Quantum spin Hall phase in honeycomb nanoribbons with two different atoms: edge shape effect to bulk-edge correspondence

Kenji Kondo and Ren Ito
Research Institute for Electronic Science, Hokkaido University, Hokkaido Sapporo Kita-ku Kita-20 Nishi-10, Japan
E-mail: kkondo@es.hokudai.ac.jp

Keywords: quantum spin Hall effect, topological insulators, bulk-edge correspondence, edge shape effect

Abstract
In this study, we consider a quantum spin Hall (QSH) phase in both the zigzag and the armchair type of honeycomb nanoribbons with two different atoms from the viewpoint of bulk-edge correspondence. Generally, the QSH phase in honeycomb nanoribbons is determined by the topology of the bulk Hamiltonian. However, the armchair type of nanoribbons seems to become the QSH phase in a very different region compared with bulk materials. On the other hand, the zigzag type of nanoribbons seems to become the QSH phase in almost the same region as bulk materials. We study the reason why the QSH phase in nanoribbons seems to be different from that of bulk materials using the extended Kane-Mele Hamiltonian. As a result, there is a clear difference in the edge states in the QSH phase between the zigzag and the armchair type of nanoribbons. We find that the QSH phase region in nanoribbons is actually different from that of bulk materials. This is because the coherence lengths of edge wave functions of nanoribbons are extremely influenced by their edge-shapes. We can conclude that the bulk-edge correspondence does not hold for relatively narrow nanoribbons compared with their coherence lengths and that the edge shapes of nanoribbons make their coherence lengths of edge wave functions different, which largely influences the QSH phase.

1. Introduction
Recently, topological materials and topological phenomena have attracted much attention in the field of condensed matter physics [1–12]. Especially, topological insulators are very important for practical use since they are considered to be promising candidates of spin current generators in the spintronics devices [13–17]. Since spin current generators are mandatory in the spintronics field, many researchers have proposed new ones [18–30]. Among them, spin sources using topological insulators are very attractive because of their dissipationless spin currents. Topological insulators originate from two-dimensional quantum spin Hall (QSH) insulators which were predicted theoretically by Kane and Mele for the first time in 2005 [31]. They suggested that graphene with spin-orbit interactions (SOI) exhibits a two-dimensional QSH phase which is a new state of matter. They also discovered that the QSH phase relates directly to the mathematical concepts of ‘topology’. The QSH insulators are distinguishable from the normal insulators by $\mathbb{Z}_2$ topological invariant and, therefore, they are also called as two-dimensional topological insulators.

Soon after the Kane-Mele suggestion, Bernevig, Hughes, and Zhang theoretically proposed that a HgTe/CdTe quantum well is another candidate of the QSH insulator in 2006 [32]. In 2007, König et al showed the existence of QSH phases in the same type of quantum well experimentally [33]. This is the first experimental realization of QSH phases. The other system which exhibits the QSH phase is an AlSb/InAs/GaSb quantum well. Liu et al predicted that this material would also show the QSH phase in 2008 [34]. This theoretical prediction has been proven to be correct by an experimental result in 2010 [35]. The concept of topological insulators is extended to three-dimension and many materials have been gradually discovered to be topological insulators such as Bi$_2$Te$_3$, Bi$_2$Se$_3$, Sb$_2$Te$_3$, and so on [36–41].
As described above, Kane and Mele’s study on the QSH phase has invoked many studies related to the topological insulators [5–7, 42]. One of the most important features of the QSH phase is the existence of gapless edge states. The helical spin current flows at all the edges of QSH insulators. These gapless edge states are robust against any perturbations which do not break the time reversal symmetry (TRS) since they are topologically protected by the TRS. Another important feature of them is that the topological feature of the QSH phase is determined only by the bulk states. This is so called ‘bulk-edge correspondence’ [43–47]. The value of $Z_2$ topological invariant is calculated by the bulk wave functions of materials under this concept. Therefore, many researchers have considered that the QSH phase is determined only by the bulk states of materials and that the QSH phase is not affected by the edge shape. Actually, Kane and Mele have not mentioned the difference between the zigzag and the armchair-type of graphene nanoribbons in the QSH phase. Also, there are very few papers dealing with the QSH phase of the armchair-type of graphene nanoribbons. The band structures of both the zigzag and the armchair-type of graphene nanoribbons in the QSH phase are shown in a review paper [48]. Looking at these band structures in detail, the energy band of the armchair-type of nanoribbons in the QSH phase seems to have a finite energy-gap at cross point of linear dispersion (edge states) in contrast to the zigzag-type in the QSH phase. The appearance of gapless edge states inside the band-gap is an important property of the QSH phase. It is a serious problem that the linear dispersion of the armchair-type of nanoribbons looks like having a finite energy-gap although the bulk graphene is situated in the QSH phase. This fact seems to suggest that the QSH phase depends on the edge shapes of graphene nanoribbons. Although the QSH phase is determined by the bulk-edge correspondence, it can be considered that the bulk wave functions are also affected by the edge shape. As a result, we can speculate that this is the reason why the QSH phase in nanoribbons seems to be different from that of bulk materials and why the QSH phase in the armchair-type of nanoribbons are especially different from that of bulk materials in comparison to the zigzag-type of nanoribbons.

