Dissipationless spin current in anisotropic *p*-doped semiconductors

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Recently, dissipationless spin current has been predicted for *p*-doped semiconductors with spin-orbit coupling. Here we investigate the effect of the breaking of spherical symmetry on the dissipationless spin current, and obtain values of the intrinsic spin Hall conducitivity for realistic semiconductor band structures with cubic symmetry.

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Spintronics is a new field of science and technology aimed at manipulating the spin of electrons to build functional logic and storage devices.[1] The creation, manipulation and transport of spin currents is a central challenge in this field. Recently, Murakami *et al.*[2] found an important law of spintronics, which relates the spin current and the electric field by the response equation,

$$j_j^i = \sigma_s \epsilon_{ijk} E_k, \tag{1}$$

where j_j^i is the current of the ith component of the spin along the direction j and ϵ_{ijk} is the totally antisymmetric tensor in three dimensions (3D). This effect arises because of spin-orbit coupling in the valence band of conventional semiconductors such as GaAs and Ge. Sinova *et al.*[3] also found a similar effect in the electron doped conduction band. Transport equation (1) is similar to Ohm's law in electronics. However, unlike Ohm's law, this new law describes a purely dissipationless spin current, in the sense that Eq. (1) is invariant under time reversal and the intrinsic part of σ_s does not depend on impurity scattering. These effects have been further discussed in recent literature.[4–9]

Fundamental to the proposal of Murakami *et al.*[2] is the spin-orbit coupling that exists in the Lüttinger effective-mass model in degenerate valence bands:

$$H = \frac{1}{2m}\left(\left(\gamma_1 + \frac{5}{2}\gamma_2\right)k^2 - 2\gamma_2(\mathbf{k}\cdot\mathbf{S})^2\right), \tag{2}$$

where $\mathbf{k}$ is the momentum operator of the valence holes, and $\mathbf{S}$ is the four-by-four spin-$3/2$ operator that describes the four hole states at a given value of k. In this "isotropic," or spherically symmetric model, the helicity $\lambda = \hat{k}\cdot\vec{S}$ is a good quantum number of the isotropic Lüttinger Hamiltonian above, and it labels the two doubly degenerate Kramers' bands that correspond to the heavy holes $\lambda = \pm 3/2$ and light holes $\lambda = \pm 1/2$. The spin current effect can be intuitively understood as a consequence of the conservation of total angular momentum: $\mathbf{J} = \hbar\mathbf{x}\times\mathbf{k} + \mathbf{S}$, where $\mathbf{x}$ is the holes' position operator. The spin current flows in such a way that the change of the orbital angular momentum $\mathbf{L} = \hbar\mathbf{x}\times\mathbf{k}$ exactly cancels the change of the spin angular momentum $\mathbf{S}$. When an electric field is applied on the arbitrary z axis, the z component of $\mathbf{J}$ is conserved. The topological nature of the spin current is manifested in the gauge-field formulation of Ref. 5, where the spin conductance is defined in terms of a linear combination of the components of a gauge field, $G_{ij} = \lambda(\lambda^2 - 13/4)\epsilon_{ijl}k_l/k^3$, clearly reflecting a monopole structure in $\mathbf{k}$ space. The singularity at $\mathbf{k}\to 0$ exemplifies the confluence of the Kramers' doublets at the Γ point where the band becomes fourfold degenerate, but the flux of the gauge field through a two-dimensional surface in $\mathbf{k}$ space is constant and set by the helicity eigenvalue.

The picture presented above is valid as long as the Hamiltonian is isotropic, that is to say, it has spherical symmetry. In the real materials in which the dissipationless spin current is predicted,[2] all of which are characterized by large anisotropy (see Table I), the angular momentum $\mathbf{J}$ and the helicity $\lambda = \hat{k}\cdot\vec{S}$ are no longer good quantum numbers. It is therefore vital to ask whether the topological spin current is preserved in materials which are not rotationally invariant. In this brief report, we investigate the effect of the breaking of spherical symmetry on the dissipationless spin current, and calculate the values of the intrinsic spin Hall conductivity for anisotropic band structure parameters.

