Spin Accumulation with Spin-Orbit Interaction

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Spin accumulation is a crucial but imprecise concept in spintronics. In metal-based spintronics it is characterized in terms of semiclassical distribution functions. In semiconductors with a strong spin-orbit coupling the spin accumulation is interpreted as a superposition of coherent eigenstates. Both views can be reconciled by taking into account the electron-electron interaction: a sufficiently strong self-consistent exchange field reduces a spin accumulation to a chemical potential difference between the two spin bands even in the presence of spin-orbit coupling. We demonstrate the idea on a clean two-dimensional electron gas by showing how the exchange field protects a spin accumulation from dephasing and introduces an easy-plane anisotropy.

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Metal-based spintronics [1] has evolved into a mature field in which spin phenomena are routinely exploited in versatile applications [2]. However, integration of spin-based functionalities into semiconductor circuits is still a pressing challenge. Much of the recent research in this area has been motivated by device concepts, such as the seminal Datta-Das transistor [3], which requires injection and detection of spins by ferromagnetic contacts to a narrow channel of a two-dimensional electron gas (2DEG) with gate-controlled spin-orbit interaction (SOI). In spite of progress to inject, modulate, transport, and detect spin polarization all-electrically [4–9], as well as evidence that the SOI can indeed be tuned by external gates [10], the route to a working spin transistor appears to be still full of obstacles. In the meantime, many insights have been obtained on the spin accumulation and its dynamics by optical methods, especially time-dependent Kerr and Faraday rotation spectroscopy [11–16]. Large Rashba splitting has been observed at metal surfaces by angle-resolved photoemission [17], which has attracted a lot of attention recently [18,19].

We define a spin accumulation as a nonequilibrium spin-polarized state injected optically or electrically into a nonmagnetic material. In metal-based spintronics a spin accumulation is synonymous with a chemical potential difference between spin-up and spin-down bands [20]. However, in semiconductors the SOI prominently affects the electronic structure and transport properties [21]. A spin accumulation is then interpreted as an intrinsically time-dependent quantum superposition of coherent eigenstates. This difference is not just a semantic question, but it is essential for the functionality of spintronic devices. Here we offer a unified mean-field theory for the spin accumulation in both metals and semiconductors. Spin can be injected either slowly, e.g., by a ferromagnetic contact with small electric bias, or rapidly, e.g., by pulsed optically induced excitation. We start below with a description of spin-accumulation eigenstates that are accessible by adiabatic excitation followed by a brief discussion of the spin-accumulation dynamics of rapidly excited states. We illustrate the general ideas at the hand of a 2DEGs with Rashba SOI [22], in which the disorder-scattering lifetime broadening is much smaller than the spin-orbit splitting at the Fermi level.

Let us consider an infinitely extended homogeneous 2DEG. To leading order in the electron wave vector $\mathbf{k} = -i\boldsymbol{\nabla}$ the Hamiltonian including the SOI is [21] $H_0 = \hbar^2 k^2/2m^* + \alpha(\sigma_x k_y - \sigma_y k_x)$, where $m^* = m_r m_e$ is the effective electron mass, m_e is the bare electron mass, σ_i are the Pauli matrices, and α is the Rashba SOI strength parameter [22]. Electron-electron interactions are treated within the density-matrix functional theory (DMFT) [23] which is a generalization of the Hohenberg-Kohn-Sham density-functional theory [24] that can handle excited states. Compared to the Hartree-Fock (HF) method, exchange and correlation effects in the DFMT can be treated within local approximations. The reduced density matrix is $\Gamma(\mathbf{z}, \mathbf{z}') = \sum_i^\infty n_i \chi_i(\mathbf{z}) \chi_i^\dagger(\mathbf{z}')$, where χ_i are eigenstates of the Kohn-Sham Hamiltonian (natural orbitals), $0 < n_i < 1$ are the corresponding eigenvalues (natural occupation numbers), and $\mathbf{z} = (\mathbf{r}, \sigma)$ is space-spin coordinate. We define Γ_s as the subset of all density matrices which correspond to a given electron density $\rho(\mathbf{r}) = \sum_{i\sigma} n_i \chi_i^\dagger(\mathbf{z}) \chi_i(\mathbf{z})$ and spin polarization $\mathbf{s}(\mathbf{r}) = \sum_i n_i \chi_i^\dagger(\mathbf{z}) \boldsymbol{\sigma} \chi_i(\mathbf{z})/N$, where N is the total number of electrons. The density-matrix functional is defined via minimization of the total energy $E[\Gamma_s] = \min_{\Psi[\Gamma_s]} \langle \Psi[\Gamma_s] | H | \Psi[\Gamma_s] \rangle$ in the space of all many-body wave functions that correspond to a given $\Gamma_\mathbf{s}$.