In this study, we investigate the electronic structures in the QSH phase for both the zigzag and the armchair type of honeycomb nanoribbons in order to verify the above speculation. Also, we deal with honeycomb nanoribbons with two different atoms in order to generalize the discussion. Then, we investigate to what extent the edge shapes of nanoribbons affect the phase diagram of the QSH insulators.

2. Theory

In this section, we discuss the QSH phase for bulk honeycomb materials using an extended Kane-Mele model. The extended Kane-Mele model is generalized by incorporating the different strengths of SOIs. This model can describe both the QSH phase and the normal insulating phase depending on parameters.

2.1. Calculation model and the Hamiltonian

We consider both the zigzag-type and the armchair-type of honeycomb nanoribbons as shown in figure 1. These models have infinite length in horizontal direction with periodic boundary conditions and have finite $N$ layers in vertical direction. The vertical layer is labeled by $n$ where $n = 1, 2, \cdots N$. Dashed rectangles show the unit cells of this model. The absolute value of translational vector is denoted by $a_Z$ and $a_A$ in the zigzag-type and the
armchair-type of nanoribbons, respectively. Red circles show sublattice A and blue ones show sublattice B. In the extended Kane-Mele model, the atoms located on sublattice A differ from those located on sublattice B. Here, we consider the following Hamiltonian:

\[
H = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}_i^{\dagger} \hat{c}_j + i \lambda_{SO}^A \sum_{\langle i,j \rangle, \sigma} \nu_{ij} \hat{b}_i^{\dagger} \sigma_z \hat{b}_j^{\sigma} + i \lambda_{SO}^B \sum_{\langle i,j \rangle, \sigma} \nu_{ij} \hat{a}_i^{\dagger} \sigma_z \hat{a}_j^{\sigma} + \lambda_{st} \sum_{i, \sigma} \xi_i \hat{c}_i^{\dagger} \hat{c}_i^{\sigma},
\]

The first term shows the nearest neighbor hopping term with its hopping energy \( t \), the second term shows the SOI originating from the atoms A with its strength \( \lambda_{SO}^A \), and the third term shows the SOI originating from the atoms B with its strength \( \lambda_{SO}^B \). The operator \( \hat{a}_i^{\sigma} \) annihilates an electron with spin \( \sigma \) from site \( i \) on sublattice A, while the operator \( \hat{b}_i^{\sigma} \) annihilates an electron with spin \( \sigma \) from site \( i \) on sublattice B. The symbols \( \langle i, j \rangle \) in the second and third term mean that the sum runs over the second nearest neighbors. \( \nu_{ij} \) is equal to \(+1\) or \(-1\) depending on whether electrons take a counterclockwise path or clockwise path. \( s_z \) is the matrix representation of the z component for electron’s spin, where z axis points to the normal direction to the plane. The fourth term is the staggered potential with its strength \( \lambda_{st} \) and works as a perturbation against the QSH phase. The symbol \( \xi_i \) takes the value of 1 (−1) in the case that electrons exist in the atoms A (B). The operator \( \hat{c}_i^{\sigma} \) in the first and the fourth terms denotes \( \hat{a}_i^{\sigma} \) or \( \hat{b}_i^{\sigma} \) depending on whether electrons are on sublattice A or on sublattice B.

