Spin-Hall Insulator

Shuichi Murakami,[1,*] Naoto Nagaosa,[1,2,3] and Shou-Cheng Zhang[4]

[1]*Department of Applied Physics, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*
[2]*CERC, AIST, Tsukuba Central 4, Tsukuba 305-8562, Japan*
[3]*CREST, Japan Science and Technology Agency (JST), Kawaguchi, Saitama 332-0012, Japan*
[4]*Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA*

(Received 31 May 2004; published 6 October 2004)

Recent theories predict dissipationless spin current induced by an electric field in doped semiconductors. Nevertheless, the charge current is still dissipative in these systems. In this work, we theoretically predict the dissipationless spin-Hall effect, without any accompanying charge current, in some classes of band insulators, including zero-gap semiconductors such as HgTe and narrow-gap semiconductors such as PbTe. This effect is similar to the quantum-Hall effect in that all the states below the gap contribute and there occurs no dissipation. However, the spin-Hall conductance is not quantized even in two dimensions. This is the first example of a nontrivial topological structure in a band insulator without any magnetic field.

DOI: 10.1103/PhysRevLett.93.156804 PACS numbers: 73.43.–f, 72.25.Dc, 72.25.Hg, 85.75.–d

Introduction.—The generation of the spin current by an external electric field [1,2] has attracted recent interest. It has been proposed theoretically that hole-doped semiconductors such as p-GaAs and p-Ge show this effect due to the intrinsic spin-orbit interaction in the Luttinger model [1]. The n-GaAs in a heterostructure is another candidate for this effect [2], although some questions regarding disorder effects still remain [3,4]. In both cases, the spin current is generated not by the displacement of the electron distribution function, but by the anomalous velocity due to the Berry curvature of the Bloch states. In this sense, the spin current does not accompany dissipation, and it is similar to both the quantum Hall effect (QHE) and also the intrinsic anomalous Hall effect (AHE). However, even though the spin current itself does not cause Joule heating, the applied electric field generates a charge current because of nonzero resistivity. Hence, strictly speaking, it is not dissipationless as a whole system. Therefore, both for low power logic device applications and for theoretical interest, we are lead to the question of whether the spin-Hall effect can exist in a band insulator without any charge current. In conventional semiconductors such as GaAs and Si without doping, the spin-Hall effect is zero; they are inert both for the spin and the charge responses, as assumed in conventional band theories.

In contrast to the conventional semiconductors, we propose in this Letter two classes of band insulators showing finite spin-Hall conductivity without any charge conductivity. One class is (distorted) zero-gap semiconductors such as HgTe, HgSe, β-HgS, and α-Sn. In these systems, in contrast to conventional semiconductors, the heavy-hole (HH) and light-hole (LH) bands have the opposite signs of the mass, with only the former being occupied at zero doping, and the finite spin-Hall effect is predicted. Furthermore, by introducing a uniaxial strain, a gap opens without destroying the spin-Hall effect. The other class is narrow-gap semiconductors such as PbTe, PbSe and PbS. Thus these two classes of materials without doping have a gap and the spin-Hall current accompanies no dissipation, similar to the QHE. Unlike the QHE, however, these band insulators have several new aspects: (i) the spin-Hall conductance is not quantized and depends on parameters characterizing the band structure; (ii) there is no magnetic field, and the system is three dimensional; and (iii) the effect is protected by the large band gap and is robust even at room temperature. From these novel aspects, this spin-Hall effect realizes a new state of matter in the simple band insulators.

These novel features originate from the fact that the gap in these materials arises due to the spin-orbit coupling, which causes the spin-Hall effect. The spin-orbit coupling gives rise to a splitting of bands into multiplets of the total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$. If all the bands in the same J multiplet are filled, they do not contribute to spin-Hall conductivity. Only when the fillings of the bands in the same J multiplet are different, the spin-Hall conductivity can be nonzero. Nonzero spin-Hall effect does not require breaking of any symmetry such as inversion or time reversal. Thus the spin-Hall effect should be a common effect, while its magnitude may vary from material to material. In particular, the spin-Hall effect is nonzero in nonmagnetic band insulators such as zero-gap and narrow-gap semiconductors, as explained below. This is distinct from the spin current in spin systems considered by Meier and Loss [5].

