Orbitronics: the Intrinsic Orbital Hall Effect in p-Doped Silicon

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The spin Hall effect depends crucially on the intrinsic spin-orbit coupling of the energy band. Because of the smaller spin-orbit coupling in silicon, the spin Hall effect is expected to be much reduced. We show that the electric field in p-doped silicon can induce a dissipationless orbital current in a fashion reminiscent of the spin Hall effect. The vertex correction due to impurity scattering vanishes and the effect is therefore robust against disorder. The orbital Hall effect can lead to the accumulation of local orbital momentum at the edge of the sample, and can be detected by the Kerr effect.

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Spin manipulation in semiconductors has seen remarkable theoretical and experimental interest in recent years with the advent of spin-electronics, and with the realization that strong spin-orbit coupling in certain materials can influence the transport of carriers in so-called spintronics devices [1]. Recently, a new way to manipulate spin has been proposed, where the spin current is created by an electric field through the intrinsic spin-orbit coupling in the semiconductor bands[2, 3]. The direction of the spin polarization and the current flow direction are mutually perpendicular and perpendicular to the electric field. The spin Hall effect has been recently observed experimentally by [4, 5].

While of possible great application in semiconductors with large spin-orbit coupling such as GaAs and InSb, the effect is expected to be smaller in the most used semiconductor of the electronics industry: silicon. Indeed, the small spin-orbit coupling in silicon, as measured by the energy of the split-off band relative to the top of the valence band, $\sim 44 \ meV$, makes the spin-Hall effect effect small at room temperature. Recently, Yao and Fang[6] computed the intrinsic spin Hall effect from first principle, for a variety of materials including silicon.

Given the dominance of silicon in semiconductor industry, it is important to find a similar dissipationless transport process which does not rely on the spin-orbit coupling. In this paper, we investigate the possibility of replacing the spin degree of freedom by the orbital degree of freedom, and call the associated field of study orbitronics. The valence band of Si consists largely of three p-orbitals. The three orbital degrees of freedom transform as a (pseudo-) spin one quantity under rotation, are odd under time reversal, and couple to the crystal momentum of the hole. We show that p-doped Si under the influence of an electric field develops an intrinsic orbital current of the p-band. The polarization of the p-orbitals, the direction of flow, and the direction of the electric field are mutually perpendicular. The transport equation is similar in form to the spin-Hall equation[2]:

$$j_j^i = \sigma_I \epsilon_{ijk} E_k. \tag{1}$$

Here j_j^i stands for the orbital current flowing along the j

direction, where the local orbitals are polarized along the i direction. For an electric field on the y-axis, we expect an orbital current flowing in the positive x direction to be polarized in the $+z = p_x + ip_y$ direction while the orbital current flowing in the negative x direction is polarized in the $-z = p_x - ip_y$ direction. Like the spin current, the orbital current is also even under time reversal, and the above response equation is dissipationless.

As a semiconductor with diamond structure the valence band of Si contains 3 p-orbitals where the holes reside [7]. While in most semiconductors the intrinsic spin$-1/2$ of the holes couples with the spin-1 p-orbitals to create the light and heavy hole bands as well as the split-off band, in silicon this coupling is small and its energy scale is easily overtaken by disorder or thermal fluctuations. We therefore neglect it. The diamond lattice symmetry therefore requires that the form of the Hamiltonian near the zone center be [8, 9]

$$H = Ak^2 - (A-B)\sum_{i=1}^{3} k_i^2 I_i^2 - 2C \sum_{i\neq j=1}^{3} \frac{1}{2}\{k_i, k_j\}\frac{1}{2}\{I_i, I_j\} \tag{2}$$

where the I_i are the orbital angular momentum matrices:

$$I_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} I_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} I_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

and A, B, C are material constants. An essential feature of the above Hamiltonian is the coupling between the local orbital moment I_i and the momentum k_i. In analogy with the spin-orbit coupling we call this orbital-orbit coupling. Within the spherical approximation $A - B = C$ and the Hamiltonian becomes

