Rapid Communication

The robustness of the quantum spin Hall effect to the thickness fluctuation in HgTe quantum wells*

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The quantum spin Hall effect (QSHE) was first realized in HgTe quantum wells (QWs), which remain the only known two-dimensional topological insulator so far. In this paper, we have systematically studied the effect of the thickness fluctuation of HgTe QWs on the QSHE. We start with the case of constant mass with random distributions, and reveal that the disordered system can be well described by a virtual uniform QW with an effective mass when the number of components is small. When the number is infinite and corresponds to the real fluctuation, we find that the QSHE is not only robust, but also can be generated by relatively strong fluctuation. Our results imply that the thickness fluctuation does not cause backscattering, and the QSHE is robust to it.

Keywords: quantum spin Hall effect, HgTe quantum wells, disorder effect

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Studies on topological states of quantum matter have attracted much attention due to the discovery of the time-reversal invariant topological insulator (TI).[1−3] A great deal of interest has been stimulated by the theoretical proposal of realizing the quantum spin Hall effect (QSHE) in graphene.[4,5] Although the spin–orbit coupling is too weak in graphene to observe the effect, the TI concept is attractive. Subsequently, this phase is indeed observed experimentally in both two and three dimensions.[6−13] Since then, more and more experimental and theoretical efforts are being devoted to this field, making it the hottest topic in condensed matter physics.[14,15]

A key feature of TIs is the existence of gapless edge or surface states within the bulk gap. These states are topologically protected and are robust to nonmagnetic impurity scattering due to their helicity, which has been verified by angle-resolved photoemission spectroscopy and scanning tunneling microscope experiments.[10,16] More interestingly, it is noted recently that the TI not only is robust to disorder, but also can be brought about by disorder. The new topological phase, referred to as the topological Anderson insulator (TAI), has been predicted to exist in both two and three dimensions.[17−20] TAI studies focus on on-site type disorder. Recent experiments in the HgTe QWs show that except for the on-site disorder, the well-width fluctuation cannot be ignored and will affect the transport properties.[21] Particularly, the thickness fluctuation which naturally exists may be helpful for studying Dirac fermion transport with random mass, which is difficult to realize experimentally at present.

In this paper, we provide a systematic theoretical study on the effect of the thickness fluctuation of HgTe QWs. Based on the tight-binding model describing HgTe QWs, the thickness fluctuation is modeled as the disorder in the Dirac mass. We start with the case of constant mass with random distributions, and show that the disordered system can be well described by a virtual uniform QW with an effective mass when the number of components is small. When the number is infinite and corresponds to the real fluctuation, we find that the QSHE is not only robust, but also can be generated by relatively large fluctuation. Finally, the similarity and difference between the effect of on-site disorder and the physics of the Dirac equation with a random mass are discussed.

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We start with the effective four-band Hamiltonian for HgTe QWs which reads[7,23]

$$\boldsymbol{H}_{\rm eff}(k_x,k_y)=\begin{pmatrix}\boldsymbol{H}_{\rm D}(\boldsymbol{k}) & 0\\ 0 & \boldsymbol{H}^*_{\rm D}(-\boldsymbol{k})\end{pmatrix}, \qquad (1)$$