The SOI terms are essential for exhibiting the QSH phase. The QSH phase emerges depending on the values of the strength of SOI and the staggered potential which are normalized by the hopping energy. Kane and Mele incorporated the Rashba term in their Hamiltonian. However, we omit this term in our Hamiltonian since this term can be omitted without the loss of generality. This manipulation makes it easier to investigate the difference of the wave functions between the zigzag-type and the armchair-type of nanoribbons.

2.2. Derivation of the QSH phase diagram in our model

We analytically derive the condition of the emergence of the QSH phase in bulk honeycomb materials using the extended Kane-Mele model. Kane and Mele have derived that a graphene exhibits the QSH phase in the case of \( \lambda_{st} < 3 \sqrt{3} \lambda_{SO} \) when ignoring Rashba term. It can be easily confirmed that the QSH phase in the extended Kane-Mele model emerges in the case of \( \lambda_{st} < 3 \sqrt{3} \lambda_{SO} \), where \( \lambda_{SO} = (\lambda_{SO}^A + \lambda_{SO}^B) / 2 \) as shown below.

We consider an infinite honeycomb lattice with periodic boundary conditions in x and y directions as shown in figure 2. The dashed parallelogram represents the unit cell of this lattice. It is enough to consider only the SOI term in order to derive the condition of emergence of the QSH phase in our model. This is because the difference between the Kane-Mele model and our model is only SOI term of the Hamiltonian.

Here, we denote the SOI term of the Hamiltonian as \( H_{SO}^{\sigma} \) with \( \sigma = +1 (-1) \) for up-spin (down-spin) electrons. The term \( H_{SO}^{\sigma} \) is calculated as follows:
\[H_{SO} = \sigma \left[ i \lambda_{SO}^B \exp[i(ka/2 + \sqrt{3} k_y a/2)] - \exp[i(-ka/2 + \sqrt{3} k_y a/2)] \right. \\
- \exp[i(ka/2) + \exp(-ika) - \exp[-i(ka/2 + \sqrt{3} k_y a/2)] \\
+ \exp[i(ka/2 - \sqrt{3} k_y a/2)])] |\hat{\alpha}_{\sigma} \rangle_{\sigma} \\
+ \sigma i \lambda_{SO}^A \left[ \exp[-i(ka/2 + \sqrt{3} k_y a/2)] - \exp[i(ka/2 - \sqrt{3} k_y a/2)] \right] \\
\left. - \exp[i(ka/2 + \sqrt{3} k_y a/2)])] |\hat{\beta}_{\sigma} \rangle_{\sigma} \right]
\]

where \(x = ka/2\) and \(y = \sqrt{3} k_y a/2\). The above equation can be transformed using the properties of trigonometric functions as follows:

\[H_{SO} = \sigma \left[ i \lambda_{SO}^B (2 \sin x - 4 \sin x \cos y) |\hat{\alpha}_{\sigma} \rangle_{\sigma} \\
- \lambda_{SO}^A (2 \sin x - 4 \sin x \cos y) |\hat{\beta}_{\sigma} \rangle_{\sigma} \right],
\]

3. Calculation results

In this section, we discuss the calculation results of the QSH phase of honeycomb nanoribbons which contains two different atoms. We perform calculations of the electronic structures of both the zigzag and the armchair-type of nanoribbons and make sure that spin currents flow at the both upper and lower edges of nanoribbons in the QSH phase. Then, we discuss the regions where the QSH phase emerges in the zigzag and the armchair-type of nanoribbons.