We now assume that the exact density matrix can be generated by a noninteracting system of pseudoparticles

$$[H_0 + V_{\text{ext}} + V_H + V_{\text{xc}}]\phi_i = \epsilon_i \phi_i, \tag{1}$$

where V_{ext}, V_H, and V_{xc} are the external, the Hartree, and the exchange-correlation potential, respectively, such that $\Gamma_\mathbf{s}(\mathbf{z}, \mathbf{z}') \cong \sum_i^N f_i \phi_i(\mathbf{z}) \phi_i^\dagger(\mathbf{z}')$ with $f_i = \{0, 1\}$ and

$V_{\rm xc}(\mathbf{z}, \mathbf{z}', [\Gamma_{\mathbf{s}}]) = \delta E_{\rm xc}[\Gamma_{\mathbf{s}}]/\delta\Gamma_{\mathbf{s}}(\mathbf{z}, \mathbf{z}')$, where $E_{\rm xc}$ is the exchange-correlation energy. HF calculations for the Rashba Hamiltonian, following Ref. [25], confirm that the effect of the SOI on the exchange potential is negligible for small spin polarizations. With the local approximation, we finally arrive at $V_{\rm xc}(\mathbf{z}, \mathbf{z}', [\Gamma_{\mathbf{s}}]) \approx \delta(\mathbf{r} - \mathbf{r}')[V_0(\rho, s) + J_{\rm xc}(\rho, s)\hat{\mathbf{s}} \cdot \sigma]$, where $\mathbf{s} = s\hat{\mathbf{s}}$, and $J_{\rm xc}(\rho, s)$ [$\simeq J(\rho)s$ for small s] is the modulus of the exchange-correlation field vector. The scalar V_0 can be dropped in homogeneous systems. We may approximate J by the HF exchange energy of the strictly 2DEG [26] $V_{\rm xc} \approx J_{\rm x}(\rho, s)\hat{\mathbf{s}} \cdot \sigma \approx J(\rho)\mathbf{s} \cdot \sigma = -\sqrt{2}m_r/(\pi r_s \epsilon^2)\mathcal{R}\mathbf{s} \cdot \sigma$, where $r_s = m_r/(a_B\epsilon\sqrt{\pi\rho})$ is the dimensionless density parameter, ϵ is the relative dielectric constant of the medium, $\mathcal{R} = 13.6$ eV, and $a_B = 0.53$ Å. The effective Hamiltonian is then

$$H(\mathbf{s}) = H_0 + J\mathbf{s} \cdot \boldsymbol{\sigma}, \tag{2}$$

where $J < 0$ is the effective exchange potential, in which correlations can be included using published parametrizations of the correlation energy for a non-SO coupled 2DEG [27]. For typical electron densities ρ the exchange energies (a few meV) are of the same order of magnitude as SOI energies at the Fermi level in III–V [10] and II–VI [28] semiconductor-based 2DEGs.

The eigenstates of the Hamiltonian in the nonpolarized ground state are split into two bands with a chiral spin pattern [Figs. 1(a) and 1(b)]. The exchange field deforms the electronic bands and spinors as shown in Fig. 1(c) for in-plane and in Figs. 2(a) and 2(b) for perpendicular direction of an injected spin accumulation. SO split bands of the surface states of in-plane magnetized Gd films have been found to be deformed by the exchange potential [18] similar to Fig. 1(c). Our task is to find the self-consistent single-determinant eigenfunction of $H(\mathbf{s})$, which according to the DMFT is unique.

