Higher-Order Topological Phase on a Honeycomb-Lattice Model with Anti-Kekulé Distortion

T. Mizoguchi, H. Araki, and Y. Hatsugai
Department of Physics, University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan
(Dated: June 20, 2019)

We propose that a honeycomb-lattice model with anti-Kekulé distortion hosts a higher-order topological phase. We demonstrate this by calculating the $Z_6$ Berry phase that serves as a bulk topological invariant of the higher-order topological phase, and by showing the existence of corner states.

A honeycomb lattice provides us of a platform to realize intriguing phenomena in solid-state physics. It serves as one of the simplest examples of a non-Bravais lattice, which gives rise to a multiband electronic structure even for a single-orbital, nearest-neighbor (NN) tight-binding model. A typical example of the honeycomb-lattice systems is graphene, where emergence of Dirac fermions in solid has attracted considerable interests for decades. Besides solid-state systems, the implementation of the honeycomb structure in mechanical systems is graphene.

A typical example of the honeycomb-lattice model is graphene, which gives rise to a multiband electronic structure even as one of the simplest examples of a non-Bravais lattice, making its structure more intriguing. One of the typical modulation patterns is Kekulé-type modulation, which results in the enlargement of the unit cell. Recently, such a modulated structure has been revisited in the context of topological phases protected by crystalline symmetry. Indeed, it has been found that the single-orbital tight-binding model hosts a topological crystalline insulator (TCI), accompanied by characteristic edge states.

Spatial modulation on a honeycomb lattice makes its physics more intriguing. One of the typical modulation patterns is Kekulé-type modulation, which results in the enlargement of the unit cell. Recently, such a modulated structure has been revisited in the context of topological phases protected by crystalline symmetry. Indeed, it has been found that the single-orbital tight-binding model hosts a topological crystalline insulator (TCI), accompanied by characteristic edge states.

Such an implementation of the topological nature is also applied to photonic crystals.

In this note, we present a different view of topological phases in the honeycomb-lattice model with anti-Kekulé modulation (i.e., the modulation opposite to the Kekulé modulation). To be specific, we propose that the present model hosts a higher-order topological phase. Higher-order topological insulators (HOTIs) are a novel topological phase of matter which exhibit unconventional bulk-boundary correspondence. Namely, in HOTIs, the characteristic boundary states appear at the boundary with co-dimension larger than one.

In this note, we present a different view of topological phases in the honeycomb-lattice model with anti-Kekulé modulation (i.e., the modulation opposite to the Kekulé modulation). To be specific, we propose that the present model hosts a higher-order topological phase. Higher-order topological insulators (HOTIs) are a novel topological phase of matter which exhibit unconventional bulk-boundary correspondence. Namely, in HOTIs, the characteristic boundary states appear at the boundary with co-dimension larger than one.

Very recently, the authors have proposed that the HOTIs are characterized by a bulk topological invariant, namely, the $Z_6$ Berry phase defined with respect to the parameters of the local twist of the Hamiltonian. Using this topological invariant, we demonstrate that the $Z_6$ Berry phase is quantized in six-fold (i.e., we obtain the $Z_6$ Berry phase as a topological invariant) due to the local six-fold symmetry around a certain hexagonal plaquette, and that the $Z_6$ Berry phase is $\pi$ for anti-Kekulé modulation, while it is zero for the Kekulé modulation. We also show the existence of corner states when the Berry phase is $\pi$.

We consider the Hamiltonian on a honeycomb lattice:

$$H = \sum_{i,j} t_{i,j} c_i^\dagger c_j + (h.c.),$$

where $\langle i, j \rangle$ represents the NN pairs on the honeycomb lattice, and the transfer integral $t_{i,j}$ is equal to $t_0$ ($t_1$) solid (dashed) bonds in Fig. 1(a).

The previous study by Kariyado and Hu has elucidated that the mirror winding number characterizes the topological phases. In fact, the mirror winding number depends on the choice of the unit cell, which coincides with the fact that emergence of the edge modes depends on the shape of the edges. The mirror winding number changes at the critical point, $t_0 = t_1$, where the Hamiltonian is reduced to the conventional NN hopping model and thus the bulk band gap closes.