$$H = Ak^2 - r(\vec{k} \cdot \vec{I})^2, \tag{3}$$

where we have defined $r \equiv A - B$ to simplify notation. This form is identical to the spherically symmetric Luttinger Hamiltonian for the light and heavy hole bands, but as a fundamental physical (and, as we shall see, mathematical) difference, the matrix I is not spin-3/2 4×4 matrix but spin-1 p-orbital 3×3 matrices. For

simplicity, we now work with the spherically symmetric Hamiltonian.
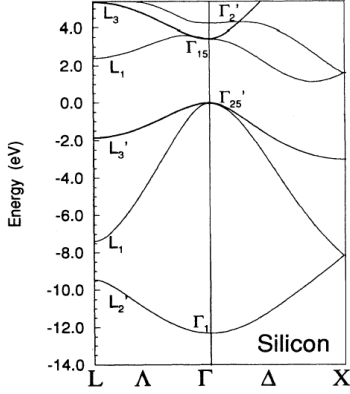

FIG. 1: Si energy bands from [10]. The effective Hamiltonian in Eq.(3) describes the $\Gamma_{25'}$ bands and is valid close to the Γ point.

Good quantum numbers for this Hamiltonian are the helicity $\lambda = \vec{k} \cdot \vec{I}/k$ and the total angular momentum $\vec{J} = \vec{x} \times \vec{p} + \vec{I}$ which is a sum of the usual motion angular momentum plus the localized orbital momentum. The energy bands contain of two degenerate bands of helicity $\lambda = \pm 1$ as well as a third band of helicity $\lambda = 0$

$$\epsilon_{\pm 1}(k) = Ak^2 \quad \epsilon_0(k) = (A - r)k^2. \tag{4}$$

Introducing five symmetric, traceless matrices[11] ξ_a^{ij}, where $a = 1, 2, 3, 4, 5$, $i, j = 1, 2, 3$, $\xi_a^{ij} = \xi_a^{ji}$ and $\xi_a^{ii} = 0$, the second term in Eq. (3) can be expanded as:

$$H(k) = \epsilon(k) + r(d_a \Gamma^a) \tag{5}$$

where

$$\epsilon(k) = \frac{k^2}{3}(3A - 2r) , \ d_a(k) = \xi_a^{ij} k_i k_j , \ \Gamma_a = \xi_a^{ij} I_i I_j,$$
$$d_1 = -\sqrt{2}k_y k_z, \quad d_2 = -\sqrt{2}k_x k_z, \quad d_3 = -\sqrt{2}k_x k_y$$
$$d_4 = -\frac{1}{\sqrt{2}}(k_x^2 - k_y^2), \quad d_5 = -\frac{1}{\sqrt{6}}(2k_z^2 - k_x^2 - k_y^2). \tag{6}$$

Following Ref. [11], one can similarly define the so called conserved spin *i.e.* the spin operator projected onto the eigenstate bands of the model. Using the projection operators onto the helicity bands in terms of the Γ^a:

$$P_{\lambda^2=0} = (1 - (\hat{k} \cdot I)^2) = \frac{1}{3} + \frac{1}{k^2} d_a \Gamma^a$$
$$P_{\lambda^2=1} = (\hat{k} \cdot I)^2 = \frac{2}{3} - \frac{1}{k^2} d_a \Gamma^a. \tag{7}$$

(with the usual projection operator properties $P_0^2 = P_0$, $P_{\pm 1}^2 = P_{\pm 1}$, $P_0 P_{\pm 1} = 0$) , the Hamiltonian can be written as $H = \epsilon_{\pm 1}(k) P_{\pm 1}(k) + \epsilon_0(k) P_0(k)$. The conserved

local orbital moment operator then commutes with the Hamiltonian:

$$I_i^{cons} = P_0 I_i P_0 + P_1 I_i P_1, \quad [H, I_i^{cons}] = 0; \quad i = 1, 2, 3. \tag{8}$$

The conserved orbital moment formalism physically implies that we consider the system in its adiabatic state, where changes to the equilibrium state, such as applied fields, etc., are slow enough as to maintain the system in its energy eigenstates. It is also the case that the local orbital moment operator I_i has no projection onto the zero-helicity band, i.e. $P_0 I_i P_0 = 0$ for $i = 1, 2, 3$. Hence, the projected motion of local orbital moments is equivalent to the projection onto the degenerate helicity $\lambda = \pm 1$ bands.