where $\boldsymbol{H}_{\rm D}(\boldsymbol{k})=\epsilon(\boldsymbol{k})+d_i(\boldsymbol{k})\boldsymbol{\sigma}_i$, $\boldsymbol{\sigma}_i$ $(i=x,y,z)$ are 2×2 Pauli matrices. To the lowest order of $\boldsymbol{k}$, $d_1(\boldsymbol{k})=Ak_x$, $d_2(\boldsymbol{k})=Ak_y$, $d_3(\boldsymbol{k})=M-Bk^2$, and $\epsilon(\boldsymbol{k})=C-Dk^2$. In the above Hamiltonian, the spin-up and spin-down subsystems can be decoupled, and $\boldsymbol{H}_{\rm D}(\boldsymbol{k})$ and $\boldsymbol{H}^*_{\rm D}(-\mathbf{k})$ describe the spin-up and spin-down subsystems, respectively. The lower block $\boldsymbol{H}^*_{\rm D}(-\mathbf{k})$ is the time-reversal counterpart of the upper block, and thus the total system preserves time-reversal symmetry. A, B, C, D, and M are specific material parameters depending on the QW geometry, which take the same values as those in previous work.[17,18] A tight-binding model of the form of Eq. (1) can be derived by the following substitutions: $k_ia\to\sin(k_ia)$ and $(k_ia)^2\to 2[1-\cos(k_ia)]$, where a is the lattice constant. The matrix elements are written as: $d_1(\boldsymbol{k})=A\sin(k_x)$, $d_2(\mathbf{k})=A\sin(k_y)$, $d_3(\boldsymbol{k})=M-4B+2B[\cos(k_x)+\cos(k_y)]$, and $\epsilon(\boldsymbol{k})=C-4D+2D[\cos(k_x)+\cos(k_y)]$. The system can exhibit a conventional insulating phase for $M>0$ and a quantum spin Hall effect phase for $M<0$. The two different phases are characterized by a Z_2-valued topological invariant.

We first consider the case of constant mass with a random distribution. The mass M is no longer a constant on each site as above, and can take several different values. There is a fixed coverage λ_i (the sum of all λ_i is 1) for each value M_i, while the sites are randomly distributed. A two-component case is shown schematically in Fig. 1(a), where λ percent sites take the value M_1 and the other ones take M_2. In the following, we will start with this simple case.

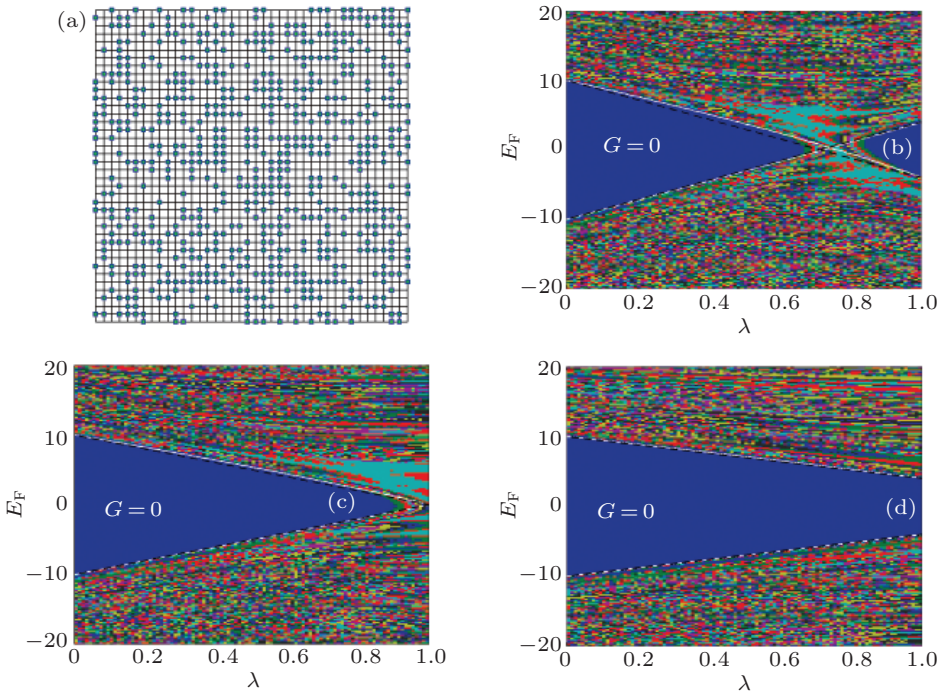


Fig. 1. (colour online) (a) Schematic drawing of the distribution of mass in the two-component case. The mass in the locations marked by filled squares takes one value and that with nothing takes another value. False color plots of conductance as a function of the coverage λ and the Fermi energy $E_{\rm F}$ on a $100(L)\times 80(W)$ strip: (b) $M_1=-10$ and $M_2=4$; (c) $M_1=-10$ and $M_2=0$; (d) $M_1=-10$ and $M_2=-4$. The blue regions in (b), (c), and (d) have zero conductance, and thus mark the regions in the gap.