3.1. Results for the honeycomb nanoribbons with two different atoms

Figure 3 shows the electronic structures of the zigzag-type of nanoribbons with \(\lambda_{SO}^A = 0.06\) and \(\lambda_{SO}^B = 0.03\). Red lines show the up-spin states of electrons and blue ones show the down-spin states. In the zigzag-type of nanoribbons, there exist four edge states which are seen as linear dispersions as shown in figure 3(a). Figure 3(a) shows the electronic structure of the QSH phase and figure 3(b) shows that of the normal insulating phase. The edge states connect the upper bulk states and lower bulk states in the QSH phase. When the staggered potential becomes larger than its critical value \(\lambda_{c} = 3 \sqrt{3} \lambda_{SO}^M\) the QSH phase is broken to become normal insulating phase as shown in figure 3(b).

We are going to discuss the edge states of the QSH phase in more detail in the followings. The red line from the lower left to the upper right in figure 3(a) indicates that up-spin electrons travel from left to right at the upper edges of nanoribbons. On the other hand, the blue one from the upper left to the lower right in the band structure indicates that down-spin electrons travel from right to left at the upper edges of the nanoribbons. Therefore, spin currents flow from left to right at the upper edges of nanoribbons. In the same way, we can make sure that spin currents also flow at the lower edges of nanoribbons in the opposite direction to the upper edges. This can be confirmed by plotting the electron densities of the edge states of the zigzag-type of nanoribbons.
From figures 4(a) and (b), it is found that electrons in the edge states concentrate at both the edges while electrons in the bulk states spread over the nanoribbons except for the edges.

So far, we notice the difference between nanoribbons with the same atoms (e.g., graphenes) and nanoribbons with two different atoms (e.g., boron nitride). When looking at figure 3(a) carefully, we can notice that pairs of edge states are not parallel in contrast with graphene nanoribbons. Therefore, the velocities of up and down spin electrons in the upper edge of nanoribbons are slower than those in the lower edge of nanoribbons. This fact indicates that a much larger spin current flows at the lower edge than at the upper edge in this case. This asymmetry of spin currents occurs from different strengths of SOI in the nanoribbons. As shown in figure 4(a), we can confirm that edge states at the upper (lower) edge have almost all electrons at the atom A (B). Therefore, the SOI from the atom B are very important at the upper edge, while the SOI from atom A are very important at the lower edge as illustrated in figure 5. As a result, the magnitude of spin current at both the edges is the same value. This asymmetry of spin currents will probably be useful when we need an asymmetry spin source. Except for the asymmetry of spin currents, the following discussion about the QSH phase is applicable to honeycomb nanoribbons with the same atoms.

On the other hand, figures 6(a) and (b) shows the electronic structures of the armchair-type of honeycomb nanoribbons with $\lambda_N = 0.06$ and $\lambda_B = 0.03$. In the armchair-type, up-spin states and down-spin states are almost degenerate in contrast to the zigzag-type. Figure 6(a) shows the electronic structure of the QSH phase nanoribbons and figure 6(b) shows that of normal insulating phase in the armchair-type of nanoribbons. The linear energy dispersions appear in the QSH phase while they don’t appear in normal insulating phase. In the same way as the zigzag-type nanoribbons, the QSH phase is broken to become normal insulating phase when the staggered potential becomes larger than its critical value $\lambda_N = 3\sqrt{3}\lambda_B$. However, in the armchair-type, even though the value of $\lambda_B$ is smaller than the phase transition critical value $\lambda_N$, the linear dispersions have a small
finite gap at $ka_A = 0$ when magnifying the cross point in the linear dispersion as shown in figure 7. As a result, the phase is a normal insulating one. Figure 7 means that the armchair-type of nanoribbons actually shows normal insulating phase in the case of $N = 20$ under $\lambda_{so}^A = 0.06$, $\lambda_{so}^B = 0.03$, and $\nu = 0.12$ although these parameters indicates that nanoribbons are considered to be in the QSH phase by ‘extended Kane-Mele condition’ according to the bulk-edge correspondence. However, if the QSH phase is affected by edge-shapes to much extent, there may be large difference in the critical staggered potential value among the zigzag-type nanoribbons, the armchair-type nanoribbons, and bulk materials. Therefore, it is worth considering the possibility that the edge-shapes could affect the QSH phase. In fact, the emerging small energy gap closes completely in the armchair-type of nanoribbons when their widths become larger enough as shown in figure 8. At that time, the regions of the QSH phase of nanoribbons become the same ones as bulk materials even though the edges of nanoribbons have any shapes. At the same time, this fact strongly suggests that the QSH phase is affected by the edge-shapes when the widths of nanoribbons are small, which is discussed in more detail later.

