Electrical generation of spin in crystals with reduced symmetry

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We propose a simple way of evaluating the bulk spin generation of an arbitrary crystal with a known band structure in the strong spin-orbit coupling limit. We show that, in the presence of an electric field, there exists an intrinsic torque term which gives rise to a nonzero spin generation rate. Using methods similar to those of recent experiments which measure spin polarization in semiconductors, this spin generation rate should be experimentally observable. The wide applicability of this effect is emphasized by explicit consideration of a range of examples: bulk wurtzite and strained zinblende (n-GaAs) lattices, as well as quantum well heterojunction systems.

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I. INTRODUCTION

A considerable amount of attention has been devoted in recent years, both experimentally and theoretically, to the field of semiconductor spintronics. There have been numerous suggestions of advantages offered by the manipulation of the spin degree of freedom, including the increased functionality of spin devices, low power consumption, integration with existing technologies and the fact that in spin transport quantum coherence can be maintained on large time scales. Semiconductors can be used in the same spintronic devices as metals, and have the additional advantages brought about by the existence of an adjustable bandgap and by the ability to manipulate the carrier density over many orders of magnitude by doping, gating and heterojunction formation. Moreover, spin accumulation in a semiconductor will generate a much larger voltage because the density of states at the Fermi energy is lower than in a metal, leading to a larger spin splitting.

To this end it would be extremely desirable if a practical method existed for the efficient generation of spin polarization inside a semiconductor, as well as for the transport of spins over a sizable length scale. Although optical spin injection has been known for decades, it is impractical for devices, since it is not sufficiently local for nanoelectronics. On the other hand, spin injection from a ferromagnetic metal into a semiconductor requires long spin lifetimes and is impeded by the resistivity mismatch between the two materials. Progress has been achieved with ferromagnetic semiconductors, but room temperature semiconductor ferromagnetism has not yet been clearly established. Recent research has focused on the electrical control of spins in semiconductors, including theoretical work on the possibility of observing a spin-Hall effect, together with various efforts to generate a spin current.

Following this energetic theoretical enterprise, recent experimental work has demonstrated the detection of a sizable spin accumulation in semiconductors to be a feasible task. Motivated by these findings, in this article we present a general theory of the intrinsic electrical spin generation that occurs generically in spin-orbit coupled systems that are not inversion-symmetric. We will concentrate on systems where the spin-orbit interactions are strong. The existence of the mechanism we discuss has been pointed out in the previous literature. Our approach is to be contrasted with earlier theories which consider directly the response of a spin polarization to an electric field, by Aronov et al. for example. When calculating the spin density directly via linear response it is, in general, not possible to separate the intrinsic generation terms from the extrinsic scattering effects, thus physical transparency is often sacrificed. On the other hand, in the present paper we recognize spin generation as an intrinsic effect so that it may be determined from first principles calculations. The interplay of the spin generation and relaxation terms, resulting in a finite spin polarization, emerges in the final analysis, as pointed out by Edelstein. So far, experiment has attempted to measure the spin generation rate separately from the spin relaxation time in the weak spin-orbit coupling limit. The idea we discuss has already been applied to the Rashba Hamiltonian, which we also examine below.

Spin-orbit interactions can be important in semiconductors for several reasons. The first is the fact that the carriers are clustered near the band extrema around high symmetry points where there exist degeneracies, and the form of these degeneracies is determined by the spin-orbit interaction. Due to the fact that in semiconductors the carriers occupy a narrow width of k-space the spin-orbit interaction can therefore play a crucial role. We will show in this article that, because of the fact that spin is not conserved, there exists a term which acts as a bulk source of spin generation. It represents the rate of change of the spin density in response to an external electric field.

Intrinsic spin-orbit effects have been shown to lead to a non-zero Berry curvature which gives a contribution to the anomalous Hall effect, while a spin-orbit-induced metal-insulator transition has been detected by Koga et al. From the references mentioned above, such intrinsic spin-orbit effects have not been taken into account previously, although several theories...
exist which account for the role intrinsic spin-orbit effects play in spin relaxation\textsuperscript{25}. Moreover, a number of articles have considered an electric-field-induced rotation of the total spin polarization\textsuperscript{30,31}, which is distinct from the electrical spin generation we discuss in our work. In the situations we consider, the total spin polarization is initially zero, therefore it cannot undergo a rotation.

Because both the rate of change of the spin density and the electric field are even under time reversal, ferromagnetism is not required for spin generation. Nevertheless, because the electric field changes sign under spatial inversion while the rate of change of the spin density does not, spin generation occurs only in crystals with broken inversion symmetry. Further details of these symmetry arguments will be given in the last section.

The outline of this paper is as follows. In section II we will present the formalism underlying our discussion of intrinsic spin generation. The mechanism we outline applies to a wide class of systems, and to illustrate this we discuss, in section III, two-dimensional heterostructures described by the Rashba model, followed by a model of the conduction bands of unstrained bulk wurtzite structures and strained bulk $n$-GaAs.