Due to the random distribution of mass, the system becomes disordered. To study the robustness of the QSHE, we employ the recursive Green function method and evaluate the conductance G of a ribbon with a width W and length L using the Landauer–Büttiker formalism.[24–26] In the following calculations, we use a periodic boundary condition in the width direction to avoid the finite-size effect, and thus determine the phase boundary more precisely. We only consider a single realization of the disorder at

each λ, but present the results in a fashion that is designed to amplify the effect of fluctuations, which turns out to be sufficient for determining the size of the gap with a very good accuracy. In Fig. 1(b), the masses are $M_1 = -10$ and $M_2 = 4$, and their coverages are $1-\lambda$ and λ, respectively. At $\lambda = 0$, the system has a uniform mass M_1 and shows the QSHE. As λ is increased, which means replacing the mass with M_2 on increasing number of sites, the system remains in the QSHE phase and the gap size is reduced. At a critical value λ_c, the gap vanishes. Hereafter, the gap is inverted and the system becomes a normal insulator. Interestingly, we find that the disordered system can be described by an effective mass $M_{\rm eff} = (1-\lambda)M_1+\lambda M_2$ (the black line in Fig. 1(b)). We also consider the cases of $M_1 = -10$, $M_2 = 0$ (see Fig. 1(c)), and $M_1 = -10$, $M_2 = -4$ (see Fig. 1(d)), and find that the effective mass description is also applicable to the results. The system we study is like an alloy composed of two materials. One of them is randomly substituted by the other at a fix percentage λ. The simplest approach to treating the substitutional disorder would be to simply interpolate between the tight binding parameters for the two materials. In our case, since only the masses are different, it is reasonable to approximate the electronic structure of the system using a translationally invariant Hamiltonian with an interpolating effective mass. At small λ (or close to 1), the band structure is not drastically changed and the effective description is expected to be more accurate, which is indeed the case, as shown in Fig. 1. We also notice that even at intermediate λ, the discrepancy is small. Thus, to some extent, the effective description is applicable for the whole λ regime. The topological properties of the system can also be studied by calculating the Z_2-valued topological invariant. The spins $s_z = \pm 1$ in Eq. (1) can be taken separately. When the system is in the QSHE phase, each copy exhibits quantized Hall conductance. Thus, we can calculate the Hall conductance to determine the topological properties using the Kubo formula:

$$\sigma_{xy} = -\frac{2e^2}{\hbar}\,\mathrm{Im}\sum_{E_n<E_{\rm F}<E_m}\frac{\langle n|\boldsymbol{v}_x|m\rangle\langle m|\boldsymbol{v}_y|n\rangle}{(E_m-E_n)^2}, \quad (2)$$