Next, we investigate the electron densities of the armchair-type of nanoribbons in the QSH regime in order to find the difference of the QSH phase between the zigzag-type and the armchair-type. The QSH phase should have the edge states because of its topological feature. Firstly, we consider the armchair-type of nanoribbons with large enough width. By plotting the electron density in the linear dispersion of the armchair-type of nanoribbons with $N = 40$ width, we can confirm that the linear dispersion exactly represents the edge states like the zigzag-type as shown in figure 9(a). Compared to bulk states shown in figure 9(b), Electrons in these edge states adequately concentrate around both the edges of the armchair-type of nanoribbons. However, in contrast to the zigzag-type, electrons do not completely gather at the edges and they spread into the bulk to some extent. Especially, when $N$ becomes much small, electrons spread into the bulk to much extent as shown in figure 10(a).
Note that these states are different from bulk states shown in figure 10(b). We can speculate that the wave functions in the edge states have much longer coherence length in the case of the armchair-type than that in the case of the zigzag-type. The coherence length $l_c$ can be defined as follows:

$$l_c = \frac{\hbar}{m_{\text{eff}} v_F},$$  

(6)
where $\hbar$ is the Planck’s constant divided by $2\pi$, $m_{\text{eff}}$ is the electron effective mass of nanoribbons, and $v_F$ is the Fermi velocity.

Here, we are going to investigate the probability densities of electrons in the armchair-type of nanoribbons quantitatively in order to estimate the coherence length $l_c$. Figure 11 shows those of the linear dispersion states in the armchair-type of nanoribbons in the case of $N = 150$. From figure 11(a), the probability density of electrons has large peaks at both the upper and lower edges and shows 0 in the center of nanoribbons although it has nonzero values even at the 25 layers far from the edge. The probability densities of the bulk states spread widely into nanoribbons as shown in figure 11(b). These facts show that the linear dispersion states is surely the edge states of the QSH phase even in the armchair-type of nanoribbons. Next, we compare the probability densities of electrons of edge states in the zigzag and the armchair-type of nanoribbons when the width is relatively small ($N = 20$) as shown in figure 12. Two probability densities of electrons are totally different from each other. The probability densities in the zigzag-type have much sharper peak at the both edges than those in the armchair-type.

From figures 11(a) and 12(a), the coherence length of the armchair-type nanoribbons (the zigzag-type nanoribbons) is estimated to be about $8a$ ($a / (2\sqrt{3})$), where $a$ is the lattice constant defined in figure 2. Namely, the coherence length of the armchair-type is about 27.7 times longer than that of the zigzag-type. Therefore, the edge states of the QSH phase in the zigzag-type manifests itself more pronouncedly than that in the armchair-type. These results mean that edge shapes of nanoribbons obviously affect the QSH phase of nanoribbons, which makes the QSH phase of nanoribbons different from that of the bulk materials in spite of bulk-edge correspondence. Without taking into consideration this edge effect, we cannot determine the QSH phase region of narrow honeycomb-nanoribbons.

It is considered that the large difference of the coherence lengths between the zigzag-type one and the armchair-type one originates from the properties of host-honeycomb materials without SOI terms. The model Hamiltonian of the host-honeycomb materials without SOI terms is the same as that of graphenes. As pointed in

![Figure 10.](image1.png)  
**Figure 10.** The electron densities in the case of $N = 8$, $\lambda_{\text{SO}}^A = 0.06$, $\lambda_{\text{SO}}^B = 0.03$, and $\lambda_e = 0.01$ at (a) edge states and (b) bulk states.