\section{II. FORMALISM}

In the physical picture we consider, the spin-orbit interaction has been taken into account in the band structure. We adopt a Boltzmann-wave-packet approach, in which the carriers in a band labeled by the index \( n \) are described by wave-packets following a Boltzmann phase-space distribution \( f_n(r,c,k,t) \). The construction of a wave-packet representing a charge and spin carrier in band \( n \), which has real and \( k \)-space coordinates \((r,c,k)\), has been thoroughly treated by Sundaram and Niu\textsuperscript{32} and will not be considered at length here. The semiclassical equations of motion for \((r,c,k)\), in the presence of a constant uniform electric field \( F \), are\textsuperscript{32}:

\begin{equation}
\begin{aligned}
\hbar \dot{k}_c &= -eE \\
\hbar \dot{c}_n &= \frac{\partial \varepsilon_n}{\partial k_c} + eE \times \Omega_n,
\end{aligned}
\end{equation}

where \( \Omega_n = 2\text{Im} \left( \frac{\partial \varepsilon_n}{\partial k_c} \right) \) represents the Berry, or geometrical curvature\textsuperscript{32}.

The theory presented in this article is a theory of spin accumulation in the strong spin-orbit coupling limit, implying that the splitting of the bands due to the spin-orbit interaction exceeds their broadening due to disorder at all wave-vectors. As a result, the bands are well defined although, due to the presence of the spin-orbit interaction, they are not pure spin-up and spin-down bands. The distribution function corresponding to each band \( n \), \( f_n \), can drift according to the semiclassical equations of motion, and can also change due to collisions. The time evolution of the distribution function is governed by the Boltzmann equation,

\begin{equation}
\frac{\partial f_n}{\partial t} + \dot{c}_n \frac{\partial f_n}{\partial c}_n + \dot{k} \frac{\partial f_n}{\partial k} = \frac{df_n}{dt} \text{coll}.
\end{equation}

The right hand side, \( \frac{df_n}{dt} \text{coll} \), is the collision term which may be modeled by a relaxation time approximation when scattering is weak enough, or it may be expressed in terms of collision integrals. For electrons in equilibrium, the solution of the Boltzmann equation is \( f_n^{(0)} \), the Fermi-Dirac distribution, while in a general nonequilibrium situation \( f_n \) can be written as \( f_n^{(0)} + \delta f_n \). In the presence of a constant uniform electric field \( E \) the shift \( \delta f_n \) is given, in the relaxation time approximation, by the well-known result\textsuperscript{32}:

\begin{equation}
\delta f_n = f_n - f_n^{(0)} = e\tau_p E \cdot \nabla f_n^{(0)}.
\end{equation}

where \( \nabla = \frac{1}{\hbar} \frac{\partial}{\partial c} \), \( \varepsilon_n \) is the energy of band \( n \), and \( \tau_p \) is the momentum relaxation time. We shall refer to terms which depend only on the equilibrium value of the distribution function, \( f_n^{(0)} \), as intrinsic, as opposed to extrinsic terms, depending on the nonequilibrium distribution, and therefore on scattering.

The study of spin generation necessarily relies on the spin equation of continuity. For the case we consider, we have shown in a previous publication\textsuperscript{14} that this equation takes the form:

\begin{equation}
\frac{\partial S_n}{\partial t} + \nabla \cdot \mathbf{J}_n^s = \mathcal{T}_n + \int d^3k \int df_n \mathbf{\hat{J}}(\hat{s})_n.
\end{equation}

The terms on the LHS represent the spin density and current in band \( n \), while the last term in the equation takes into account collisions. The abbreviation \( \langle \hat{s} \rangle_n \) stands for the expectation value in band \( n \) of the spin operator corresponding to any one component of the spin. We specialize henceforth in homogeneous systems, in which the divergence of the spin current in \( 41 \) will be zero and the equation of continuity may be written as:

\begin{equation}
\frac{\partial S_n}{\partial t} = \mathcal{T}_n + \int d^3k \left( f_n^{(0)} - f_n \right) \mathbf{\hat{J}}(\hat{s})_n,
\end{equation}

where \( \tau_p \) is the relaxation time. The first term on the RHS, which accounts for spin generation in the absence of collisions, is the focus of this paper. This term, which we shall call the torque density, exists due to the fact that spin is in general not conserved and therefore the average spin of a wave-packet is not constant in time. As discussed in Culcer \textit{et al.}\textsuperscript{14}, this torque density is defined as:

\begin{equation}
\mathcal{T}_n(r,t) = \int d^3r_c \int d^3k f_n(r_c,k,t)\langle \hat{s} \delta (\hat{r} - r) \rangle_n,
\end{equation}

in which \( \hat{r} \) is understood as \( \frac{1}{\hbar} [\hat{H}, \hat{s}] \), \( \hat{H} \) is the Hamiltonian, \( \hat{r} \) is the quantum-mechanical position operator and
\[ \langle \rangle \] stands for the expectation value in a wave-packet constructed starting from the eigenfunction corresponding to band \( n \). Throughout this paper we assume that products of non-commuting operators have been symmetrized. We note that the equation of continuity \[ \begin{align*}
\end{align*} \] is derived directly from the first-principles definitions of \( S_n, J_n^s \) and \( \mathcal{T}_n \). In homogeneous systems the torque density simplifies to

\[ \mathcal{T}_n = \int d^3 k f_n \langle \dot{\tau} \rangle_n, \]  

which will be referred to as the spin generation term. The fact that we are considering homogeneous systems also implies that we may regard the wave-packets as being wide in real space, thus sharp in \( k \)-space, and evaluate the expectation value \( \langle \dot{\tau} \rangle_n \) using Bloch wavefunctions. It should be pointed out that, although we arrive at our results semiclassically, one does not require a local description to obtain them, and they can be found using, for example, a Kubo formula approach. The connection to this latter approach will be detailed in what follows. Moreover, our theory is not restricted to the generation of spin, since \( \langle \dot{s} \rangle_n \) may represent the wave-packet expectation value of any component of any other non-conserved observable.