where $\boldsymbol{v}_{\boldsymbol{k}} = \partial \boldsymbol{H}(\boldsymbol{k})/\partial \boldsymbol{k}$, with $H(k)$ being the Hamiltonian of the system. For the disordered systems, the above calculation can be generalized by taking the disordered system as a "supercell" and introducing the twisted boundary conditions.[27–29] However, the increasing amount of calculation will greatly limit the size we can access. Hence, to calculate larger sizes, we preserve the inversion symmetry. Then the problem can be greatly simplified.[6] It has been shown that the topological invariant can be determined from the knowledge of the parity $\xi_{2m}(\boldsymbol{\Gamma}_i)$ of the $2m$-th occupied energy band at the four time-reversal invariant momenta (TRIM) $\boldsymbol{\Gamma}_i$ that satisfy $\boldsymbol{\Gamma}_i = \boldsymbol{\Gamma}_i + \boldsymbol{G}$ ($\boldsymbol{G}$ is the reciprocal lattice vector). The four TRIMs can be expressed in terms of primitive reciprocal lattice vectors as $\boldsymbol{\Gamma}_{i=(n_1,n_2)} = (n_1\boldsymbol{b}_1 + n_2\boldsymbol{b}_2)/2$, with $n_j = 0, 1$. Then Z_2 is the product $\prod_{n_j=0,1}\delta_{n_1n_2}$, where the parity product for the occupied bands $\delta_i = \prod_{m=1}^{N}\xi_{2m}(\boldsymbol{\Gamma}_i)$. We want to mention that for a large enough system, such consideration will not change the underlying physics. We show the results in Fig. 2. For different disorder realizations, the energy levels for

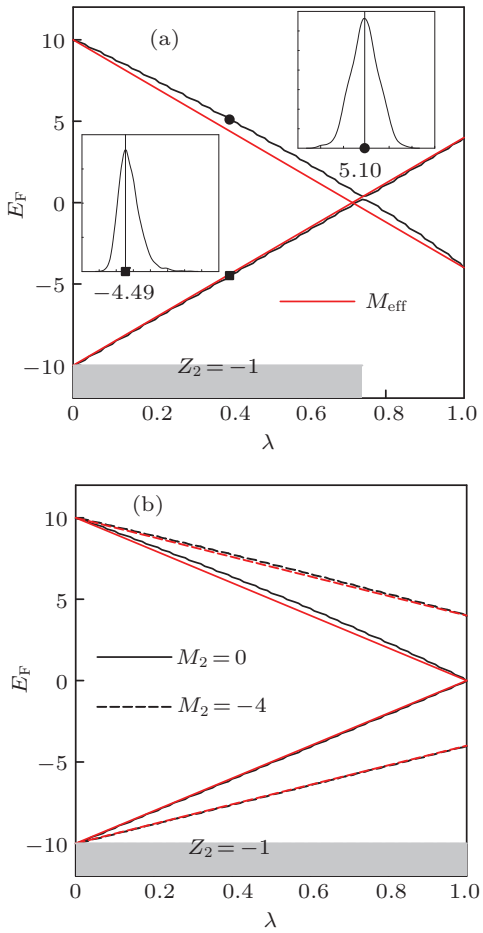


Fig. 2. (colour online) The gap value extracted from the calculations of topological invariant (black solid line) and of the effective mass $M_{\rm eff} = (1-\lambda)M_1 + \lambda M_2$ (red solid line) for: (a) $M_2 = 4$, (b) $M_2 = 0$, and $M_2 = -4$. The insets in Fig. 2(a) show the broadened energy levels which restrict the gap size to be $\lambda = 0.4$. The shaded regions in both figures mark the range on the λ axis where the system has a nontrivial Z_2.

the electrons at half filling and the one just above are broadened (as shown in the inset of Fig. 2(a)). For the parameters used, the physical gap size is determined by the value at $\boldsymbol{k} = (0,0)$ TRIM. We can approximate the gap value from the peaks of the distributions, which are the energy levels for the most energetic electrons. Such consideration is reasonable in that disorder broadens the energy bands, and the states in the tail are mostly localized, as in the case of integer quantum Hall effect. Our calculations are carried on 1000 different disorder realizations and the extracted gap size fits well with that from the calculations of conductivity. Additionally, in all 1000 realizations, $Z_2 = -1$ for $\lambda < \lambda_c$, while $Z_2 = 1$ for $\lambda > \lambda_c$, which implies that the topological quantum phase transition at λ_c is a sharp one. These results are well consistent with those from the calculations of conductivity. We also consider the case of three components, and the results are similar.