TABLE I. Valence-band parameters for some common materials (after Ref. 10). Following Ref. 11 we define $\delta = (\gamma_3 - \gamma_2)/\gamma_1$ as a measure of the anisotropy.

	γ_1	γ_2	γ_3	δ
Si	4.22	0.39	1.44	0.248
Ge	13.35	4.25	5.69	0.108
GaAs	7.65	2.41	3.28	0.114
InSb	35.08	15.64	16.91	0.036
InAs	19.67	8.37	9.29	0.047
GaP	4.20	0.98	1.66	0.162

The most general Hamiltonian which respects time-reversal and cubic symmetries was derived by Lüttinger:[12]

$$H_0 = \frac{1}{2m}\left(\gamma_1 + \frac{5}{2}\gamma_2\right)k^2 - \frac{\gamma_2}{m}(k_x^2S_x^2 + k_y^2S_y^2 + k_z^2S_z^2) - 2\frac{\gamma_3}{m}[\{k_x,k_y\} \times\{S_x,S_y\} + \{k_y,k_z\}\{S_y,S_z\} + \{k_z,k_x\}\{S_z,S_x\}], \tag{3}$$

where we define $\{A,B\}=\frac{1}{2}(AB+BA)$ and $k^2=k_x^2+k_y^2+k_z^2$. The parameters, γ_1,γ_2, and γ_3, are material dependent. In the special case of $\gamma_2=\gamma_3$ (which we call isotropic), the last two terms simply combine to yield $-\gamma_2/m(\vec{k}\cdot\vec{S})^2$.

In real materials, however, the values of γ_2 and γ_3 are very different. Table I lists the values of these parameters in some important materials. The anisotropy, characterized by the parameter $\delta\equiv(\gamma_3-\gamma_2)/\gamma_1$, is relevant and substantial for all the materials, and especially relevant for Si. In order to understand the dissipationless spin current generated in these real materials, including its dependence on the orientation of the field and current with respect to the crystal axes, we must consider the full anisotropic Hamiltonian Eq. (3).

When $\gamma_2\neq\gamma_3$, the Hamiltonian is no longer isotropic and the helicity is not a good quantum number. However, the energy spectrum of the Hamiltonian retains the same structure as in the isotropic case, albeit with a different dispersion relation. After diagonalizing the Hamiltonian, we obtain two doubly degenerate energy levels, which we call light and heavy holes in analogy within the isotropic case:

$$E(k) = \frac{1}{2m}\gamma_1 k^2 \pm \frac{\gamma_3}{m}d(k),$$

$$d^2(k) = \left(\frac{\gamma_2}{\gamma_3}\right)^2(k_x^4 + k_y^4 + k_z^4) + \left(3 - \left(\frac{\gamma_2}{\gamma_3}\right)^2\right)(k_y^2k_x^2 + k_x^2k_z^2 + k_y^2k_z^2). \tag{4}$$

Following Ref. 5 we can expand the spin-dependent terms in the anisotropic Lüttinger Hamiltonian in terms of Clifford algebra of dirac Γ matrices $\{\Gamma^a,\Gamma^b\}=2\delta_{ab}I_{4\times4}$:

$$H_0 = \epsilon(\mathbf{k}) + \frac{\gamma_3}{m}d_a\Gamma^a, \tag{5}$$

$$\epsilon(\mathbf{k}) = \frac{\gamma_1}{2m}k^2,$$

$$d_1 = -\sqrt{3}k_zk_y, \quad d_2 = -\sqrt{3}k_xk_z, \quad d_3 = -\sqrt{3}k_xk_y,$$

$$d_4 = -\frac{\sqrt{3}}{2}\frac{\gamma_2}{\gamma_3}(k_x^2 - k_y^2), \quad d_5 = -\frac{1}{2}\frac{\gamma_2}{\gamma_3}(2k_z^2 - k_x^2 - k_y^2) \tag{6}$$