To calculate the spin-Hall conductivity σ_s, we follow the method developed by the authors [6]. We restrict ourselves to systems with time-reversal and inversion symmetries; therefore, all the states form Kramers doublets. By picking up two doubly degenerate bands near the Fermi energy, the Hamiltonian is written as a linear combination of 4×4 matrices $\Gamma_a (a = 1, 2, 3, 4, 5)$, which form the Clifford algebra $\{\Gamma_a, \Gamma_b\} = 2\delta_{ab}$. Following [6],

we write the Hamiltonian [7] as

$$H = \epsilon(\mathbf{k}) + \sum_{a=1}^{5} d_a(\mathbf{k})\Gamma_a, \tag{1}$$

where $\epsilon(\mathbf{k})$ and $d_a(\mathbf{k})$ are even functions of $\mathbf{k}$. Its eigenvalues are given by $\epsilon_{\pm}(\mathbf{k}) = \epsilon(\mathbf{k}) \pm d(\mathbf{k})$, where $d = |\mathbf{d}|$.

Zero-gap semiconductors.—As a first example, we consider zero-gap semiconductors with diamond or zinc-blende structures. Examples are α-Sn for the former and HgTe, HgSe, and β-HgS for the latter. In the zinc-blende structure, the inversion symmetry breaking is small and can be neglected. In experiments [8] and first-principle calculations [9] for HgSe, however, there exists some controversy on their band structure near the Γ point, whether the gap is zero or finite. Here we consider the zero-gap case, while the following discussions and estimates are not essentially affected by minute difference of band structures at the Γ point.

Before going to the zero-gap semiconductors, let us review the calculation of the spin-Hall effect for p-type conventional semiconductors with diamond or zinc-blende structures [6]. In the Hamiltonian Eq. (1), the Γ_a matrices are the five traceless matrices quadratic in spin-3/2 matrices [10,11], given in [6]. In [6], to overcome the difficulty in defining a spin current, which comes from spin nonconservation due to the spin-orbit interaction, the spin $\mathbf{S}$ has been separated into a conserved part $\mathbf{S}^{(c)}$ and a nonconserved part $\mathbf{S}^{(n)}$: $\mathbf{S} = \mathbf{S}^{(c)} + \mathbf{S}^{(n)}$. The conserved part $\mathbf{S}^{(c)}$ consists of intraband matrix elements of the spin. From this conserved spin $\mathbf{S}^{(c)}$ we can uniquely define a conserved spin current from the Noether's theorem. The spin-Hall conductivity calculated by the Kubo formula is given as

$$\sigma^{l}_{ij(\mathrm{c})} = \frac{4}{3V}\sum_{\mathbf{k}}[n_L(\mathbf{k}) - n_H(\mathbf{k})]\eta^{l}_{ab}G^{ab}_{ij}, \tag{2}$$

where $n_L(\mathbf{k})$, $n_H(\mathbf{k})$ are the Fermi distributions of holes in the LH and the HH bands. We take the hole picture in this model, where the LH and HH bands have positive energies. The geometric tensor G^{ab}_{ij} is calculated as

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

where ϵ_{abcde} is the totally antisymmetric tensor with $\epsilon_{12345} = 1$. Each element of the tensor η^{l}_{ab} is a constant, and its expression is given in [6]. For cubic semiconductors we can write $\sigma^{l}_{ij(\mathrm{c})} = \epsilon_{ijl}\sigma_s$, where σ_s is a constant.

The zero-gap semiconductors have "inverted" band structure, compared with conventional semiconductors, as shown in the inset of Fig. 1. The energy of the original conduction band becomes lower than the Fermi energy E_F. At the same time, the LH band moves up to become a conduction band, while the HH band remains a top of the valence band. The "LH" and "HH" bands touch at the Γ point ($\mathbf{k} = 0$). Although the band structure is largely different from conventional ones, its gauge-field