Now we study the case of constant masses with random distributions. This kind of disorder is not realistic in the HgTe QWs, but the underlying physics is general. Namely, the Dirac equation with several constant masses can be well described by a uniform one with an effective mass which is just the arithmetical average of different values. It can be realized in graphene via adatom deposition to engineer a robust QSHE.[30] In real materials, the thickness fluctuation is anywhere and the amplitude is estimated to be of the order of 0.2–0.3 nm.[21] In the tight-binding model, it is described by replacing the mass on site n with $M+\epsilon_n$. The disorder ϵ_n satisfies the distribution probabilities:

$$P_{\rm d}(\epsilon_n) = \begin{cases} 1/W, & -W/2 \le \epsilon_n \le W/2 \\ 0, & \text{otherwise}, \end{cases} \tag{3}$$

where W is the distribution width describing the strength of disorder. The fluctuation can be also viewed as the case of constant masses with random distributions, while the number of components is infinite and the coverages are all equal.

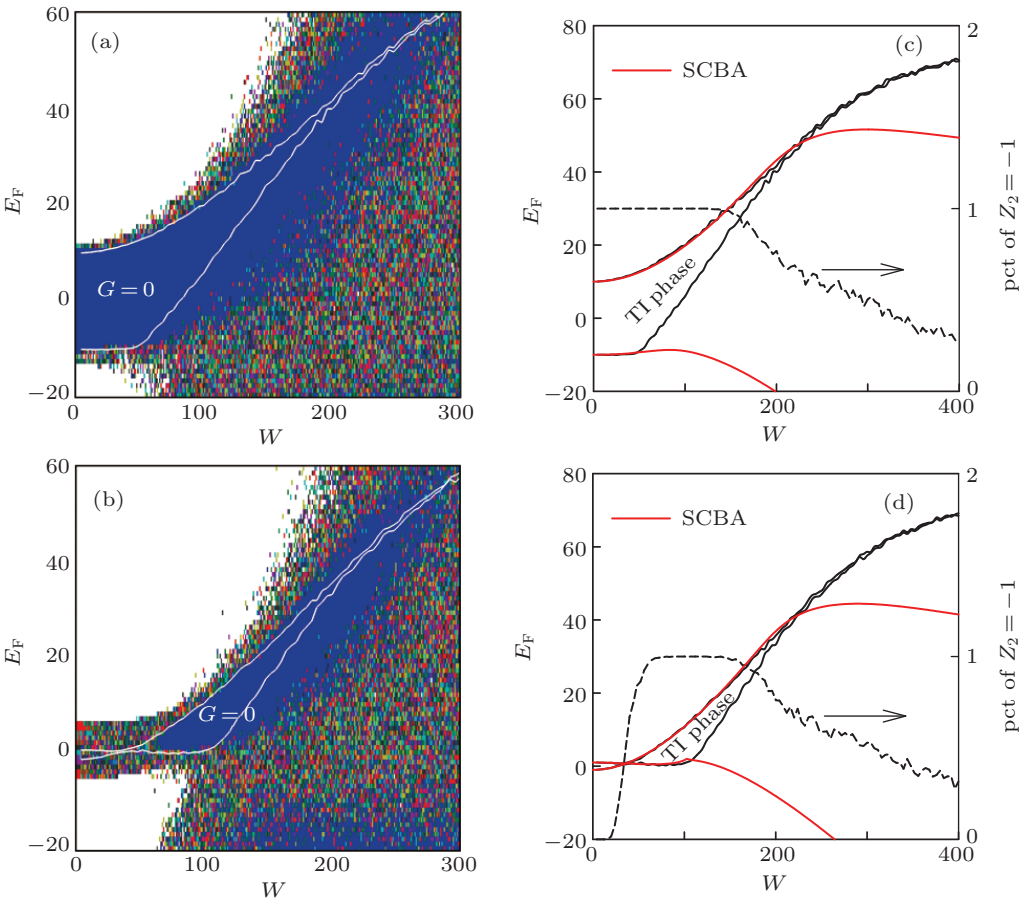


Fig. 3. (colour online) False color plot of conductance G as a function of disorder strength W and the Fermi energy $E_{\rm F}$ for (a) $M = -10$ and (b) $M = 1$. The conductance in the white region also fluctuates and is not shown here. The phase boundaries extracted from the calculations of topological invariant and SCBA are shown for (c) $M = -10$ and (d) $M = 1$.

We evaluate the conductance G of a ribbon with the same geometry as those in Fig. 1 in the presence of the disorder described by Eq. (2). In Fig. 3(a), the disorder is introduced to a TI in its clean form, and it can be seen that the TI phase persists to a fairly large strength of disorder. In Fig. 3(b) the disorder is introduced to a normal insulator. Interestingly, it can invert the gap and turn the normal insulator into a TI. These behaviors are similar to those induced by an on-site one, where a topological Anderson insulator is predicted.[17] The phase diagrams extracted from the calculations of topological invariant are shown in Figs. 3(c) and 3(d). It can be seen that the weak-disorder boundary fits well with that from the calculations of conductivity, while the strong-disorder one fits well only when the strength of disorder W is small. The percentage of the disorder realizations with $Z_2 = -1$ is also shown in the figure. When its value is 0 (1), the system is in the trivial (nontrivial) insulating phase. At