with $d_ad_a=d^2$. Whereas in the isotropic Lüttinger model the matrix used to diagonalize the Hamiltonian belongs to the $SO(3)$ group of rotations in $\mathbf{k}$ space,[2] in the anisotropic materials the matrix that diagonalizes the anisotropic Hamiltonian belongs to the $SO(5)$ rotations in d_a space. The $SO(5)$ Clifford algebra representation of the Hamiltonian (5) naturally unifies both the isotropic and the anisotropic Lüttinger model on the same footing. Since this form of the Hamiltonian depends on $\mathbf{k}$ only through the five-dimensional (5D) vector d_a, a large part of the results in Ref. 5 is directly applicable to the anisotropic case. In this sense, the $SO(5)$ Clifford algebra formalism shows its full power in the anisotropic case studied here. The projection operators onto the two-dimensional subspace of states of the heavy-hole (HH) and light-hole (LH) bands read:

$$P^L = \tfrac{1}{2}(1 + \hat{d}_a\Gamma^a), \quad P^H = \tfrac{1}{2}(1 - \hat{d}_a\Gamma^a). \tag{7}$$

For finite $\mathbf{k}$, the Hamiltonian maintains the $SO(4)$ symmetry observed in Ref. 5. This symmetry reflects the degeneracy of the two Kramers' doublets at each value of $\mathbf{k}$, corresponding to the doubly degenerate HH and the LH bands. Each of the bands has a $SU(2)$ symmetry, which we denote by $SU(2)_{\mathrm{HH}}$ and $SU(2)_{\mathrm{LH}}$. Therefore, the total symmetry is $SU(2)_{\mathrm{HH}}\times SU(2)_{\mathrm{LH}}=SO(4)$. At the Γ point, $\mathbf{k}=0$, there is a enhanced $SO(5)$ symmetry.

The symmetry generators read:

$$\rho^{ab} = \Gamma^{ab} + d_bd_c\Gamma^{ca} - d_ad_c\Gamma^{cb} = P^L\Gamma^{ab}P^L + P^H\Gamma^{ab}P^H, \tag{8}$$

where $\Gamma^{ab}=-i/2[\Gamma^a,\Gamma^b]$ and $[\rho^{ab},H_0]=0$ trivially since the Hamiltonian is diagonal in the HH and LH bands. The spin operators S^i are related to the Γ^{ab} matrices through the tensor η^i_{ab}, whose entries were given in Ref. 5: $S^i=\eta^i_{ab}\Gamma^{ab}$. The concept of a conserved spin current is still valid in anisotropic materials, since the projected spin is a constant of motion in virtue of its being a linear combination of the symmetry generators, $S^l_{(c)}=\eta^l_{ab}\rho^{ab}=P^LS^lP^L+P^HS^lP^H$. We can therefore define the conserved spin current as $J^l_i=\frac{1}{2}\{\partial H/\partial k_i,S^l_{(c)}\}$. Note that the richer anisotropic Lüttinger Hamiltonian yields a very similar structure to the isotropic one when cast in $SO(4)$ language.

Although the concept of helicity $\lambda=k_iS^i$ is not valid in anisotropic materials, we can define a corresponding conserved helicity, λ_{new}, as

$$\lambda_{\mathrm{new}} = k_iS^i_{(c)} = \lambda + 2k_i\eta^i_{ab}d_bd_c\Gamma^{ca} = P^L\lambda P^L + P^H\lambda P^H. \tag{9}$$

Since it is a linear combination of the symmetry generators of H_0 ($\lambda_{\mathrm{new}}=k_iS^i_{(c)}=k_i\eta^i_{ab}\rho^{ab}$), it is clear that $[H,\lambda_{\mathrm{new}}]=0$. In the isotropic limit, $\lambda_{\mathrm{new}}=\lambda$, as can be seen using the identities $[\lambda,P^L]=[\lambda,P^H]=0$, valid in the isotropic case.