![Figure 11.](image2.png)  
**Figure 11.** The probability densities of electrons in the armchair-type of nanoribbons in (a) the edge states and (b) bulk states in the case of $N = 150$, $\lambda_{\text{SO}}^A = 0.06$, $\lambda_{\text{SO}}^B = 0.03$, and $\lambda_e = 0.01$.
some literatures [49–52], the zigzag-type graphenes without SOI have zero-energy states attributing to edge states and the armchair-type graphenes without SOI never have zero-energy states attributing to edge states. Therefore, the zigzag-type graphenes are always metallic and the electrons in the zigzag-type graphenes always concentrate on edge states. On the other hands, the armchair-type graphenes are almost like semiconductors. As a result, in the zigzag-type honeycomb materials, the electrons tend to concentrate at the edges intrinsically and in the armchair-type honeycomb materials, the electrons tend to spread over the bulk intrinsically, which is the origin of the large difference of the coherence lengths between the zigzag-type one and the armchair-type one.

3.2. Results for the QSH phase diagram of honeycomb nanoribbons

From here, we will discuss the QSH phase diagram region in honeycomb nanoribbons. The QSH phase diagram of bulk honeycomb materials consisting of two different atoms is derived in the ‘Theory’ section. The analytical result of critical staggered potential \( \lambda_c \) is given by \( 3 \sqrt{3} \lambda_{SO}^M \), where \( \lambda_{SO} \) is the average value of the strengths of SOI of two different atoms A and B. This result matches the analytical result obtained by Kane and Mele in the case of graphene.

However, when we apply this criterion to the honeycomb nanoribbons, there are times when the gapless edge states disappear in the nanoribbon even though \( \lambda_c \) is smaller than the analytical value of \( \lambda_c \). This phenomena is especially pronounced in the armchair-type of nanoribbons. Since the existence of gapless edge states is one of the important properties for the QSH phase, the case in which edge states have a finite energy gap is no more in the QSH phase but in normal insulating phase. Since the analytical \( \lambda_c \) is obtained by considering the bulk honeycomb materials with no edges, the information of the edge shapes is not included in the analytical result. The lacking information of edge shapes is considered to cause the deviation from the QSH phase diagram obtained by the extended Kane-Mele condition. Although the bulk-edge correspondence always holds mathematically, the edge shape effect should be considered from a practical view point. Therefore, we have to calculate the QSH phase diagram taking into consideration the edge shapes in order to obtain the QSH phase diagram for more realistic finite nanoribbons. Figure 13 shows the difference of critical values of staggered potential \( \lambda_c \) between a numerical calculation (blue surface) and an analytical solution of bulk (light blue surface) in the zigzag-type and the armchair-type of nanoribbons in the case of \( N = 20 \). When the width of nanoribbons is relatively small \( (N = 20) \), the numerical critical values \( \lambda_c \) obviously become much smaller than the analytical solutions in the armchair-type nanoribbons as shown in figure 13(b) while they are almost the same as the analytical solution in the zigzag-type nanoribbons. Note that even in the zigzag-type nanoribbons, there is a little difference between the numerical critical values and the analytical ones derived by bulk states. The apparent difference between the armchair-type and the zigzag-type nanoribbons originates from the magnitude of their coherence lengths. As the above mentioned, these values are about \( 8a \) and \( a/(2\sqrt{3}) \) for the armchair-type nanoribbons and the zigzag-type ones, respectively.

Namely, when the width of a nanoribbon is not large enough in comparison to its coherence length, the QSH phase of the nanoribbon largely deviates from that of bulk materials. The above results are consistent with the results of electronic structures and electron densities in the armchair-type nanoribbons and the zigzag-type nanoribbons. When the width of nanoribbons becomes large enough, the numerical results of the QSH phase diagram coincide with the analytical solutions of bulk in both the zigzag and the armchair-type nanoribbons as shown in figure 14. The bulk-edge correspondence recovers completely.
Therefore, we conclude that these results show that the bulk-edge correspondence does not hold for relatively narrow nanoribbons compared with their coherence lengths and that the edge shapes make their coherence lengths of edge wavefunctions different in nanoribbons, which influences the QSH phase of nanoribbons. Of course, the bulk-edge correspondence revives totally when the widths of nanoribbons become relatively wide compared with their coherence lengths.