We now consider the effect of a uniform electric field $\vec{E}$ in our system. The application of an electric field introduces an extra-potential $V(x) = e\vec{E} \cdot \vec{x}$. This changes the equation of motion by acting on the particle momentum with the obvious result of accelerating the particles in the momentum direction. Since however, the momentum is coupled to the local orbital moment, the electric field will influence its motion and orientation, in a similar way as the spin-Hall effect. In particular, a non-zero local orbital current appears which selectively polarizes moving electrons into certain p-orbitals.

One can define two orbital currents, though one is perhaps more appropriate. First we have the conventional orbital-current given by $J_j^i = \frac{1}{2}\left\{ \frac{\partial H}{\partial k_j}, I^i \right\}$ with the brackets denoting an anticommutator. This current is not conserved by the Hamiltonian dynamics and thus a more appropriate current to consider is that given by the motion of the conserved orbital moment $J_{j(c)}^i = \frac{1}{2}\left\{ \frac{\partial H}{\partial k_j}, P_0 I^i P_0 + P_1 I^i P_1 \right\} = \frac{1}{2}\left\{ \frac{\partial H}{\partial k_j}, P_1 I^i P_1 \right\}$. This conserved current is the current of the orbital moment in the helicity ± 1 band. We calculate the DC-response of both of these currents using the Kubo formula.

The Green's function for the above Hamiltonian is matrix-valued and reads :

$$G(E, k) = (E - (\epsilon(k) + (A - B)d_a \Gamma^a))^{-1} \tag{9}$$

which involves inverting a 3×3 matrix. The lack of a Clifford-algebra property for the 3×3 Γ^a matrices makes the solution of this problem much harder than in the similar spin-Hall effect formalism [11]. However, after some algebra and the use of the identity $P_0 P_1 \equiv 0$, the Green's function can be written as:

$$G(E, k) = \frac{3(rk^2 - 3E(k)) - 9rd_a\Gamma^a}{(-3E(k) + 2rk^2)(3E(k) + rk^2)}, \tag{10}$$

with $E(k) \equiv E - \epsilon(k)$. We compute the response function of the spin current to an electric field. From the Kubo

formula we get:

$$Q_{ij}^l(i\nu_m) = \frac{1}{V\beta}\sum_{k,n} Tr(J_i^l G(i(\omega_n + \nu_m),k)J_j G(i\omega_n,k)) \tag{11}$$

with Matsubara frequencies $\nu_m = 2\pi m/\beta, \omega_n = (2n+1)\pi/\beta$, and charge current operator $J_j = \partial H/\partial k^j$. After performing the summation over the Matsubara frequencies, and after tracing over all the matrices, the complicated sum is reduced to a simpler form. For example the Q_{23}^1 component for the conserved current is given by:

$$Q_{23}^1(i\nu_m) = -\frac{1}{V}\sum_k \frac{(n_F(\epsilon_{\pm 1}) - n_F(\epsilon_0))r^2 k_x^2 \nu_m}{2((i\nu_m)^2 - r^2 k^4)}. \tag{12}$$

In this equation n_F is the Fermi-Dirac distribution function. The next step is to consider the zero-frequency limit of the orbital conductivity which is obtained from the response function as $\sigma_{ij}^l = \lim_{i\nu_m \to 0} \frac{Q_{ij}^l(i\nu_m)}{\nu_m}$. After the momentum integration, we obtain a beautiful tensor structure:

$$\sigma_{jk}^i = \epsilon_{ijk}\sigma_I. \tag{13}$$

It is especially suggestive that this tensor structure is identical to the one in the spin Hall effect [2] although the gauge (matrix) structure of the Hamiltonian is fundamentally different. The conductivity σ_I gives:

$$\sigma_I = \int_{k_0^F}^{k_{\pm 1}^F} \frac{d^3k}{(2\pi)^3}\frac{k_x^2}{2k^4} = \frac{1}{12\pi^2}(k_{\pm 1}^F - k_0^F). \tag{14}$$