We will be concerned with a system in which only a constant uniform electric field is present. Making a convenient choice of gauge, this electric field can be included in the Hamiltonian through the electromagnetic vector potential \( \mathbf{A} \) \( \mathbf{r}, t \) only. This results in a nonadiabatic mixing of the bands, so that the Bloch wavefunctions \( |u_n\rangle \) have the following form:

\[ |u_n\rangle = |\phi_n\rangle - \sum_{m \neq n} \frac{\langle \phi_m | h \frac{d}{d t} | \phi_n \rangle}{\epsilon_n - \epsilon_m} |\phi_m\rangle, \]  

where the \( \{|\phi_n\rangle\} \) are the unperturbed Bloch eigenstates. The only time dependence comes from the fact that \( k \) drifts under the action of the electric field, as in \[ \begin{align*}
\end{align*} \]. Therefore it is legitimate to make the replacement \( \frac{d}{d t} \rightarrow -e \mathbf{E} \cdot \frac{d}{d k} \) in \[ \begin{align*}
\end{align*} \]. In this way, the wave functions \( |u_n\rangle \) depend on the electric field through a reactive term, in other words the field induces a change in the wave functions at each \( k \). The \( \{|u_n\rangle\} \) form a complete set. Moreover, the expectation value \( \langle \dot{s} \rangle_n \equiv \langle u_n | \dot{s} | u_n \rangle \) is a function of \( k \) only, and its time dependence arises implicitly through its dependence on the wave vector. We have thus included the effect of the electric field in mixing the bands but neglected inter-band scattering.

In the limit of wide wave-packets, it is straightforward to prove, starting from Eq. \[ \begin{align*}
\end{align*} \], that \( \langle \dot{\tau} \rangle_n \) evaluated in the \( \{|u_n\rangle\} \) basis is equal to \( \frac{\partial \langle \dot{s} \rangle_n}{\partial k} \), where \( \langle \dot{s} \rangle \) is evaluated in the unperturbed \( \{|\phi_n\rangle\} \) basis and \( k = -\frac{e \mathbf{E}}{\hbar} \) from \[ \begin{align*}
\end{align*} \]. The former approach is equivalent to using the Kubo formula to find the response of \( \dot{\tau} \) to an electric field. Following this line of thought, we find that the spin generation term is always at least first order in the electric field. Then, to first order in the electric field, we may replace \( f_n \) by its equilibrium value \( f_n^{(0)} \). This spin generation term is then purely intrinsic, as defined at the beginning of this section. The final form of this term is:

\[ \mathcal{T}_n = -\frac{e \mathbf{E}}{\hbar} \int d^3 k f_n^{(0)} \frac{\partial \langle \dot{s} \rangle_n}{\partial k}. \]  

Our theory thus shows that there exists a spin generation rate which can be interpreted as due to a displacement of the wave-packet in \( k \)-space, but also as the expectation value of the operator \( \dot{\tau} \) in a state which is not an eigenstate of the crystal Hamiltonian. Experiment has been attempting to measure this rate of generation, but for the time being success has been achieved only in the weak spin-orbit coupling limit.

In the steady state the equation of continuity becomes simply:

\[ \int d^3 k f_n^{(0)} \langle \dot{s} \rangle_n = \mathcal{T}_n \]  

Remembering that \( \int d^3 k f_n^{(0)} \langle \dot{s} \rangle_n = 0 \) and assuming a momentum relaxation time independent of wave-vector, the LHS is simply \( \frac{\dot{\mathcal{T}}_n}{\tau_p} \). We can then rewrite the above equation to express the steady state spin density as:

\[ S_n = \mathcal{T}_n \tau_p \]  

The characteristic time governing the relaxation of the spin density distribution is the momentum relaxation time. This is to be expected, since the theory describes non-degenerate, well defined bands.

We note that the torque term must be present even in a clean system if the Hamiltonian contains spin-non-conserving terms. In the presence of scattering mechanisms, the intrinsic spin generation term is balanced by the extrinsic spin relaxation term so that a net spin polarization can be reached in the steady state. In addition, in the systems we consider, we assume scattering is strong enough to keep the distribution function near equilibrium and the scattering time small, but not strong enough to make inter-band mixing important.

### III. Examples

In order to clarify the significance of the examples presented below, we start with some comments regarding the spin-orbit interaction and asymmetry. The terms in the spin-orbit interaction which are odd in \( k \) rely upon the inversion asymmetry of the system under study. This asymmetry can be of two kinds, depending on the dimensionality of the system. In three dimensions, the inversion asymmetry is a property of the underlying material, and is referred to as bulk inversion asymmetry (BIA). In two dimensions, an asymmetric confinement potential can provide an additional source of inversion asymmetry,
known as structure inversion asymmetry (SIA). Moreover, the application of strain along a particular direction further reduces the symmetry of the structure, with important consequences which will be examined below.