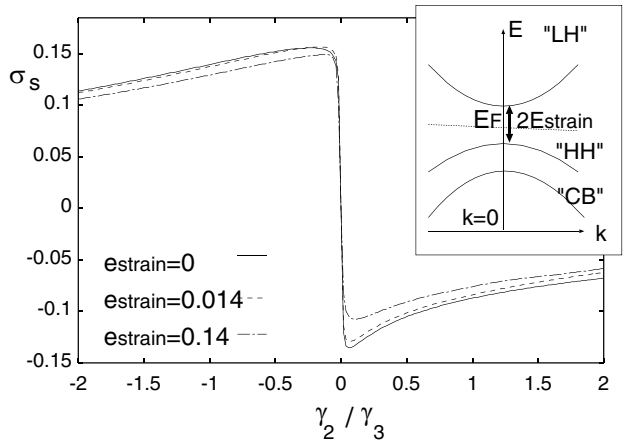

FIG. 1. Spin-Hall conductivity σ_s as a function of γ_2/γ_3, calculated from the tight-binding Hamiltonian modeling a zero-gap semiconductor without doping. $e_{\mathrm{strain}} = ma^2E_{\mathrm{strain}}/\gamma_3$ is a dimensionless parameter representing the uniaxial compressive strain, where $2E_{\mathrm{strain}}$ is an energy splitting at $\mathbf{k} = \mathbf{0}$ due to the strain. $e_{\mathrm{strain}} \sim 0.014$ corresponds to the value of α-Sn in a compressive stress $3.18 \times 10^9 \mathrm{dyn/cm}^2$ [14]. Inset: a schematic picture of the band structure for the zero-gap semiconductors with uniaxial strain. The labels LH, HH, and CB corresponds to the light-hole, heavy-hole, and the conduction bands in the conventional semiconductors with cubic symmetry, respectively. E_F is the Fermi energy.

structure giving rise to the intrinsic spin-Hall effect remains the same, and we can still use Eq. (2). In Eq. (2), the summand is proportional to $n_L(\mathbf{k}) - n_H(\mathbf{k})$. Therefore, in conventional semiconductors, hole doping is required for nonzero spin-Hall conductivity σ_s; in remarkable contrast, σ_s is nonzero in the zero-gap semiconductors even without doping, because $n_L(\mathbf{k}) = 1$, and $n_H(\mathbf{k}) = 0$ [12].

In conventional semiconductors $n_L - n_H$ is nonzero only near the Γ point, and to calculate σ_s we could use the Luttinger Hamiltonian valid only for small $\mathbf{k}$ [1,6]. On the contrary, to calculate the spin-Hall conductivity for the zero-gap semiconductors, we need a Hamiltonian valid for all $\mathbf{k}$. Hence, we shall construct a tight-binding Hamiltonian. The primitive vectors are $\mathbf{a}_1 = \frac{1}{2}(0, a, a)$, $\mathbf{a}_2 = \frac{1}{2}(a, 0, a)$, and $\mathbf{a}_3 = \frac{1}{2}(a, a, 0)$, where a is a lattice constant. Necessary conditions for the Hamiltonian are time-reversal, inversion, and cubic symmetries. Under these conditions, the simplest model which reproduces the Luttinger Hamiltonian near the Γ point is written as

$$d_1 = \sqrt{3}\gamma_3 C[\cos\theta_1 - \cos(\theta_2 - \theta_3)],$$

$$d_2 = \sqrt{3}\gamma_3 C[\cos\theta_2 - \cos(\theta_3 - \theta_1)],$$

$$d_3 = \sqrt{3}\gamma_3 C[\cos\theta_3 - \cos(\theta_1 - \theta_2)],$$

$$d_4 = \sqrt{3}\gamma_2 C[\cos\theta_2 - \cos\theta_1 + \cos(\theta_3 - \theta_1) - \cos(\theta_2 - \theta_3)],$$

$$d_5 = \gamma_2 C[\cos\theta_1 + \cos\theta_2 - 2\cos(\theta_1 - \theta_2) + \cos(\theta_3 - \theta_1) + \cos(\theta_2 - \theta_3) - 2\cos\theta_3],$$

where $C = 2/(a^2 m)$, m is the electron mass, and $\theta_j = \mathbf{k}\cdot\mathbf{a}_j$ ($j = 1, 2, 3$). The constants γ_2 and γ_3 correspond to the Luttinger parameters [11]. In the real-space representation, the spin-dependent part of the Hamiltonian involves only the nearest-neighbor hopping:

$$H_{\text{spin-dep}} = \frac{1}{a^2 m}\sum_{t_y,t_z=\pm 1,\mathbf{x}} c^{\dagger}_{\mathbf{x}+(a/2)(0,t_y,t_z),\alpha} c_{\mathbf{x}\beta}\cdot[-2\gamma_2 S^{x2} + \gamma_3 t_y t_z (S^y S^z + S^z S^x)]_{\alpha\beta} + (\text{two cyclic permutations of } x, y, z).$$

Although this Hamiltonian is a simplified one, we expect that it correctly captures basic physics and an order estimate of the spin-Hall effect.

