{mm_2}J_{m_2m_1}J_{m_1m}I, \tag{B6}$$

where the symbol I denotes the integral

$$I(\mathbf{E}) = e^{-3S_T}\int_{-\infty}^{\infty} dt_1 \int_0^{\infty} dt_2 \Bigg(\exp\Bigg\{ \sum_{\mathbf{q}} \frac{\Gamma_q}{2\sinh(\hbar\omega_q\beta/2)} \times \Bigg[\cos\omega_q\left(t_1 + i\hbar\frac{\beta}{2}\right) + \cos\omega_q\left(t_2 + i\hbar\frac{\beta}{2}\right) + \cos\omega_q\left(t_1 - t_2 + i\hbar\frac{\beta}{2}\right)\Bigg]\Bigg\} - 1\Bigg) \times \exp\left\{\frac{i}{\hbar} e\mathbf{E}\cdot\mathbf{R}_{mm_1} t_1 - \frac{i}{\hbar} e\mathbf{E}\cdot\mathbf{R}_{mm_2} t_2\right\}. \tag{B7}$$

Again, the integral is independent of the direction of **g**, and the resulting expression is isotropic.

Taking two times the real part, the integral over t_2 would extend from $-\infty$ to ∞. This would be the expression to be calculated for the small polaron Hall-effect.[32,33] Here, we cannot take this step, because we also need to calculate the imaginary part of the expression (B7).

The three-site rate obeys the principle of detailed balance

$$W^{(3)}_{mm_2m_1} = W^{(3)}_{m_1m_2m} e^{-\beta e\mathbf{E}\cdot\mathbf{R}_{mm_1}} \tag{B8}$$

and has the further symmetry

$$W^{(3)}_{m_1mm_2} = W^{(3)}_{m_1m_2m}. \tag{B9}$$

Using these symmetries, the long wave-length limit of the third-order term, Eq. (12), for a triangular lattice (hexagonal crystal symmetry) can be calculated as

$$\mathbf{W}^R(\mathbf{q}) = i\mathbf{K}\circ\mathbf{q}\cdot(\mathbf{E}\times\mathbf{K})\frac{3a^4 e}{k_BT}\mathrm{Re}(W^{(3)}_{012}). \tag{B10}$$

In order to calculate $\mathbf{W}^I$ 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 $I(\mathbf{0})$ 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 $(i2\hbar\beta/3, i\hbar\beta/2)$. Under the condition $\hbar\omega_q \ll k_BT$ (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

$$I \approx \frac{\hbar^2\pi}{E_a k_BT 4\sqrt{3}} e^{-4E_a/3k_BT}\left(1 - i\sqrt{\frac{3k_BT}{E_a\pi}} e^{E_a/3k_BT}\right), \tag{B11}$$

where

$$E_a = \sum_{\mathbf{q}} \frac{\hbar\omega_q\Gamma_q}{4}. \tag{B12}$$

Combining Eq. (B11) with Eq. (B10), the mobility μ_{yx} connected with the anomalous Hall-effect and the spin Hall-effect reads

$$W^R K^2 = \mu_{yx} = \mu_0 \frac{\sqrt{3}\pi}{4} \frac{(Ka)^2 J^3}{E_a (k_BT)^2} e^{-4E_a/3k_BT}, \tag{B13}$$

where $\mu_0 = ea^2/\hbar$, a is the distance between nearest neighbors (lattice constant), and $J = J_{01}$ is the overlap integral between two nearest neighbors. This expression can be compared with the Hall mobility μ_H for small polaron hopping[32] to give the relation

$$\frac{\mu_{yx}}{\mu} = 2(Ka)^2 \frac{\mu_H}{\mu_0} = \frac{2\hbar K^2 \mu_H}{e}. \tag{B14}$$

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. (B11)], 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 $k_BT \ll E_a$.

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

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

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

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 $\mathbf{H}_I$.[20] 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 $I = eb\mu E\rho$ within the strip reads

$$\mathbf{H}_I(y,z) = \frac{I\mathbf{e}_y}{4\pi b}\arctan\left(\frac{2az}{y^2 + z^2 - b^2}\right) + \frac{I\mathbf{e}_z}{8\pi b}\log\left(\frac{z^2 + (y-b)^2}{z^2 + (y+b)^2}\right). \tag{C2}$$

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