Finite size effects on the quantum spin Hall state

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Abstract. We theoretically study the helical edge states in the quantum spin Hall (QSH) effect based on an effective 4-band tight-binding model for HgTe/CdTe quantum wells. We microscopically describe the spatial dependence of the helical edge modes in the QSH state. It is found that the helical edge states are gapped when the width of sample narrows. This is because the edge states on the opposite boundary of the sample overlap each other, and then the backward scattering channel opens up.

1. Introduction
Recently, Kane and Mele proposed the quantum spin Hall (QSH) effect in a graphene layer with spin-orbit coupling [1,2]. The QSH state has a bulk energy gap, but has gapless edge states with different spins moving in opposite directions. No net charge current but spin current is carried by this edge state. Since the spin current is protected by the time reversal symmetry, it is quite robust against nonmagnetic disorder. Thus the QSH effect is expected to play an important role in spintronics.

Soon after the proposal of the QSH effect in a graphene, Bernevig et al. proposed the QSH effect in HgTe/CdTe quantum wells [3]. They predicted a quantum phase transition in HgTe/CdTe quantum wells as a function of a thickness $d$ of the quantum wells. The quantum well system is a conventional insulator for $d < d_c$ and the QSH state for $d > d_c$, which has a single pair of helical edge state. This QSH effect in HgTe/CdTe quantum wells was observed by König et al. [4]. More recently, it is known that a certain class of three-dimensional topological insulator material can have protected surface states which is a higher-dimensional analogue of one-dimensional helical edge states in the QSH effect [5,6,7,8,9].

In order to utilize the QSH effect in microscopically fabricated devices, it is important to reveal the system size effects on the QSH state. Recently, Zhou et al. presented an analytical study of the continuum effective 4-band model for a strip of finite width for the HgTe/CdTe quantum wells [10]. They showed that edge states on the two sides can couple together to produce a gap in the spectrum, destroying the QSH state.

In this paper, we carry out the similar analysis on the finite size effect on the QSH state, but based on the tight-binding scheme. Because the tight-binding model can easily describe atomic scale roughness around the edge of the sample and simulate various device geometry.

2. Method
The effective 4-band model for HgTe quantum wells proposed by Bernevig et al. is given as
Here, we derive a corresponding Hamiltonian based on the square lattice tight-biding scheme
the upper block
\[ H = \epsilon(k) I_{2 \times 2} + \sum_{a=1,2,3} d_a(k) \sigma^a, \]
where \( k_x \) and \( k_y \) are momenta in the plane of the two-dimensional electron gas, \( I_{2 \times 2} \) is a 2 \times 2
unit matrix, \( \sigma_a \) are the Pauli matrices, \( \epsilon(k) = C - D(k_x^2 + k_y^2), d_1 + id_2(k) = A(k_x + ik_y), \) and
\( d_3 = M - B(k_x^2 + k_y^2) \). \( A, B, C, D, \) and \( M \) are material parameters that depend on the quantum
well geometry. The most important property of this model is that the gap parameter \( M \) can be continuously tuned from a positive value for thin quantum well with thickness \( d < d_c \) to a negative
value for thick quantum well with \( d > d_c \). A quantum phase transition between a
insulating state and the QSH state occurs at a critical thickness \( d_c \).

Because the Hamiltonian is block diagonal and the lower block \( H^\dag(-k) \) is time reversal of
the upper block \( H(k) \), it is sufficient to solve the upper block \( H(k) \) on the finite strip geometry.
Here, we derive a corresponding Hamiltonian based on the square lattice tight-biding scheme
given as,
\[
\mathcal{H} = e_1 \sum_{i,l=1,2} c_{i,l}^\dagger c_l + e_2 \sum_i c_{i,1}^\dagger c_{i,1} - e_2 \sum_i c_{i,2}^\dagger c_{i,2} + e_3 \sum_{<i,j>} c_{i,1}^\dagger c_{j,1} + e_4 \sum_{<i,j>} c_{i,2}^\dagger c_{j,2}^\dagger

+ie_5 \sum_i (c_{i,1}^\dagger c_{i,1} - c_{i,1}^\dagger c_{i,1} + c_{i,2}^\dagger c_{i,2} + c_{i,2}^\dagger c_{i,2} - c_{i,2}^\dagger c_{i,2} + h.c.)