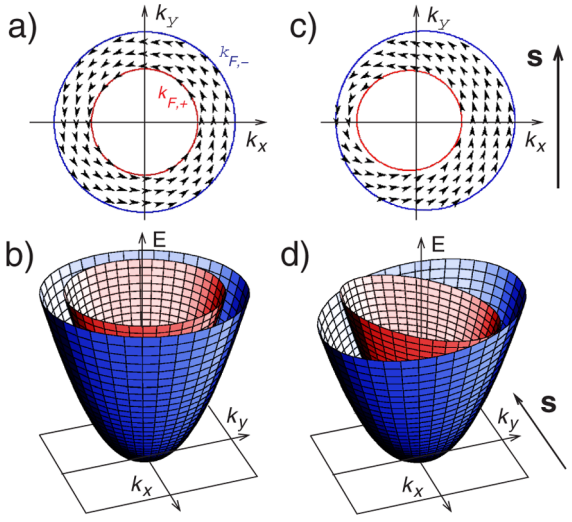

FIG. 1 (color online). Left: Spins (a) and energies (b) of the ground-state spin-split bands in a noninteracting Rashba 2DEG. The inner and outer circles correspond to the Fermi energies of the spin-split bands. Right: Modulation of the electronic structure in the presence of an in-plane spin accumulation $\mathbf{s}$ by its exchange field. Circles in (c) are fixed-energy contours. The shifted occupation number distributions that minimize the energy are shown in (d).

Introducing the occupation numbers $f_{\mathbf{k}\lambda} = \{0, 1\}$ of the spin-split states $\phi_{\mathbf{k}\lambda}$, the spin polarization reads

$$\mathbf{s} = \sum_{\mathbf{k}\lambda} f_{\mathbf{k}\lambda}\langle\phi_{\mathbf{k}\lambda}|\boldsymbol{\sigma}|\phi_{\mathbf{k}\lambda}\rangle/N, \tag{3}$$

where $\lambda = \{+, -\}$ is the band index. The state we are looking for minimizes the energy under the constraint (3), with the $f_{\mathbf{k}\lambda}$ as constrained variational variables. We solve the problem either analytically in limiting cases or numerically by a stochastic minimization method, which uses penalty functions to fix the spin polarization and the Metropolis sampling method to find the global energy minimum. An unequal occupation of spin bands, $N_- = \sum_{\mathbf{k}-} f_{\mathbf{k}-} > N_+$, can be parametrized by a chemical potential difference or a band polarization $p_b = (N_- - N_+)/N > 0$. Occupations can also shift in momentum space [Fig. 1(d)].

A spin accumulation in the plane of the 2DEG can be generated at minimized energy by shifting the Fermi circles, which induces currents [29] via a "spin-galvanic Hall effect": the minimum energy state at fixed s_x is associated with a charge current in the perpendicular y direction,

$$j_{c,y} = -e\frac{\alpha}{\hbar}\left(1 + \frac{Jm^*}{\pi\rho\hbar^2}\right)s_x. \tag{4}$$

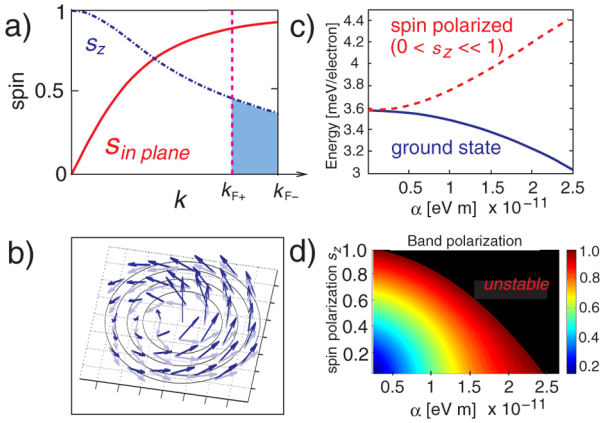

FIG. 2 (color online). (a),(b) Spin direction of the lower spin-split ($-$) band in the presence of a spin polarization normal to the 2DEG plane. The total spin polarization is determined by the shaded area between $k_{F,-}$ and $k_{F,+}$. (c) The ground state (solid line) and excited eigenstates (dashed line) with nonzero, small spin polarization perpendicular to the 2DEG surface are separated with an energy gap. (d) Band polarization of spin-accumulation states at fixed $J = -2$ meV. Material parameters are $\epsilon = 12.7$, $m^* = 0.067m_e$, $\rho = 2 \times 10^{15}/\mathrm{m}^2$.