The recent work reported in Ref. 5 shows that the Kubo formula for the conserved spin current response can be expressed purely in terms of a geometric quantity,

$$G_{ij} = G^{ab}_{ij}\Gamma^{ab} = \frac{1}{4d^3}\epsilon_{abcde}d_c\frac{\partial d_d}{\partial k_i}\frac{\partial d_e}{\partial k_j}\Gamma^{ab}, \tag{10}$$

which describes mapping from the 3D k vector space to the 5D d vector space. This results also include a quantum correction to the semiclassical result in Ref. 2. We shall apply this formula to the anisotropic case here. However, there is one essential difference. Whereas in the isotropic case, the field strength can be brought, through proper choice of gauge, to the diagonal form $G_{ij}=\lambda(\lambda^2-13/4)\epsilon_{ijl}k_l/k^3$, in the anisotropic case this is impossible. Non-Abelian field strengths are, in general, gauge-variant. However, there is a fundamental difference between fields that can be diagonalized through gauge transformation and fields for which this is not possible. The former are ultimately Abelian in nature, whereas the latter are truly non-Abelian. The nondiagonal gauge field which describes evolution in anisotropic materials reflects the richer structure of the anisotropic Lüttinger Hamiltonian.

We can express the field strength in terms of the (unprojected) spin degrees of freedom if we first note that the ten $SO(5)$ generators Γ^{ab} decompose into the three spin matrices S^i and the seven cubic, symmetric and traceless combinations of the spin operators of the form $S^iS^jS^k$, namely,

$$A^1 = (S_x)^3, \quad A^2 = (S_y)^3, \quad A^3 = (S_z)^3,$$

$$A^4 = \{S_x, (S_y)^2 - (S_z)^2\},$$

$$A^5 = \{S_y, (S_z)^2 - (S_x)^2\},$$

$$A^6 = \{S_z, (S_x)^2 - (S_y)^2\},$$

$$A^7 = S_xS_yS_z + S_zS_yS_x. \tag{11}$$

Then we can write

$$G_{ij} = \frac{1}{4d^3}\epsilon_{ijl}k_l[V_\mu A^\mu + U_l S^l], \quad l = 1, \ldots, 3, \quad \mu = 1, \ldots, 7, \tag{12}$$

where

$$U_l = \frac{1}{2}\frac{\gamma_2}{\gamma_3}\left[\left(13 + 28\frac{\gamma_2}{\gamma_3}\right)k_l^3 + \left(13 - 28\frac{\gamma_2}{\gamma_3}\right)k^2 k_l\right],$$

$$V_l = -2\frac{\gamma_2}{\gamma_3}\left[\left(1 + 4\frac{\gamma_2}{\gamma_3}\right)k_l^3 + \left(1 - 4\frac{\gamma_2}{\gamma_3}\right)k^2 k_l\right],$$

$$V_4 = -3\frac{\gamma_2}{\gamma_3}k_x(k_y^2 - k_z^2),$$

$$V_5 = -3\frac{\gamma_2}{\gamma_3}k_y(k_x^2 - k_z^2),$$

$$V_6 = -3\frac{\gamma_2}{\gamma_3}k_z(k_x^2 - k_y^2),$$

$$V_7 = -12k_xk_yk_z, \tag{13}$$

$l = 1, \ldots, 3$.

When cast in $SO(4)$ language, the expression for the spin conductance in anisotropic materials has the same form as that in the spherical model:

TABLE II. Material-dependent coefficients of spin conductivity for values of $\gamma_1, \gamma_2, \gamma_3$ that corresponding to common semiconductors. Also given are the actual spin conductivities at $n = 10^{19}$ cm^{-3} for both real anisotropic materials, and their spherical approximations ($\delta = 0$).

	$S(\gamma_1,\gamma_2,\gamma_3)$	$\sigma_s(\Omega^{-1}\text{ cm}^{-1})$	$\sigma_s\vert_{\delta=0}(\Omega^{-1}\text{cm}^{-1})$
Si	0.028	14.60	21.10
Ge	0.063	32.79	34.31
GaAs	0.062	32.64	34.33
InSb	0.083	43.63	44.67
InAs	0.079	41.61	42.55
GaP	0.051	26.50	29.17

$$\sigma_{ij}^l = \frac{8e^2}{V\hbar}\sum_k (n_L(\mathbf{k}) - n_H(\mathbf{k}))\frac{1}{3}\eta_{ab}^l G_{ij}^{ab}, \tag{14}$$

where $n_L = n_F(\epsilon_L)$ and $n_H = n_F(\epsilon_H)$ are the Fermi functions of the LH and HH bands. This expression can be put into the following elegant form:

$$\frac{1}{3}\eta_{ab}^l G_{ij}^{ab} = \frac{1}{8d^3}\frac{\gamma_2}{\gamma_3}\epsilon_{ijm}k_m k_l\left[\left(1 - \frac{\gamma_2}{\gamma_3}\right)k_l^2 + \left(1 + \frac{\gamma_2}{\gamma_3}\right)k^2\right], \tag{15}$$

where we see that the first term in square brackets vanishes in the isotropic case. The l index specifies the direction of the spin orientation, and it is not summed on the right-hand side of Eq. (15). It is now obvious that the only components of σ_{ij}^l that survive after summing the contributions from the whole Fermi surface are those for which $i \neq j \neq l$. Indeed, upon integration over $\mathbf{k}$, σ_{ij}^l becomes proportional to ϵ_{ijk}, just as it should for crystals with cubic symmetry.[13]

Our result for the spin current can thus be put in the form

$$\sigma_s = \frac{e^2}{\hbar}n^{1/3}S(\gamma_1, \gamma_2, \gamma_3), \tag{16}$$

where the material-specific coefficient, S, is independent of the Fermi energy, and is of the order ~ 0.05 for most materials (see Table II). The $\sigma_s \sim n^{1/3}$ scaling is the hallmark of the dissipationless spin current, and has been proposed as a means by which to distinguish from other extrinsic effects.[2,4] To compare the spin conductance in different ma-

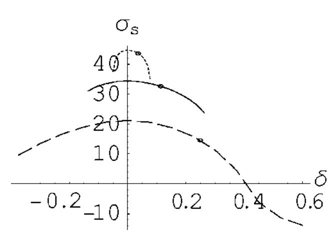

FIG. 1. Spin conductivity plotted as a function of the anisotropy, parameterized by $\delta \equiv (\gamma_2 - \gamma_3)/\gamma_1$, with $\mu = (6\gamma_3 + 4\gamma_2)/5$ and $n = 10^{19}$ cm^{-3} held fixed at values corresponding to Si (bottom curve), GaAs and InSb (top curve). The circles indicate the real values of the parameters in Si, GaAs and InSb.

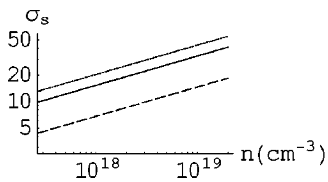

FIG. 2. Dependence of the spin conductivity on the carrier density, n, using the band parameters of Si (bottom curve), GaAs and InSb (top curve).

terials, we separate the dependence on the total carrier density, which for the anisotropic Lüttinger model depends on the band parameters: $n=(2m\epsilon_F)^{3/2}\frac{2}{3}\int(1/[(\gamma_1-2\gamma_3 d/k^2)^{3/2}]+1/[(\gamma_1+2\gamma_3 d/k^2)^{3/2}])d^2\hat{k}/(2\pi)^3$. Using this relation, we can find ϵ_F as a function of n, and use it to define the anisotropic Fermi distribution functions, $n_{L,H}(\mathbf{k})=\Theta(k_F^{L,H}-k)$. We have calculated σ_s for band parameters that correspond to a selection of real materials, as well as for band parameters that correspond to isotropic materials with the same values of γ_1 and $\mu\equiv(6\gamma_3+4\gamma_2)/5\gamma_1$. The results, listed in Table II, show that the nonzero anisotropy leads to a decrease in spin conductivity of as much as 30% (for Si), although the reduction in materials with smaller anisotropy is typically only $\sim$5%.

To illustrate the systematic dependence of spin conductance on anisotropy, we plot σ_s as a function of $\delta=(\gamma_3-\gamma_2)/\gamma_1$ with γ_1 and $\mu=(6\gamma_3+4\gamma_2)/5$ held fixed at values corresponding to Si, GaAs and InSb (Fig. 1). The spin conductance at fixed carrier concentration is maximum at $\delta=0$, whereas all real materials have $\delta>0$. This observation should guide in the selection of materials with relatively low anisotropy for spin-injection devices and other applications where strong spin current is desired. Finally, the variation of σ_s with the carrier concentration, n, is shown in Fig. 2.

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