It is a straightforward task to calculate the spin-Hall conductivity by substituting the $\mathbf{d}$ vector into Eqs. (2) and (3). In Fig. 1 is shown the value of σ_s as a function of γ_2/γ_3. Nominally $\gamma_2/\gamma_3 \sim 1$ for zero-gap semiconductors, and we get $\sigma_s \sim -0.1\frac{e}{a}$. We note that the absolute value of the spin-Hall conductivity σ_s increases as γ_2/γ_3 decreases, while in hole-doped conventional "uninverted" semiconductors σ_s is maximum around $\gamma_2/\gamma_3 \sim 1$ [13].

In such a case without doping, the longitudinal conductivity $\sigma \sim 0$ and the system is an insulator, whereas the spin-Hall conductivity is nonzero. In a three-dimensional sample, the gap is zero, and finite temperature easily provides the sample with n- and p-type carriers, producing the longitudinal (charge) conductivity. In order to circumvent this temperature effect and to keep the system insulating, it is desirable to make a finite gap at the Γ point. Because the degeneracy of the valence and conduction bands at the Γ point originates from the cubic symmetry, it is lifted by lowering the crystal symmetry, for example, by a uniaxial strain. This is indeed experimentally observed in α-Sn, where the compressive uniaxial stress opens a gap at the Γ point [14]. One can calculate an effect of a strain on the band structure by the method proposed by Pikus and Bir [15]. For simplicity, we focus on a uniaxial strain along the z axis. Within the present framework with Γ matrices, one can incorporate this uniaxial strain as an additional term $E_{\text{strain}}\Gamma_5$ in the Hamiltonian [15]. We calculated the spin-Hall conductivity for various values of a dimensionless constant $e_{\text{strain}} = ma^2 E_{\text{strain}}/\gamma_3$, and the result is shown in Fig. 1. For α-Sn, a compressive strain of $3.18 \times 10^9 \text{dyn/cm}^2$ induces an energy splitting of $2E_{\text{strain}} \sim 44.2$ meV at $\mathbf{k} = \mathbf{0}$. This splitting corresponds to $e_{\text{strain}} \sim 0.014$, considerably smaller than unity. Hence, as seen from Fig. 1, the splitting of this size does not affect much the value of σ_s. Thus, by opening a gap at the Γ point by a uniaxial strain, the spin Hall conductivity remains nonzero, while the charge conductivity is suppressed. We name it a spin-Hall insulator, though the term "Hall insulator" have been used in a different context; the Hall insulator [16] refers to an insulator where both σ_{xy} and σ_{xx} vanish while R_{xy} is finite.

Narrow-gap semiconductors.—Another example of the spin-Hall effect in band insulators is the narrow-gap semiconductors such as PbTe, PbSe, and PbS [17]. The crystal has the rocksalt structure, with the primitive vectors $\mathbf{a}_i$ ($i = 1, 2, 3$) given above. The direct gap is formed at the four equivalent L points $\mathbf{p}_1 = \frac{\pi}{a}(1, 1, 1)$, $\mathbf{p}_2 = \frac{\pi}{a}(1, -1, -1)$, $\mathbf{p}_3 = \frac{\pi}{a}(-1, 1, -1)$, and $\mathbf{p}_4 = \frac{\pi}{a}\times(-1, -1, 1)$, and is of the order of 0.15–0.3 eV. The valence and the conduction bands both form Kramers doublets. Near these L points, the Hamiltonian is given by [18,19]

$$H = v\mathbf{k}\cdot\hat{p}\tau_1 + \lambda v\mathbf{k}\cdot(\hat{p}\times\sigma)\tau_2 + Mv^2\tau_3. \quad (5)$$

Here $\mathbf{k}$ is a wave vector measured from $\mathbf{p}_i$, and $\hat{p}_i = \mathbf{p}_i/|\mathbf{p}_i|$. τ_j and σ_j are the Pauli matrices, corresponding to the orbital and the spin, respectively.