Since electrons move with constant drift velocity, there are no intrinsic spin-Hall currents [30]. Nonequilibrium spin currents are induced, but vanish to first order in s_x.

A spin accumulation perpendicular to the 2DEG surface can be generated by the exchange field that pops the in-plane spin textures out of the plane [Fig. 2(b)]. However, the SOI counteracts the spin alignment and the band polarization p_b must be increased from that of the ground state to support a spin accumulation [31]. Consequently, excited eigenstates corresponding to a finite s_z are, in contrast to the in-plane case, separated from the nonpolarized ground state by a finite energy gap

$$E_g = \left(\frac{\alpha m^*}{\hbar J}\right)^2 \left(J + \frac{\hbar^2 \pi \rho}{m^*}\right) + \mathcal{O}(\alpha^4). \quad (5)$$

The divergence in E_g at $J \to 0$ reflects the absence of an s_z component in the noninteracting Rashba model. The gap is shown in Fig. 2(c) in which Eq. (5) corresponds to the low α limit of the energy difference. This gap energy must be overcome to achieve spin-polarized eigenstates at arbitrarily small $s_z \neq 0$. Except for this singular behavior at $s_z = 0$ we find that the energy of eigenstates is isotropic (to second order in s) to the numerical accuracy for $s_z \neq 0$. We suspect that there may be a more general physical reason behind this out-of-plane isotropy. The contribution of spin-galvanic currents to $E(\mathbf{s})$ is not significant for material parameters shown in Fig. 2.

The maximum spin accumulation that can be accommodated perpendicular to the 2DEG surface is determined by the total spin polarization of a single occupied band ($p_b = 1$). In the exchange-only approximation the self-consistency criterion (3) can be fulfilled only when

$$\alpha < 2|J|/k_F = 2|J|/\sqrt{4\pi\rho} = 0.32 \text{ eV nm}/\epsilon. \quad (6)$$

Figure 2(d) shows the stability limit as a function of s_z.

Per definition, eigenstates do not dephase. The dynamics of the semiclassical spin accumulations discussed above is therefore governed by the Bloch equation $\dot{\mathbf{s}} = -\gamma \mathbf{s} \times \mathbf{B}_{\text{eff}} - \mathbf{s}/T_1$ [1], in which $\mathbf{B}_{\text{eff}} = -\partial E(\mathbf{s})/\partial \mathbf{s}$ and T_1 is the spin relaxation time. Because of the singular anisotropy of $E(\mathbf{s})$ the Bloch equation is mathematically not well defined in the mean-field theory employed here. Qualitatively, the absence of an angle dependence of $E(\mathbf{s})$ (for $s_z \neq 0$) implies that exchange-stabilized spin accumulations do not feel an internal SOI field and precess only when an external magnetic field is applied. A spin accumulation exactly in the 2DEG plane is trapped and precesses around an in-plane external magnetic field that exceeds a threshold value governed by the energy gap (5).

A large phase space available for scattering processes makes a large spin accumulation susceptible to fast decay. Therefore the stability limit of eigenstates (6) is not a sharp phase boundary. For not too highly excited systems, the Dyakonov-Perel [32] mechanism by random scattering at defects is believed to be the dominant source of finite T_1 spin lifetimes in clean systems. Since in an exchange-stabilized 2DEG the precession in the SO field is suppressed, the efficiency of the Dyakonov-Perel mechanism is strongly diminished for systems in the clean limit considered here. The opposite (dirty) regime can be handled by spin-coherent kinetic [33,34] and diffusion [35–37] equations or numerical simulations [14,38].

The Datta-Das transistor is a spin valve consisting of a 2DEG spacer with transparent ferromagnetic contacts [3]. Even when the magnetizations of the two electrodes are parallel to each other, transport depends on the magnetization direction when exchange is taken into account. When magnetizations are oriented in the current direction, the spin accumulation can be injected into the 2DEG as an eigenstate with shifted distributions [Fig. 1(c)], which does not precess and, hence, does not react to a gate voltage that modulates the SOI. For magnetizations not in the 2DEG plane spin-accumulation eigenstates are separated from the ground state by an energy gap and spin cannot be injected adiabatically at low energies. A nonadiabatic spin injection, on the other hand, could lead to a coherent superposition of eigenstates and spins would precess in the SOI field, as envisioned by Datta and Das.