large strength of disorder, its value is between 0 and 1, indicating that the system is in a mixed phase. We also compare the result with that from the self-consistent Born approximation. They differ on the strong-disorder boundary and the curves bend to opposite directions. It has been argued that the strong-disorder boundary cannot be described by effective medium theory, where a mobility edge is crossed.[19] However, the boundary from the calculation of the topological invariant seems narrower than that from the conductivity. The reason is that in the TI phase the conductance keeps an exact quantized value, while in a finite region near the strong-disorder boundary the fluctuation is also very small and cannot be distinguished by the false color plot. In fact, the strong-disorder transition is in the universality class of the quantum Hall effect which can be evidenced by the localization length scaling.

The above results show that a random mass has similar effect as on-site potential. However, they have different effects on the transport properties of Dirac fermions, where fluctuations of the on-site potential allow for metallic conduction at the Dirac point while fluctuations of the mass do not.[31] The reason is that the low-energy effective Hamiltonian of HgTe QWs is a modified Dirac equation.[32] In the presence of disorder, the quadratic term acting on the decaying state dominates the physics. Since both kinds of disorder make the state exponentially decay, they have similar effects.

In conclusion, we have made systematic studied the effect of the thickness fluctuation of HgTe QWs which naturally exists in experiments. We first consider the case of constant masses with a random distribution and show that the disordered system can be well described by virtual uniform QWs with an effective mass when the number of components is small. Though this kind of disorder is not realistic in HgTe QWs, the underlying physics is interesting and may be realized in graphene via adatom deposition. We then study the effect of realistic thickness fluctuation. We find that the QSHE is not only robust, but also can be generated by relatively large fluctuation. Though it can be viewed as a special case of constant masses with an infinite number of components, the mechanism is different and it is due to the existence of the quadratic term in the low-energy effective Hamiltonian. Our results imply that the thickness fluctuation does not cause backscattering and the QSHE is robust to it.