+e_5 \sum_i (-c_{i,1}^\dagger c_{i,1} - c_{i,1}^\dagger c_{i,1} + c_{i,2}^\dagger c_{i,2} + c_{i,2}^\dagger c_{i,2} - c_{i,2}^\dagger c_{i,2} + h.c.),
\]
where \( i, j \) are the square lattice sites, \( l = 1, 2 \) is the orbital degree of freedom, \( e_1 = 2(C - 4D), e_2 = -4B(2 - \frac{M}{2D}), e_3 = 2(D + B), e_4 = 2(D - B) \) and \( e_5 = \frac{A}{2}; <i, j> \) is the sum runs over all nearest neighbor sites, \( \delta_i (i = 1, 2) \) are the nearest neighbor vectors. We obtain the energy spectrum and dispersion by numerical diagonalization.

3. Result
To study the system-size dependence of the QSH state, we choose model parameters so as to
describe the QSH state regime, for instance, \( M = -3.0 \) [meV], \( A = 1.0 \) [meV nm], \( B = -0.5 \)
[meV nm\(^2\)], \( C = 0.0 \) [meV], \( D = 0.3 \) [meV nm\(^2\)]. Figure 2 (a) and (b) show the energy dispersion
relation for \( L = 40 \) sites. We can clearly see that gapless helical edge modes exist inside the bulk
energy gap of the system. We note here that, since we are treating \( H(k) \) only, the helical edge
mode with positive and negative group velocity are located around opposite side of the sample,
We also show the results for $L = 10$ sites in Figure 2 (c) and (d). Contrary to the $L = 40$ sites case, we can see that the energy spectrum for the edge states is parabolic near $k_x = 0$ and energy gap opens. Thus the system is insulating. This mechanism can be understood as follows. As the strip narrows, the edge states on each boundary start to couple together. Thus the backward scattering channels open up and then the time reversal protection of the edge states has been broken.

To confirm this coupling of the edge states, we plot the density distribution of the edge states for the strip with $L = 40$ sites and $L = 10$ sites in Figure 3. For the strip with $L = 40$ sites, the density distribution is located at each side of the strip and decays exponentially toward the center. Because there are no overlap of the edge states near the center, the edge states can survive in the strip with $L = 40$ sites. On the other hand, for the strip with $L = 10$ sites, it is found that the density distribution for the edge states on opposite boundary overlap each other near the center and then the backscattering channel opens up. Because of this the phase transition from QSH states to the band insulator occurs.

These behaviors are quite similar to those observed by Zhou et al. based on the continuum model [10]. However, we also find non-monotonic atomic scale spatial dependences of the edge states as shown in Figure 3.
Figure 3. The density distribution of the edge states (a) for \( L = 40 \) sites and (b) for \( L = 10 \) sites. The red solid line corresponds to \( |\Psi(k_x = -0.2, y)|^2 \), and the blue solid line corresponds to \( |\Psi(k_x = 0.2, y)|^2 \).

4. Conclusion and Discussion
We have theoretically studied the system-size effect on the helical edge state in two-dimensional strip geometry based on the effective 4-band tight-binding model for the HgTe/CdTe quantum well. It has been found that the QSH state can be broken when the width of the system is narrow enough for the edge states around each edge to overlap to open the backward scattering channels.

The present model can describe various impurity distributions, or atomic scale roughness of the sample edge. Relating studies including such disorder are being carried out.

Acknowledgments
A part of numerical computations in this work was carried out at the Yukawa Institute Computer Facility, and also at Cyberscience Center, Tohoku University. This work is partly supported by Grant-in-Aid for Scientific Research (C) and also by Next Generation Supercomputing Project, Nanoscience Program, from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

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