A. Rashba-type spin-orbit interaction

Our theory allows us to treat bulk semiconductors and quantum wells on the same footing. We begin with a study of the Rashba Hamiltonian. This Hamiltonian describes, based on symmetry arguments, the SIA of quantum well or heterojunction based two dimensional electron systems and is usually the dominant source of spin-orbit coupling in these systems. The effective Hamiltonian has the form:

$$H = \frac{\hbar^2 k^2}{2m} + \alpha (\sigma \times k) \cdot \hat{z},$$

(12)

in which $\alpha$ is the spin orbit constant and $\sigma$ is the vector of Pauli spin matrices. $\alpha$ is usually taken to have the form $a_{46} E_z$, where $a_{46}$ is a material specific parameter while $E_z$ is the component of the electric field in the $z$ direction. This electric field is in general a function of position in the quantum well, and there exists in principle an additional contribution if the interface on one side of the quantum well is different from the interface on the other side. This effective Hamiltonian therefore provides only an approximate description of the Rashba effect. The magnitude of the Rashba interaction can be tuned by an external gate voltage by an amount which has been shown to be as much as 50\%. It is customary to view the term multiplying the spin as a momentum-dependent effective magnetic field in which the spin precesses. In the absence of an external magnetic field, the bands in the Rashba model are degenerate at $k = 0$, and each band contains the same number of spin up and spin down carriers. The Hamiltonian has eigenvalues $\epsilon_{\pm} = \pm \frac{\hbar^2 k^2}{2m} \pm \alpha k$, which will be labeled by $+$ and $-$ respectively. The Berry curvatures are $\Omega_{\pm} = \pm \frac{1}{2} \lim_{h \to 0} \frac{\alpha^2 \hbar^2}{(\pi m^2 + \pi \hbar^2)^2}$. The spin generation term takes the following form:

$$\langle \hat{T} \rangle_\pm = \mp \frac{e \hbar \alpha}{2k^3} (k \times E) \cdot \hat{z},$$

(13)

with $\langle \hat{T} \rangle$ defined in Eq. 6. Interestingly, the spin torque does not depend on the spin-orbit constant. However, the total torque term, summed over the two bands, depends on the difference in Fermi wave vectors, which is proportional to the spin-orbit constant. We find that

$$T = \frac{e \alpha m}{4\pi \hbar^2} E \times \hat{z},$$

(14)

which vanishes in the limit in which $\alpha \to 0$, is in agreement with Magari\textsuperscript{23}. This result does not depend on the number density and has a universal form, but it should be noted that its validity is not universal, rather it is restricted to systems in which disorder is weak as discussed at the end of the previous section.

Using symmetry arguments, we find that the spin-orbit coupling in the conduction band of bulk wurtzite structures is also described by a Rashba-type Hamiltonian, with a spin-orbit constant defined analogously. This conclusion is supported by group theory arguments\textsuperscript{24}. The only terms linear in $k$ (and therefore dominant except at high densities) which are allowed by symmetry are $\beta(\sigma_x k_y - \sigma_y k_x)$, and the Hamiltonian is:

$$H = \frac{\hbar^2 k^2}{2m} + \beta(\sigma_x k_y - \sigma_y k_x)$$

(15)

with eigenvalues (labeled as before) $\frac{\hbar^2 k^2}{2m} \pm \beta k$. The spin generation term has a form very similar to \textsuperscript{19}:

$$\langle \hat{T} \rangle_\pm = \mp \frac{e k_{\perp}}{2k_{\perp}} (k_{\perp} \times E) \cdot \hat{z}$$

(16)

In the above, $k_{\perp} = (k_x, k_y, 0)$. The total torque term is:

$$T = \frac{e m \beta}{4\pi^2 \hbar^2} (3\pi^2 n)^{1/3} E \times \hat{z}$$

(17)

which again vanishes as $\beta \to 0$ and as the number density $n \to 0$.

B. Cubic Dresselhaus spin-orbit interaction

Finally, we turn our attention to the conduction band of zincblende semiconductors, which has been the focus of experiment recently\textsuperscript{19}. In order to be close to experiment, we consider a degenerate electron gas in an $n$-doped In$_x$Ga$_{1-x}$As heterostructure grown on GaAs, with $x=0.07$, with a strain of 0.46\% directed along (001), as given in the recent paper of Kato et al\textsuperscript{24} and references therein. The Fermi surface is only slightly displaced from equilibrium, as revealed by the drift velocities and by the mobility measurements in the supplementary table. We will not, however, attempt to simulate experiment, as many aspects seem to remain incompletely understood. For example, it is known that the strain tensor acquires off-diagonal shear terms\textsuperscript{17}, but experiment does not so far provide an unambiguous way of determining their role\textsuperscript{19,38}. Therefore, we will consider an idealized situation in which the $x$ and $y$ lattice constants are equal to their substrate values, while the lattice constant in the $z$ direction expands according to the elastic equations. Moreover, there is no convincing pattern in the variation of the BIA with increasing strain in the experiment. In fact, the only sizable increase is observed at the largest value of the strain, which is 0.46\%. Thus, it is not clear whether the linear or cubic term in the BIA is dominant in the samples investigated.

The symmetry of zincblende does not allow terms linear in $k$ in the conduction band in the bulk. As a result, when strain is applied these linear-in-$k$ terms will be first order in the strain. These terms will be important at small wave vectors, but we will concentrate on
situations in which the number density makes the Fermi wave-vector \( k_F \) high enough that the cubic Dresselhaus term is dominant. We therefore neglect the effect of the terms linear in \( k \) in this calculation, although we take into account the effect of strain on the effective masses.