$k_{\pm 1,0}^F$ are the Fermi momenta of the two bands. An identical picture emerges if we consider the response of the non-conserved orbital current to an electric field, the only difference being in the value of the constant σ_I which in the non-conserved case is $\sigma_I = \frac{1}{12\pi^2}(\frac{5}{3} + 4\frac{A}{A-B})(k_{\pm 1}^F - k_0^F)$. Estimates for the orbital and charge conductivities for silicon at a given carrier density are given in Table I. These calculations assume the mobility of holes in silicon is $450\ cm^2/V\cdot s$[12].

In the computation above we have made 3 approximations. We now discuss their validity. The first approximation is the neglect of the Si spin-orbit (SO) coupling. As commented at the beginning of the paper, the Si SO coupling is small (44 meV) and is likely to get suppressed by the energy scale of disorder and temperature. The energy scale at room temperature is of the same order of magnitude as the Si SO coupling $\sim 26\ meV$, while the difference of energies between $\epsilon_{\pm 1} - \epsilon_0$ bands at the Fermi energy is much larger $e.g.$ $\Delta E \sim 120\ meV$ at $n = 10^{20}/cm^3$ (refer to Table I for values at other densities). Hence the orbital Hall effect proposed here is much larger than the spin Hall effect that Si might have due to its small SO coupling. Moreover, our approximation gets better as the temperature is increased.

Another caveat in this calculation is our neglect of anisotropy when considering the spherical Luttinger Hamiltonian as a model for silicon. We have assumed that in the Luttinger Hamiltonian $(A-B) \approx C$ for silicon though this is not necessarily true. When $((A-B)-C)/A$ is large we cannot form the rotationally invariant $(\vec{k}\cdot\vec{I})^2$ term and the problem becomes more mathematically challenging. However, the anisotropy only slightly modifies the numerical factors given in the formulas for σ_I.

Now we turn to the effect of impurities. In the context of the spin Hall effect, analytical calculations have shown that the spin Hall effect in the Rashba model[3] is cancelled by the vertex corrections due to impurity scattering[13]. On the other hand, the vertex correction vanishes identically[14] for the spin Hall effect in the Luttinger model describing the holes[2]. This result rests on the fact that the current vertex is odd under parity, where the Hamiltonian is even under parity. A similar argument is valid here: the orbital current operator is odd under parity while the Hamiltonian is even. For this reason, the vertex correction due to impurity scattering vanishes for the orbital Hall effect discussed here and the effect should be robust.

Consider now an electric field parallel to the y-axis. In this case, per the transport equation $J_j^i = \epsilon_{ijy}E_y$ we have an orbital current flowing in the $j = x$ direction with orbital local moment polarized in the $i = z$ direction. Since there is no net charge current in the xz plane, what is happening at a microscopic level is that there are an equal number of holes flowing in the $\pm x$ direction. However, the holes flowing in the $+x$ direction tend to populate more the $p_x + ip_y$ local orbitals so as to give a net $+z$ polarization, while the holes flowing in the $-x$ direction tend to occupy predominantly $p_x - ip_y$ local orbitals so as to give the net $-z$ polarization. At one of the boundaries of the sample there will be a net accumulation of $p_x + ip_y$ occupied orbitals while at the opposite boundary the holes will tend to occupy predominantly $p_x - ip_y$ orbitals.

We now turn to the experimental detection of our effect. There have been several recent experiments that are setup to detect spin currents via the associated spin accumulation at the boundary [4, 5] and these provide us with a basis for detecting the intrinsic orbital current in silicon. Due to the fact that Si is an indirect-gap material with low efficiency for light emission, an LED-type experiment like [5], where the polarization of the emitted light gives information about the orbital where the emitting electron resides, is not experimentally viable. However, Kerr and Faraday rotation measurements are insensitive to the Si indirect gap and can be used to probe orbital polarization.