In optical pump and probe experiments, spin-polarized electrons and holes are generated by short resonant pulses of circularly polarized light, followed by fast thermalization and spin relaxation of the holes. A fast excitation creates a coherent superposition of individual spin eigenstates which dephases with time. We calculate the dynamics of the spin accumulation from the initial state ψ_0 for times $t > 0$ from $|\psi(t)\rangle = \int dt e^{iH(t)t/\hbar}|\psi_0\rangle$, where the Hamiltonian depends on t by the exchange field $J\mathbf{s}(t)$. The state at t is solved iteratively

$$|\psi(t)\rangle \approx e^{iH(t-\Delta t)\Delta t/\hbar} \ldots e^{iH(t=\Delta t)\Delta t/\hbar} e^{iH(t=0)\Delta t/\hbar}|\psi_0\rangle \quad (7)$$

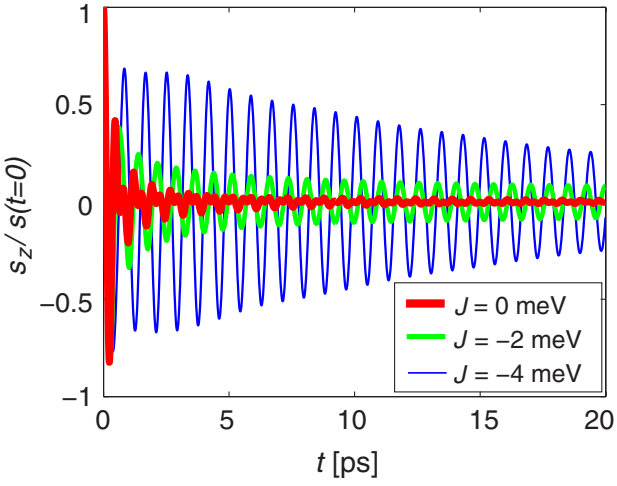

FIG. 3 (color online). Oscillation and dephasing of a spin ensemble in a SO field. The state is a coherent superposition of spin eigenstates, $s(t = 0) = 10\%$, and $\alpha = 4 \times 10^{-11}$ eV m.

for short time steps $\Delta t \simeq 1$ fs. We assume that dephasing is fast compared to the spin relaxation processes so that the occupation numbers are unchanged. Figure 3 shows the time evolution of the spin accumulation, which has been excited at time $t = 0$ into a coherent superposition of eigenstates. A single spin oscillates in the SO field by a frequency $\omega_{SO} = 2\alpha k/\hbar$. The spin polarization excited over a finite band width is therefore expected to decay on the scale of the dephasing time T_2, that decreases with increasing s. However, a strong exchange field aligns spins along a common axis and synchronizes spin precession which protects the spin polarization from dephasing. The exchange-induced enhancement of T_2 becomes significant when the exchange splitting, which is proportional to s, becomes of the same order of magnitude as the spin-orbit splitting. Such an effect has been observed in experiments [39], but can be explained by the exchange effect in the dirty limit as well [33,34].

In the space of the parameters provided by material and excitation conditions the spin accumulation features both semiclassical and quantum properties. The exchange field and thus the spin accumulation can be engineered by electron density, excitation intensity, spin direction, and electric currents, and should therefore be considered in advanced spintronic device concepts [4,15]. Our theoretical framework is general and can be extended to treat three-dimensional, inhomogeneous, and finite systems as well as the Dresselhaus SOI [40]. The electronic structures of other nonmagnetic conductors with significant SOI, e.g., hole gases in doped semiconductors or nonmagnetic transition metals, are more complicated, but still amenable to a computational implementation of our method.