We will take into account only the spin-orbit terms cubic in \( k \) which are present in the unstrained lattice, namely \( \lambda \sigma_x [k_x (k_y^2 - k_z^2) + c.p.] \), where \( \lambda \) is the spin-orbit constant and c.p. stands for cubic permutations. To determine the range of validity of this approach, we estimate the doping density \( n \) at which the bands overlap. By increasing \( n \) is performed in a doped semiconductor in the extrinsic regime. We lies in the weak spin-orbit coupling limit, \( k^3 \) term dominates the linear-in-\( k \) BIA and SIA terms. Based on the data in Kato et al., we estimate that the term cubic in \( k \) will dominate if \( n \geq 2.7 \times 10^{16} \text{ cm}^{-3} \), which puts the experiment, in which \( n = 3 \times 10^{16} \text{ cm}^{-3} \), narrowly in the range in which this term is dominant. Our prediction is, however, consistent with the bulk BIA findings of Kato et al.

Our theory is valid in the limit of strong spin-orbit interactions or weak disorder. For our theory to be valid, the following must hold:

\[
\frac{\hbar}{\tau_p} < \Delta_{so}(k_F), \tag{18}
\]

where \( \tau_p \) is the momentum relaxation time and \( \Delta_{so}(k_F) \) is the spin-orbit splitting at the Fermi wave vector. From the mobility, \( \tau_p \) is estimated at 0.22 ps, yielding \( \frac{\hbar}{\tau_p} = 2.9 \text{ meV} \).

In order for the spin-orbit to overwhelm this, the number density must exceed \( 3.5 \times 10^{16} \text{ m}^{-3} \), which is a more stringent requirement than the requirement that the cubic Dresselhaus term exceed the linear one. In other words, when the system is in the strong spin-orbit coupling limit it is already in the regime where the \( k^3 \) term dominates. This calculation also shows that the experiment of Kato et al. lies in the weak spin-orbit coupling limit, outside the validity limit of our theory. The experiment is performed in a doped semiconductor in the extrinsic regime, where extrinsic (as defined in section II) refers to situations in which scattering effects are dominant, that is the spin-orbit splitting at \( k_F \) is broadened beyond the point at which the bands overlap. By increasing \( n \) one increases \( k_F \) and therefore \( \Delta_{so}(k_F) \), passing into the intrinsic regime.

The Hamiltonian for this system is:

\[
H = \frac{\hbar^2 k_x^2}{2m_\perp} + \frac{\hbar^2 k_z^2}{2m_z} + \lambda \sigma_x [k_x (k_y^2 - k_z^2) + c.p.], \tag{19}
\]

where \( k_\perp \) has been defined above. It has eigenvalues

\[
\varepsilon_\pm = \frac{\hbar^2 k_x^2}{2m_\perp} + \frac{\hbar^2 k_z^2}{2m_z} \pm \Delta \text{ (labeled as before), with } \Delta \text{ given by } \sqrt{[k_y^2 (k_y^2 - k_z^2)]^2 + c.p.}. \]

The Berry curvatures are given by \( \Omega_{\pm} = \pm \frac{(k_x^2 - k_y^2)(k_y^2 - k_z^2)(k_z^2 - k_x^2)}{2\Delta^3} \).

In this model the \( x \)-component of spin takes the form:

\[
\langle s^x \rangle_\pm = \frac{\hbar k_x (k_y^2 - k_z^2)}{2\Delta}, \tag{20}
\]

with the other components given by cubic permutations of this expression. The \( x \)-component of the spin generation term is:

\[
\langle \dot{\tau} x \rangle_\pm = \mp \frac{e \lambda E_x (k_y^2 - k_z^2)(k_y k^4 + k_y^4 k_y^4 - k_y^4 k_y^2 - k_y^4 k_z^2)}{2\Delta^3}. \tag{21}
\]

Again the other components can be found by cubic permutation. Note that, if strain were absent so that the cubic Dresselhaus term exceed the linear one. In contrast to the Rashba model, the diagonal components of the tensor are finite, whereas the off-diagonals vanish. To obtain an explicit expression for the total spin torque, we must integrate over the Fermi surface, which in this case is ellipsoidal. We use the equilibrium distribution and the fact that \( f(\varepsilon \pm \lambda \Delta) = f(\varepsilon) \pm \lambda \Delta \frac{\partial f(\varepsilon)}{\partial \varepsilon} \), with \( \varepsilon = \frac{\hbar^2 k_x^2}{2m_\perp} + \frac{\hbar^2 k_z^2}{2m_z} \) and \( - \frac{\partial f(\varepsilon)}{\partial \varepsilon} = \delta(\varepsilon - \varepsilon_F) \).

We write the mass ratio as \( \frac{m_\perp}{m_\perp} = 1 + \gamma \), where \( \gamma \) is a small quantity, and we find that for the system under study \( \gamma = 0.023 \). The total result is:

\[
\chi_{xx} = \frac{3 e \lambda m_\perp \mathcal{I}}{8 \pi \hbar^2} (1 + \gamma)^{1/2}, \tag{22}
\]

where \( \mathcal{I} \) is a dimensionless angular integral, which contains the angular part of \( f(\theta, \phi) \), given by:

\[
\mathcal{I} = \int_0^\pi d \theta \int_0^{2\pi} d \phi \sin \theta [\sin^2 \theta \sin^2 \phi - (1 + \gamma) \cos^2 \theta] \times \frac{f(\theta, \phi)}{g(\theta, \phi)}, \tag{23}
\]

where the functions \( f \) and \( g \) are as follows:

\[
f(\theta, \phi) = (1 + \gamma)^2 \cos^4 \theta \sin^2 \phi + (1 + \gamma) \cos^2 \theta \sin^2 \theta \sin^2 \phi - \sin^4 \theta \cos^4 \phi \sin^2 \phi - (1 + \gamma) \cos^2 \theta \sin^2 \theta \cos^4 \phi \]
\[
g(\theta, \phi) = \sin^4 \theta \cos^2 \phi \sin^2 \phi + (1 + \gamma) \sin^2 \theta \cos^2 \theta \cos^2 \phi + \sin^4 \phi + (1 + \gamma) \cos^2 \theta \sin^2 \theta \cos^2 \phi \sin^2 \phi. \]
Using a Monte Carlo integration method, we find that \( \mathcal{I} = -0.03037 \). Based on symmetry arguments, \( \mathcal{I} \) vanishes when \( \gamma = 0 \), i.e., when \( m_z = m_y \). This can be seen from Eq. (21) by switching \( k_y \) and \( k_z \). At small \( \gamma \), \( 0 < \gamma < 0.1 \), our calculations show that \( \mathcal{I} \) is linear in \( \gamma \) and is given approximately by \( \mathcal{I} = -1.28 \gamma \). We expect that, for \( n = 10^{13} \text{ cm}^{-3} \), \( \chi_{xx}^z = -1.15 \times 10^{-7} \text{ c/m}^2 \). This result is four orders of magnitude larger than that observed in the current experiments in the weak spin-orbit coupling limit, which should offer an incentive for doping the samples in order to move into the strong spin-orbit limit. Meanwhile, for the density \( n = 3 \times 10^{16} \text{ cm}^{-3} \) used in experiment we find \( \chi_{xx}^z = -3.83 \times 10^{-10} \text{ c/m}^2 \), a number that is one order of magnitude larger than that observed. We stress again however that the experiment was performed in the weak spin-orbit coupling limit.

### IV. SYMMETRY CONSIDERATIONS

The form of the electric torque response tensor in different systems can be understood based on symmetry arguments. In Table I we have listed a number of possible spatial transformations which are relevant to our problem as well as the behavior of the electric field and spin torque under these transformations. The transformations considered are not assumed to be symmetry operations of the materials under study. \( I_m \) refers to spatial inversion along the \( m \)-axis, that is \( m \to -m \), while \( R_m \) refers to a rotation of arbitrary magnitude anticlockwise about the \( m \)-axis. For simplicity and without loss of generality we take the electric field to be directed along \( x \) and consider the generation of spin along all three Cartesian axes in response to this electric field.

Referring to the first part of the table, first row, it can be seen that under spatial inversion in the \( x \)-direction the electric field changes sign while \( \langle \hat{\tau} \rangle_x \) remains the same. On the other hand, under the same transformation \( \langle \hat{\tau} \rangle_y \) and \( \langle \hat{\tau} \rangle_z \) change sign, behaving in the same way as the electric field. As a result, if spatial inversion along \( x \) is a symmetry operation of the material the torque term \( \langle \hat{\tau} \rangle_x \) will vanish, but no information can be inferred about \( \langle \hat{\tau} \rangle_y \) and \( \langle \hat{\tau} \rangle_z \). An analogous argument holds for inversion along the \( y \) and \( z \) axes. Therefore if spatial inversion along all three axes is a symmetry of the material all components of the torque must vanish. This is consistent with the observation that \( \langle \hat{\tau} \rangle = 0 \) under a three dimensional inversion. Furthermore, this table helps explain the form of the torque in systems with Rashba spin-orbit interaction. The Rashba Hamiltonian has \( I_x \) and \( I_y \) as symmetries while \( I_z \) is broken. Examining Table I we see that in response to \( E_x \) only \( \langle \hat{\tau} \rangle_y \) can be nonzero, consistent with our findings in the previous section.

Next let us consider the effect of rotations by \( \pi \) about the three Cartesian axes. In the second part of the table, first row, we examine a rotation about \( x \). This rotation does not affect \( E_x \) and \( \langle \hat{\tau} \rangle_x \), but \( \langle \hat{\tau} \rangle_y \) and \( \langle \hat{\tau} \rangle_z \) change sign. Therefore, if \( R_x^\pi \) is a symmetry operation \( \langle \hat{\tau} \rangle_y \) and \( \langle \hat{\tau} \rangle_z \) will be zero in response to \( E_x \). By extension, if rotations by \( \pi \) about all Cartesian axes are symmetry operations then all the off-diagonal components of the electric torque response tensor are zero. For example, in GaAs, with or without strain applied along the \( z \)-axis, rotations by \( \pi \) about all three axes are symmetry operations so the off diagonal components of \( \chi^z \) are zero.