As the second term in the right-hand side of Eq. (5) resembles the Rashba Hamiltonian, we expect a nonzero spin-Hall conductivity with doping, in analogy with the Rashba model [2]. In fact, the subsequent calculation reveals that the spin-Hall conductivity in this model is nonzero even without doping, which is another realization of the "spin-Hall insulator." To calculate the spin-Hall conductivity, we construct an effective tight-binding model, which reduces to Eq. (5) near the L points. The simplest tight-binding model is given by the Hamiltonian Eq. (1) where $\Gamma_i = \tau_2\sigma_i (i = 1, 2, 3)$, $\Gamma_4 = \tau_1$, $\Gamma_5 = \tau_3$, and

$$d_1 = C_1[\sin\theta_2 - \sin\theta_3 + \sin(\theta_1 - \theta_2) - \sin(\theta_1 - \theta_3)],$$

$$d_2 = C_1[\sin\theta_3 - \sin\theta_1 + \sin(\theta_2 - \theta_3) - \sin(\theta_2 - \theta_1)],$$

$$d_3 = C_1[\sin\theta_1 - \sin\theta_2 + \sin(\theta_3 - \theta_1) - \sin(\theta_3 - \theta_2)],$$

$$d_4 = C_2[\sin(\theta_2 + \theta_3) - \sin(2\theta_3 - \theta_1) - \sin(2\theta_2 - \theta_1) + \sin(\theta_2 + \theta_3 - 2\theta_1)] + (\text{two cyclic permutations of the subscripts } 1, 2, 3),$$

$$d_5 = Mv^2,$$

where $C_1 = (\lambda v/\sqrt{3}a)$ and $C_2 = (v/4\sqrt{3}a)$. It contains a nearest-neighbor and a third-neighbor hopping. Let us calculate the spin-Hall conductivity corresponding to a spin current $J^l_i = \frac{1}{2}\{J_i, \sigma_l\}$ in response to an external electric field E_j. Henceforth, the Greek indices run from 1 to 3, while the Roman indices run from 1 to 5. From the Kubo formula, we obtain the result

$$\sigma^l_{ij} = \frac{1}{V}\sum_{\mathbf{k}}\frac{n_F(\epsilon_-) - n_F(\epsilon_+)}{2d^3}\cdot\left(\epsilon_{\alpha mn\beta\gamma}\epsilon_{lmn}\frac{\partial d_\alpha}{\partial k_i}\frac{\partial d_\gamma}{\partial k_j}d_\beta + 2\epsilon_{lmn}\frac{\partial\epsilon}{\partial k_i}\frac{\partial d_n}{\partial k_j}d_m\right),$$

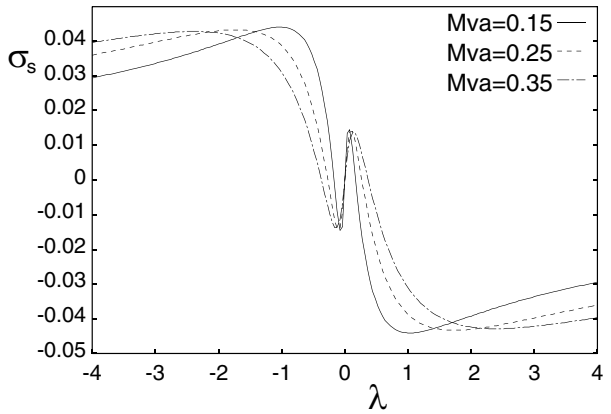

FIG. 2. Spin-Hall conductivity σ_s as a function of λ for various $m = Mva$, calculated from the tight-binding Hamiltonian modeling a narrow-gap semiconductor without doping.

where $n_F(\epsilon) = [1 + e^{\beta(\epsilon-\mu)}]^{-1}$. When we consider again the conserved spin current, we get

$$\sigma^l_{ij(c)} = \frac{1}{V}\sum_{\mathbf{k}} \frac{n_F(\epsilon_-) - n_F(\epsilon_+)}{2d^3} \epsilon_{\alpha mn\beta\gamma}\epsilon_{lmn} \frac{\partial d_\alpha}{\partial k_i}\frac{\partial d_\gamma}{\partial k_j} d_\beta.$$

It no longer depends on $\epsilon(\mathbf{k})$. For the gapped case with only the lower band is occupied, the spin-Hall conductivity σ_s is plotted for various values of two dimensionless parameters Mva and λ in Fig. 2. It is an odd function of both Mva and λ. Since the Hamiltonian Eq. (5) has eigenenergies

$$\epsilon_\pm = \pm\sqrt{v^2(\mathbf{k}\cdot\hat{p})^2 + \lambda^2 v^2(\mathbf{k}\times\hat{p})^2 + (Mv^2)^2}$$

near each L point, the values of the parameters can be extracted from experimental data; $2Mv^2$ is a direct gap at the L points, M is an effective mass along the $\hat{p}$ direction, and M/λ^2 is an effective mass perpendicular to the $\hat{p}$ direction. In PbS, PbSe, and PbTe, the values of the parameters are given as $\lambda \sim 1.2, 1.4, 3.3$, and $Mva \sim 0.26, 0.16, 0.35$, respectively. The nominal values of the spin-Hall conductivity for these compounds is around $-0.04e/a$, as seen from Fig. 2.