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[1] I. Žutić, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. **76**, 323 (2004).
[2] D. D. Awschalom and M. E. Flatté, Nature Phys. **3**, 153 (2007).
[3] S. Datta and B. Das, Appl. Phys. Lett. **56**, 665 (1990).
[4] X. Lou *et al.*, Nature Phys. **3**, 197 (2007).
[5] P. Chen *et al.*, Phys. Rev. B **74**, 241302(R) (2006).
[6] E. J. Koop *et al.*, Phys. Rev. Lett. **101**, 056602 (2008).
[7] S. M. Frolov *et al.*, arXiv:0801.4021.
[8] S. A. Crooker *et al.*, Science **309**, 2191 (2005).
[9] M. Ciorga *et al.*, arXiv:0809.1736.
[10] J. Nitta, T. Akazaki, H. Takayanagi, and T. Enoki, Phys. Rev. Lett. **78**, 1335 (1997).
[11] J. M. Kikkawa, I. P. Smorchkova, N. Samarth, and D. D. Awschalom, Science **277**, 1284 (1997).
[12] S. A. Crooker, D. D. Awschalom, and N. Samarth, IEEE J. Sel. Top. Quantum Electron. **1**, 1082 (1995).
[13] A. Pugžlys *et al.*, J. Phys. Condens. Matter **19**, 295206 (2007).
[14] W. J. H. Leyland *et al.*, Phys. Rev. B **77**, 205321 (2008).
[15] L. Meier *et al.*, Nature Phys. **3**, 650 (2007).
[16] Y. K. Kato, R. C. Myers, A. C. Gossard, and D. D. Awschalom, Science **306**, 1910 (2004).
[17] S. LaShell, B. McDougall, and E. Jensen, Phys. Rev. Lett. **77**, 3419 (1996).
[18] O. Krupin *et al.*, Phys. Rev. B **71**, 201403(R) (2005).
[19] K. He *et al.*, Phys. Rev. Lett. **101**, 107604 (2008); J. Hugo Dil *et al.*, Phys. Rev. Lett. **101**, 266802 (2008); E. Frantzeskakis *et al.*, Phys. Rev. Lett. **101**, 196805 (2008).
[20] A. G. Aronov, Pis'ma Zh. Eksp. Teor. Fiz. **24**, 37 (1976) [JETP Lett. **24**, 32 (1976)]; M. Johnson and R. H. Silsbee, Phys. Rev. Lett. **55**, 1790 (1985); F. J. Jedema, A. T. Filip, and B. J. van Wees, Nature (London) **410**, 345 (2001).
[21] Roland Winkler, *Spin-Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems*, Springer Tracts in Modern Physics Vol. 191 (Springer-Verlag, Berlin, 2003).
[22] Y. A. Bychkov and E. I. Rashba, J. Phys. C **17**, 6039 (1984); Y. A. Bychkov and E. I. Rashba, JETP Lett. **39**, 78 (1984).
[23] G. Zumbach and K. Maschke, J. Chem. Phys. **82**, 5604 (1985).
[24] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
[25] S. Chesi, G. Simion, and G. F. Giuliani, arXiv:cond-mat/0702060.
[26] U. von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972).
[27] C. Attaccalite, S. Moroni, P. Gori-Giorgi, and G. B. Bachelet, Phys. Rev. Lett. **88**, 256601 (2002).
[28] Y. S. Gui *et al.*, Physica (Amsterdam) **12E**, 416 (2002).
[29] S. D. Ganichev *et al.*, Nature (London) **417**, 153 (2002).
[30] J. Wunderlich, B. Kaestner, J. Sinova, and T. Jungwirth, Phys. Rev. Lett. **94**, 047204 (2005).
[31] We find that at large SOI it becomes energetically favorable to instead depopulate a large fraction of states in the majority spin band around $k = 0$.
[32] M. I. Dyakonov and V. I. Perel, Fiz. Tverd. Tela (Leningrad) **13**, 3581 (1971) [Sov. Phys. Solid State **13**, 3023 (1971)].
[33] M. M. Glazov and E. L. Ivchenko, JETP Lett. **75**, 403 (2002).
[34] M. Q. Weng and M. W. Wu, Phys. Rev. B **68**, 075312 (2003).
[35] A. A. Burkov, A. S. Núñez, and A. H. MacDonald, Phys. Rev. B **70**, 155308 (2004).
[36] E. G. Mishchenko, A. V. Shytov, and B. I. Halperin, Phys. Rev. Lett. **93**, 226602 (2004).
[37] İ. Adagideli and G. E. W. Bauer, Phys. Rev. Lett. **95**, 256602 (2005).
[38] E. J. Koop, B. J. van Wees, and C. H. van der Wal, arXiv:0804.2968.
[39] D. Stich *et al.*, Phys. Rev. Lett. **98**, 176401 (2007).
[40] G. Dresselhaus, Phys. Rev. **100**, 580 (1955).