Let us also consider the combined effect of rotation and inversion, taking GaAs as an example. GaAs does not have inversion along any of the three Cartesian axes as a symmetry operation. Therefore we cannot infer the vanishing or survival of the electric torque response tensor in GaAs based on considerations of inversion alone. With the electric field still along \( x \), we consider an anticlockwise rotation by \( \pi \) about the \( x \)-axis followed by inversion along \( x \), \( y \) and \( z \). The rotation does not affect \( E_x \) and \( \langle \hat{\tau} \rangle_x \). Looking at the third part of the table, first row, the electric field changes sign under \( I_x R_x^\pi \) while \( \langle \hat{\tau} \rangle_x \) does not. Therefore, if \( I_x R_x^\pi /2 \) is a symmetry of the system, the \( x \)-component of the torque in response to \( E_x \) will vanish. A similar argument holds for the \( y \) and \( z \) axes. Therefore if \( I_m R_m^\pi /2 \) is a symmetry for all Cartesian axes all the diagonal components of the electric torque response tensor will be zero. This operation is a symmetry of bulk GaAs and in order to remove the rotational symmetry we consider strain applied along the \( z \) axis. In this case \( I_x R_x^\pi /2 \) and \( I_y R_y^\pi /2 \) are not symmetries anymore, allowing \( \chi_{xx} \) and \( \chi_{yy} \) to be nonzero, while \( \chi_{zz}^z \) is zero.

### V. CONCLUSIONS

We have shown that in crystals with inversion asymmetry and strong spin-orbit interactions a spin accumulation will be generated in the presence of an electric field due to an intrinsic spin torque term. In the steady state, the spin accumulation is given simply by the product of this torque term with the momentum relaxation time. This term is expected to be observable both in systems with Rashba spin-orbit interactions and with Dresselhaus interactions. In the latter we have shown that by doping so as to bring the system into the intrinsic regime, the
effect can be observed using currently available technology.

Finally, we would like to mention a novel experimental method which has been recently proposed. In condensed matter it is usually not possible to isolate a single charge carrier in order to measure effects occurring on the scale of an individual wave-packet. Therefore, to be able to verify the existence and properties of the spin generation term one may resort to atomic physics. Using a cold-atom system to construct an individual wave-packet and mimic the spin-orbit interaction, an experiment can measure, for example, the size, wave vector and electric field dependence of \( \langle \hat{r} \rangle \) for this wave-packet. This method and the physics underlying it are described in detail by Dudarev et al.\textsuperscript{40}.