References

[1] Moore J E 2010 *Nature* **464** 194

[2] Hasan M Z and Kane C L 2010 *Rev. Mod. Phys.* **82** 3045

[3] Qi X L and Zhang S C 2011 *Rev. Mod. Phys.* **83** 1057

[4] Kane C L and Mele E J 2005 *Phys. Rev. Lett.* **95** 226801

[5] Kane C L and Mele E J 2005 *Phys. Rev. Lett.* **95** 146802

[6] Fu L and Kane C L 2007 *Phys. Rev.* B **76** 045302

[7] Bernevig B A, Hughes T L and Zhang S C 2006 *Science* **314** 1757

[8] König M, Wiedmann S, Brüne C, Roth A, Buhmann H, Molenkamp L W, Qi X L and Zhang S C 2007 *Science* **318** 766

[9] Hsieh D, Qian D, Wray L, Xia Y, Hor Y S, Cava R J and Hasan M Z 2008 *Nature* **452** 970

[10] Hsieh D, Xia Y, Wray L, Qian D, Pal A, Dil J H, Osterwalder J, Meier F, Bihlmayer G, Kane C L, Hor Y S, Cava R J and Hasan M Z 2009 *Science* **323** 919

[11] Zhang H, Liu C X, Qi X L, Dai X, Fang Z and Zhang S C 2009 *Nature Phys.* **5** 438

[12] Xia Y, Qian D, Hsieh D, Wray L, Pal A, Lin H, Bansil A, Grauer D, Hor Y S, Cava R J and Hasan M Z 2009 *Nature Phys.* **5** 398

[13] Chen Y L, Analytis J G, Chu J H, Liu Z K, Mo S K, Qi X L, Zhang H J, Lu D H, Dai X, Fang Z, Zhang S C, Fisher I R, Hussain Z and Shen Z X 2009 *Science* **325** 178

[14] Guo H M and Feng S P 2012 *Chin. Phys.* B **21** 077303

[15] Yuan J H, Cheng Z, Zhang J J, Zeng Q J and Zhang J P 2012 *Chin. Phys.* B **21** 047203

[16] Roushan P, Jungpil S, Parker C V, Hor Y S, Hsieh D, Qian D, Richardella A, Hasan M Z, Cava R J and Yazdani A 2009 *Nature* **460** 1106

[17] Li J, Chu R L, Jain J K and Shen S Q 2009 *Phys. Rev. Lett.* **102** 136806

[18] Jiang H, Wang L, Sun Q F and Xie X C 2009 *Phys. Rev.* B **80** 165316

[19] Groth C W, Wimmer M, Akhmerov A R, Tworzydlo J and Beenakker C W J 2009 *Phys. Rev. Lett.* **103** 196805
[20] Guo H M, Rosenberg G, Refael G and Franz M 2010 *Phys. Rev. Lett.* **105** 216601
[21] Tkachov G, Thienel C, Pinneker V, Buttner B, Brune C, Buhmann H, Molenkamp L W and Hankiewicz E M 2011 *Phys. Rev. Lett.* **106** 076802
[22] Büttner B, Liu C X, Tkachov G, Novik E G, Brüne C, Buhmann H, Hankiewicz E M, Recher P, Trauzettel B, Zhang S C and Molenkamp L W 2011 *Nature Phys.* **7** 418
[23] Guo H M, Feng S P and Shen S Q 2011 *Phys. Rev.* B **83** 045114
[24] Metalidis G and Bruno P 2005 *Phys. Rev.* B **72** 235304
[25] Landauer R 1970 *Philos. Mag.* **21** 863
[26] Büttiker M 1988 *Phys. Rev.* B **38** 9375
[27] Niu Q, Thouless D J and Wu Y S 1985 *Phys. Rev.* B **31** 3372
[28] Essin A M and Moore J E 2007 *Phys. Rev.* B **76** 165307
[29] Guo H M 2010 *Phys. Rev.* B **82** 115122
[30] Weeks C, Hu J, Alicea J, Franz M and Wu R Q 2011 *Phys. Rev.* X **1** 021001
[31] Bardarson J H, Medvedyeva M V, Tworzydlo J, Akhmerov A R and Beenakker C W J 2010 *Phys. Rev.* B **81** 121414(R)
[32] Shen S Q, Shan W Y and Lu H Z 2011 *Spin* **1** 33