In summary, it has been definitely confirmed that the QSH phase is affected by the edge shapes in the case of narrow nanoribbons. This fact suggests that it is very important to take care of the edge shapes when we search for QSH insulators of nanoscale materials experimentally and/or we utilize nanoscale QSH insulators for spintronic devices. Moreover, since the coherence length is considered to be determined by the edge-shapes, we consider that a numerical calculation is need every time in order to estimate the QSH phase criteria for nanoribbons with different edge shapes.

4. Conclusion

We have studied the QSH phase for bulks and nanoribbons of honeycomb materials with two different atoms. The numerical calculation has been performed for electronic structures of the zigzag-type and the armchair-type nanoribbons with changing their widths. We have estimated the parameter regions where the QSH phase emerges and their coherence lengths of edge wavefunctions for both the zigzag-type and the armchair-type nanoribbons.
As a result, there is a large difference in the edge states in the QSH phase between the zigzag and the armchair type of nanoribbons. It has been found that the QSH phase region in nanoribbons is actually different from that of bulk materials. This is because the coherence lengths of edge wave functions of nanoribbons are extremely influenced by their edge-shapes. The coherence lengths are about $8a$ and $a/(2\sqrt{3})$ for the armchair-type nanoribbons and the zigzag-type ones, respectively.

From numerical calculation results, we can conclude that the bulk-edge correspondence does not hold for relatively narrow nanoribbons compared with their coherence lengths and that the edge shapes of nanoribbons make their coherence lengths of edge wavefunctions different, which largely influences the QSH phase. Therefore, we should pay much attention to the edge shapes when looking for nanoscale QSH insulators experimentally and applying nanoscale QSH insulators to spintronic devices.

**Acknowledgments**

This work is partially supported by a Grant-in-Aid for Scientific Research (Grant No. 16K04872) from JSPS, Center for Spintronics Research Network (CSRN) Tohoku University, and Dynamic Alliance for Open Innovation Bridging Human, Environment and Materials.