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1. A. Fert, J. M. George, H. Jaffres, and G. Faini, J. Phys. D 35, 2443 (2002).
2. D.K. Young, J. A. Gupta, E. Johnston-Halperin, R. Epstein, Y. Kato, and D. D. Awschalom, Semicond. Sci. Technol. 17, 275 (2002).
3. J.M. Kikkawa and D.D. Awschalom, Phys. Rev. Lett. 80, 4313 (1998).
4. G. Schmidt and L.W. Molenkamp, Semicond. Sci. Technol. 17, 310 (2002); G. Schmidt, D. Ferrand, L. W. Molenkamp, A. T. Filip, and B. J. van Wees, Phys. Rev. B 62, R4790 (2000); G. Schmidt, G. Richter, P. Grabs, C. Gould, D. Ferrand, and L. W. Molenkamp, Phys. Rev. Lett. 87, 227203 (2001).
5. Y. Ohno, R. Terauchi, T. Adachi, F. Matsukura, and H. Ohno, Phys. Rev. Lett. 83, 4196 (1999); Y. Ohno, D. K. Young, B. Beschoten, F. Matsukura, H. Ohno, and D. D. Awschalom, Nature 402, 790 (1999).
6. R. Fiederling, M. Keim, G. Reuscher, W. Ossau, G. Schmidt, A. Waag, and L. W. Molenkamp, Nature 402, 787 (1999); I. Malajovich, J. M. Kikkawa, D. D. Awschalom, J. J. Berry, and N. Samarth, Phys. Rev. Lett. 84, 1015 (2000).
7. X. Jiang, R. Wang, S. van Dijken, R. Shelby, R. Macfarlane, G. S. Solomon, J. Harris, and S. S. P. Parkin, Phys. Rev. Lett. 90, 256603 (2003).
8. B.T. Jonker, Proceedings IEEE 91, 727 (2003).
9. H.J. Zhu, M. Ramstein, H. Kostial, M. Wassermeier, H.-P. Schnherr, and L. W. Molenkamp, Phys. Rev. Lett. 87, 016601 (2001).
10. H. Ohno, Science 281, 951 (1998).
11. G.A. Prinz, Science 282, 1660 (1998).
12. S.A. Wolf, Science 294, 1488 (2001).
13. S. Datta and B Das, Appl. Phys. Lett. 56, 665 (1990).
14. D. Culcer, J. Sinova, N. A. Sinitsyn, T. Jungwirth, A. H. MacDonald, and Q. Niu, Phys. Rev. Lett. 93, 046602 (2004).
15. J. Sinova, D. Culcer, Q. Niu, N. A. Sinitsyn, T. Jungwirth, and A. H. MacDonald, Phys. Rev. Lett. 92, 126603 (2004); S. Murakami, N. Nagaosa, and S.-C. Zhang, Science 301, 1348 (2003); S. Murakami, N. Nagaosa, and S.-C. Zhang, Phys. Rev. B 69, 235206 (2004); M.I. Dyakonov and V. I. Perel, JETP 33, 1053 (1971); J.E. Hirsch, Phys. Rev. Lett 83, 1834 (1999); S. Zhang, Phys. Rev. Lett 85, 393 (2000); T. Damk~er, H. Bottger, and V. V. Brykshin, Phys. Rev. B 69, 205327 (2004).
16. There is already a vast theoretical literature on spin currents from the past few years. The following is a selection: S. Zhang and Z. Yang, Phys. Rev. Lett. 94, 066602 (2005); L. Hu, J. Gao, and S. Q. Shen, Phys. Rev. B 70, 235323 (2004); E.G.Mishchenko, A.V.Shytov, and B. I. Halperin, Phys. Rev. Lett. 93, 226602; J. Inoue, G.W.Bauer, L. W. Molenkamp, Phys. Rev. B 67, 033104 (2003); Florian Schuetz, M. Kollar, and P. Kopietz, Phys. Rev. B 69, 035133 (2004); A.M. Bratkovsky and V.V. Ospiov, J. Appl. Phys. 96 (8), 4525 (2004); N.M..Chchkelatkevich, JETP. Lett. 78, 230 (2003); A. Slobodskyy, C. Gould, T. Slobodsky, C. R. Becker, G. Schmidt, and L. W. Molenkamp, Phys. Rev. Lett. 90, 246601 (2003).
17. Y. K. Kato, R. C. Myers, A. C. Gossard, and D. D. Awschalom, Science 306, 1910 (2004).
18. J. Wunderlich, B. Kaestner, J. Sinova, and T. Jungwirth, Phys. Rev. Lett. 94, 047204 (2005).
19. Y. Kato, R. C. Myers, A. C. Gossard, and D. D. Awschalom, Phys. Rev. Lett. 93, 176601 (2004); Y. Kato, R. C. Myers, A. C. Gossard, and D. D. Awschalom, Nature 427, 50 (2004); J. Stephens, J. Berezovsky, J. P. McGuire, L. J. Sham, A. C. Gossard, and D. D. Awschalom, Phys. Rev. Lett. 93, 097602 (2004).
20. P.R. Hammar and M. Johnson, Phys. Rev. Lett. 88, 066806 (2002).
21. L. S. Levitov, Y. V. Nazarov, and G. M. Eliashberg, Sov. Phys. JETP 61 (1), 133 (1985).
22. V. M. Edelstein, Solid State Comm. 73, 233 (1990).
23. A.G.Aronov, Yu.B.Lyanda-Geller, and G.E.Pikus, Sov.Phys. JETP. 73, 537 (1991).
24. L. I. Magarill, A. V. Chaplik, and M. V. ntin, Semiconductors 35 (9), 1081 (2001).
25. D. Culcer, A. H. MacDonald, and Q. Niu, Phys. Rev. B 68, 045327 (2003).
26. T. Jungwirth, Q. Niu, and A. H. MacDonald, Phys. Rev. Lett. 88, 207208 (2002).
27. Yugu Yao, Leonard Kleinman, A. H. MacDonald, Jairo Sinova, T. Jungwirth, Ding-sheng Wang, Enge Wang, and Qian Niu, Phys. Rev. Lett. 92, 037204 (2004).
28. T. Koga, J. Nitta, T. Akazaki, and H. Takayangi, Phys. Rev. Lett. 89, 046801 (2002).
29. Y. Qi and S. Zhang, Phys. Rev. B 65, 214407 (2002), ibid. 67, 052407 (2003); V. K. Dugaev, J. Barnas, A. Lusakowski, and L. A. Turski, Phys. Rev. B 65, 224419 (2002); J. M. V. Lopes, J. M. B. Lopes dos Santos, and Y. G. Pogorelov, J. Mag. Mag. Mat. 242, 482-484 (2002); J. Fabian, and S. DasSarma, Phys. Rev. B 66, 024436 (2002).
30. Recent theories include: O.Bleibaum, Phys. Rev. B 69, 205202, (2004); M.Q.Weng, M.W.Wu and L. Jiang, Phys.
Rev. B 69, 245320 (2004).
31 S. Saikin, M. Shen, M.-C. Cheng, and V. Privman, J. Appl. Phys. 94, 1769 (2003); Y. Pershin, Physica E 23, 226 (2004); S. Saikin, J. Phys. Cond. Matt. 16, 5071 (2004).
32 G. Sundaram and Q. Niu, Phys. Rev. B 59, 14915 (1999).
33 N. W. Ashcroft and N. D. Mermin, Solid State Physics, 2nd edition (Saunders College Publishing, 1976).
34 J. Nitta, T. Akazaki, and H. Takayanagi, Phys. Rev. Lett. 78, 1335 (1997).
35 R. Winkler, Spin-Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems (Springer Tracts in Modern Physics Vol. 191, Springer, Berlin, 2003).
36 L. C. Lew Yan Voon, M. Willatzen, M. Cardona, and N. E. Christensen, Phys. Rev. B 53 (16), 10703 (1996).
37 K. L. Kavanagh, M. A. Capano, L. W. Hobbs, J. C. Barbour, P. M. J. Maree, W. Schaff, J. W. Mayer, D. Pettit, J. M. Woddall, J. A. Stroscio, and R. M. Feenstra, J. Appl. Phys. 64 (10), 4843 (1988).
38 B. Bernevig and S.-C. Zhang, cond-mat/0408442.
39 I. Vurgaftman, J. R. Meyer, and L. R. Ram-Mohan, J. Appl. Phys. 89 (11), Part 1, 5815 (2001).
40 A. Dudarev, R. B. Diener, I. Carusotto, and Q. Niu, Phys. Rev. Lett. 92 (15), 153005 (2004).
41 The experiment described in Ref. [18] uses a magnetic field to rotate the spins in the $z$ direction, then measures the accumulation of $s_z$. This procedure is appropriate in the weak spin-orbit limit. In the limit of strong spin-orbit interaction, if one attempts to rotate the spins, one must also take into account the effect of the spin-orbit interaction on the spins.