As seen from the detection of the spin-Hall effect in GaAs the time-resolved Kerr (Faraday) microscope is an effective experimental apparatus for spintronics. A very similar experiment to that performed in [4] could be per-

n(cm^{-3})	σ_I ($\frac{1}{\Omega \cdot cm}$)	σ_c($\frac{1}{\Omega \cdot cm}$)	$\ell(\mu m)$	ΔE(meV)	ρ_I ($\frac{\mu_B}{cm^2}$)
10^{21}	20.7	72000	3.9	540	2×10^{15}
10^{20}	9.63	7200	1.8	120	9×10^{14}
10^{19}	4.47	720	0.85	24	4×10^{14}
10^{18}	2.07	72	0.39	5.4	2×10^{14}
10^{17}	0.963	7.2	0.18	1.2	9×10^{13}
10^{16}	0.447	0.72	0.085	0.25	4×10^{13}

TABLE I: Parameter values are given as a function of the density n. We have presented the orbital conductivity σ_I, the charge conductivity σ_c, the spin diffusion length ℓ, the energy difference between the two hole bands at the Fermi energy ΔE, and the orbital polarization density ρ_I.

A (eV/m^2)	B (eV/m^2)	C (eV/m^2)	A-B (eV/m^2)
0.951	1.51	-2.06	-0.558

TABLE II: Specific material parameters for silicon calculated using [7, 15].

formed with a Si sample. The orbital current will create two regions at the edge of the sample where electrons occupy orbitals polarized in opposite directions and thus will have different optical properties with respect to circularly polarized light. The change in the angle of the beam reflected (or transmitted, in the case of Faraday rotation) from the surface of the sample gives information about the orbital moment polarized on the direction of the beam. One obstacle to performing this measurement in Si is the possibly short relaxation time of the orbital angular momentum. Since there are no systematic study of the orbital relaxation in Si, we take the hole spin relaxation time as a rough estimate, since these two quantities transform the same way, and couple to the crystal momentum in the same way. The resolution of the Kerr microscope in [4] is $\approx 1 \mu m$ and must be comparable to the size of the region where the orbitally polarized electrons accumulate. This size is $L = \sqrt{D\tau_s}$ where τ_s is the spin-relaxation time (although this is an orbital polarization, we expect the relaxation time to be comparable to the spin relaxation time). D is the hole diffusion coefficient and has the expression $v_F^2\tau/3$ where τ is the momentum relaxation time and v_F is the Fermi velocity. The size of the orbital polarization region hence depends heavily on the hole-spin relaxation time. Hole-spin relaxation times in semiconductors have been measured to be anywhere from $\tau_s \approx 4 \ ps$[16] to $\tau_s \approx 1 \ ns$ [17]. Hole-spin relaxation times for Si structures have been measured to be on the order of $\sim 10 \ ps$ at low temperatures[18, 19]. However, these measurements are "bipolar" measurements where both electrons and holes are excited and spin-polarized. A "monopolar" spin measurement, which excites carriers only in intraband or intrasubband transitions, would measure spin relaxation times without electron-hole in-

teraction and exciton formation[20]. This measurement was carried out in [20] for p-type quantum wells in a regime of intraband or intersubband transitions and they measured a hole-spin lifetime of $\sim 30 \ ps$. This regime is the most relevant for our calculations so we will use this value in our subsequent estimations. We have estimated the hole-spin diffusion constant (which we expect to be close to the orbital diffusion constant) and the spatial distribution of the orbital moments. The values for the length over which the holes are distributed are given in Table I as ℓ. For a steady electric current J_y we can estimate the orbital current density to be $j_I \sim (\sigma_I/\sigma_c)J_y$[2]. The values of orbital polarization density are given by the expression $j_I\tau_s$[2]. Assuming that $3 \times 10^5 V/cm$ is an upper bound for the electric field in Si[12] we have calculated several values of the maximum orbital polarization density in Table I under ρ_I.

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