**ORCID iDs**

Kenji Kondo @ https://orcid.org/0000-0003-3447-0038

**References**

[1] Hasan M Z and Kane C L 2010 Rev. Mod. Phys. 82 3045–67
[2] Qi X L, Wu Y S and Zhang S C 2006 Phys. Rev. B 74 085308
[3] Sheng L, Sheng D N, Ting C S and Haldane F D M 2005 Phys. Rev. Lett. 95 136802
[4] Bernevig B A and Zhang S C 2006 Phys. Rev. Lett. 96 106802
[5] Fu L, Kane C L and Mele E J 2007 Phys. Rev. Lett. 98 106803
[6] Fu L and Kane C L 2007 Phys. Rev. B 76 045302
[7] Fu L 2011 Phys. Rev. Lett. 106 106802
[8] Moore J 2009 Nat. Phys. 5 378
[9] Burkov A and Balents L 2011 Phys. Rev. Lett. 107 127205
[10] Burkov A, Hook M and Balents L 2011 Phys. Rev. B 84 235126
[11] Soluyanov A A, Gresch D, Wang Z, Wu Q, Troyer M, Dai X and Bernevig B A 2015 Nature 527 495
[12] Yang K Y, Lu Y M and Ran Y 2011 Phys. Rev. B 84 075129
[13] Rosciewsky N, Walker E, Gowtham P, Muschinske S, Hellman F, Bank S and Salahuddin S 2019 Bulletin of the American Physical Society APS March Meeting, arXiv:1810.05674
[14] Tokura Y, Kawasaki M and Nagaosa N 2017 Nat. Phys. 13 1056
[15] Ma M, Jalil M, Tan S, Li Y and Suiz 2012 Appl. Adv. 3 032162
[16] Kondo K 2014 J. Appl. Phys. 115 17C701
[17] Gotte M, Joppe M and Dahm T 2016 Sci. Rep. 6 36070
[18] Lustikova J, Shiom Y, Qiu Z, Kikkawa T, Iuchi R, Uchida K and Saitoh E 2014 J. Appl. Phys. 116 135302
[19] Yang X, Liu Y, Zhang X, Zhou L, Wang X, Chi F and Feng J 2014 Phys. Chem. Chem. Phys. 16 11349–55
[20] Zhao H K and Wang Q 2015 Phys. Lett. A 338 425–32
[21] Liu Y, Yang X, Chi F, Si M and Guo Y 2012 Appl. Phys. Lett. 101 213109
[22] Governale M, Taddei F and Fazio R 2003 Phys. Rev. B 68 155324
[23] Zhang Q, Chan K S and Lin Z 2011 Appl. Phys. Lett. 98 032106
[24] Mal’tishukov A, Tang C, Chu C and Chao K A 2003 Phys. Rev. B 68 233307
[25] Scheid M, Bercioux D and Richter K 2007 New J. Phys. 9 401
[26] Choi G M, Min B C, Lee K J and Cahill D G 2014 Nat. Comm. 5 4334
[27] Tang Z, Shikoh E, Aso H, Kawahara A, Ando Y, Shino J and Shiraiishi M 2013 Phys. Rev. B 87 140401
[28] Kimura T, Hashimoto N, Yamada S, Miyag M and Hamaya K 2012 NPG Asia Mater. 4 e9
[29] Kondo K 2015 New J. Phys. 18 013002
[30] Kondo K 2012 J. Appl. Phys. 111 07C713
[31] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 146802
[32] Bernevig B A, Hughes T L and Zhang S C 2006 Science 314 1757–61
[33] König M, Wiedmann S, Brüne C, Roth A, Buhmann H, Molenkamp L W, Qi X L and Zhang S C 2007 Science 318 766–70
[34] Liu C, Hughes T L, Qi X L, Wang K and Zhang S C 2008 Phys. Rev. Lett. 100 236601
[35] Knez I, Du R R and Sullivan G 2011 Phys. Rev. Lett. 107 136603
[36] Zhang H, Liu C X, Qi X L, Dai X and Fang Z 2009 Nat. Phys. 5 438–42
[37] Liu C X, Qi X L, Zhang H, Dai X, Fang Z and Zhang S C 2010 Phys. Rev. B 82 045122
[38] Chen Y et al 2009 Science 325 178–81
[39] Hasan M Z and Moore J E 2011 Annus. Rev. Condens. Matter Phys. 2 55–78
[40] Zhang W, Yu R, Zhang H J, Dai X and Fang Z 2010 New J. Phys. 12 065013
[41] Kuroda K et al 2010 Phys. Rev. Lett. 105 146801
[42] Fu L and Kane C L 2006 Phys. Rev. B 74 195312
[43] Kellendonk J, Richter T and Schulz-Baldes H 2002 Rev. Math. Phys. 14 87–119
[44] Avila J C, Schulz-Baldes H and Villegas-Blas C 2013 Mathematical Physics, Analysis and Geometry 16 137–70
[45] Graf G M and Porta M 2013 Commun. Math. Phys. 324 851–95
[46] Kubota Y 2017 Commun. Math. Phys. 349 493–525
[47] Hayashi S 2018 Commun. Math. Phys. 364 343–56
[48] Murakami S 2008 Prog. Theor. Phys. Suppl. 176 279–301
[49] Nakada K, Fujita M, Dresselhaus G and Dresselhaus M S 1996 Phys. Rev. B 54 17954–61
[50] Gunlycke D and White C T 2008 Phys. Rev. B 77 115116
[51] Zhang X, Kuo J L, Gu M, Bai P and Sun C Q 2010 Nanoscale 2 2160–3
[52] Liu X et al 2015 Chem. Rev. 115 6746–810