Concluding remarks.—We theoretically predict the spin-Hall effect in zero-gap semiconductors like HgTe and in narrow-gap semiconductors like PbTe. From a simple tight-binding model, the spin-Hall conductivity is estimated to be of the order of e/a, where a is a lattice constant. This effect is protected by the band gap E_G, which is of the order of 0.15–0.3 eV for narrow-gap semiconductors, and hence is robust against the thermal agitations, impurity scatterings, and electron-electron inelastic scatterings as long as the energy scale of these is smaller than E_G. In contrast to the doped semiconductors, the dissipationless spin current in band insulators does not lead to spin accumulation at the boundary, because it lacks any mechanisms which breaks time-reversal symmetry. Nonetheless, it can be detected by the electric field due to the Aharonov-Casher effect [5], which propagates for a macroscopic distance via the spin current.

We thank D. Culcer, E. Fradkin, A. H. MacDonald, Q. Niu, and J. Sinova for helpful discussions. This work is supported by NAREGI and Grant-in-Aids for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology of Japan, the U.S. NSF under Grant No. DMR-0342832, and the U.S. Department of Energy, Office of Basic Energy Sciences under Contract No. DE-AC03-76SF00515.

*Electronic address: murakami@appi.t.u-tokyo.ac.jp

[1] S. Murakami, N. Nagaosa, and S. C. Zhang, Science **301**, 1348 (2003).
[2] J. Sinova *et al.*, Phys. Rev. Lett. **92**, 126603 (2004).
[3] J. Inoue, G. E.W. Bauer, and L.W. Molenkamp, Phys. Rev. B **70**, 041303 (2004).
[4] S. Murakami, Phys. Rev. B **69**, 241202(R) (2004).
[5] F. Meier and D. Loss, Phys. Rev. Lett. **90**, 167204 (2003).
[6] S. Murakami, N. Nagaosa, and S. C. Zhang, Phys. Rev. B **69**, 235206 (2004).
[7] Here we changed the normalization of **d** by a constant factor from [6] for convenience.
[8] K.-U. Gawlik *et al.*, Phys. Rev. Lett. **78**, 3165 (1997), and references therein; T. Dietl *et al.*, Phys. Rev. Lett. **81**, 1535 (1998); K.-U. Gawlik *et al.*, *ibid.* **81**, 1536 (1998); D. Eich *et al.*, Phys. Rev. B **61**, 12666 (2000).
[9] A. Delin, Phys. Rev. B **65**, 153205 (2002); A. Delin and T. Klüner, *ibid.* **66**, 035117 (2002).
[10] J. E. Avron, L. Sadun, J. Segert, and B. Simon, Phys. Rev. Lett. **61**, 1329 (1988).
[11] J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).
[12] We take the hole picture where only the LH is occupied.
[13] B. A. Bernevig, J. P. Hu, E. Mukamel, and S. C. Zhang, Phys. Rev. B **70**, 113301 (2004).
[14] B. J. Roman and A.W. Ewald, Phys. Rev. B **5**, 3914 (1972).
[15] G. E. Pikus and G. L. Bir, Fiz. Tverd. Tela **1**, 1642 (1959) [Sov. Phys. Solid State **1**, 1502 (1960)].
[16] S. C. Zhang, S. Kivelson, and D. H. Lee, Phys. Rev. Lett. **69**, 1252 (1992).
[17] These materials have been studied theoretically for the model of parity anomaly for a possibilitiy of the Hall effect at the domain boundary. See E. Fradkin, E. Dagotto, and D. Boyanovsky, Phys. Rev. Lett. **57**, 2967 (1986); **58**, 961(E) (1987); D. Boyanovsky, E. Dagotto, and E. Fradkin, Nucl. Phys. **B285**, 340 (1987).
[18] O. Tchernyshyov, Phys. Rev. B **62**, 16751 (2000).
[19] B. A. Volkov, O. A. Pankratov, and A.V. Sazonov, Zh. Eksp. Teor. Fiz. **85**, 1395 (1983) [Sov. Phys. JETP **58**, 809 (1983)].