In this note, we examine a different topological invariant from the mirror winding number, namely the $Z_6$ Berry phase, which does not depend on the choice of the unit cell. Following Refs., we define the $Z_6$ Berry phase in the present model. To do this, we first pick up one of the hexagonal plaquettes all of whose bonds have the hopping $t_0$ [see a red hexagon in Fig. 1(a)]. We write the Hamiltonian on this plaquette as $H_0$, and the Hamiltonian can be divided in two parts, as $H = H_0 + (H - H_0)$. We then introduce the twist of the Hamiltonian only in $H_0$, while keeping $(H - H_0)$ unchanged. To be spe-
specific, we consider the twisted Hamiltonian $h_0(\Theta)$, where $\Theta = (\theta_1, \theta_2, \theta_3, \theta_4, \theta_5)$ with $\theta_i \in [0, 2\pi]$ are parameters describing the twist angles. The explicit form of $h_0(\Theta)$ is

$$h_0(\Theta) = t_0 \sum_{a=1}^{6} e^{i\theta_a+i\gamma_{a+1}} c_a + (\text{h.c.}),$$

(2)

where we have introduced $\theta_6 := -(\theta_1 + \theta_2 + \theta_3 + \theta_4 + \theta_5)$ and have defined $\gamma$ in modulo 6 such that $a+\gamma \equiv a$; for the positions of sites 1-6, see Fig. 1(a). The total Hamiltonian with the twist is given as $H(\Theta) = h_0(\Theta) + (H-h_0)$. Then, for the many-body ground state of $H(\Theta)$, we write as $|\Psi(\Theta)\rangle$, we define the Berry connection as $A(\Theta) = -i|\Psi(\Theta)\rangle \langle \partial_\Theta \Psi(\Theta)|$. The Berry phase, $\gamma$, is defined as a contour integral of the Berry connection as

$$\gamma = \int_{L_1} d\Theta \cdot A(\Theta) \pmod{2\pi},$$

(3)

where $L_1$ is a path in a five-dimensional parameter space given as $L_1 = E_0 \rightarrow G \rightarrow E_1$ with $E_0 = (0,0,0,0,0)$, $G = \frac{1}{b}(2\pi, 2\pi, 2\pi, 2\pi, 2\pi)$, and $E_1 = (2\pi, 0, 0, 0, 0)$. The Berry phase defined in this way is quantized in $Z_6$ because there are five alternative paths $L_i$ $(i = 2, 3, 4, 5, 6)$ which is equivalent to $L_1$ due to the six-fold symmetry of $h_0$, and the sum of the six Berry phases defined on each path $L_i$ is 0 in modulo 2$\pi$, meaning that $\gamma = \frac{2\pi}{6} n$ ($n = 0, 1, 2, 3, 4, 5$); see Refs. 17,23 for the details.

In Fig. 2(b), we plot $\gamma$ as a function of $t_0/t_1$. Clearly, $\gamma = 0$ for $t_0/t_1 < 1$, and $\gamma = \pi$ $(= \frac{2\pi}{6} \cdot 3)$ for $t_0/t_1 > 1$. This means that the topological phase exists in $t_0/t_1 > 1$. In fact, the nontrivial Berry phase indicates that the ground state is adiabatically connected to the “irreducible cluster” state, which cannot be reduced to individual atomic states. In the present case, for $t_0 > t_1$, the ground state is connected to the “hexamer state” [Fig. 2(a)]. For $t_0 < t_1$, in contrast, the ground state is connected to the “dimer state” [Fig. 2(b)], which is identified by using the $Z_2$ Berry phase.

Next, to demonstrate that the nontrivial Berry phase results in a topologically-protected boundary states at the corners, which is a defining feature of the HOTI phase, we show the energy spectrum and wave functions under the open boundary conditions in both of two directions. The aforementioned picture of the hexamer state indicates that the boundary states in the present model crucially depend on the shape the boundary; this coincides with the results in the previous work. In this note, we consider the finite system shown in Fig. 3(b), where the boundaries intersect hexagonal plaquettes at the edges and the corners.

In Fig. 3(a), we plot the energy spectrum as a function of $t_0/t_1$. We do not see the in-gap state around zero energy for $t_0/t_1 < 1$, whereas there exist the in-gap states for $t_0/t_1 > 1$ which have quasi-two-fold degeneracy. Note that the energy is slightly deviated from zero due to the finite-size effect. Figure 3(b) shows the real-space distribution of the wave function, averaged over two in-gap states. Clearly, it is localized at the 120-degree corners where the hexagonal plaquettes are cut off. Note that, if we remove one of the corner sites, the energy of the in-gap state is exactly pinned to zero due to the imbalance between two sublattices of the original honeycomb lattice. From these results, we conclude that the ground state is in the HOTI phase for $t_0/t_1 > 1$.

In summary, we have shown that the HOTI phase is realized in a honeycomb-lattice model with anti-Kekulé-type modulation. This is due to the fact that the ground state for $t_0 > t_1$ can be adiabatically connected to the hexamer state, which hosts topologically nontrivial structure in that it cannot be adiabatically connected to the atomic states. We demonstrate the existence of the HOTI phase by showing the non-trivial $Z_6$ Berry phase, and the corner states under a certain shape of the boundaries.

So far, we have discussed the non-interacting fermion system, but we expect that our proposal of the HOTI phase opens up a way to search corner states in the various systems, such as correlated electron systems and photonic crystal. Regarding the correlation effect, we remark that the Berry phase can be defined even in the presence of interactions.

We thank T. Kariyado for variable comments. This work is supported by the JSPS KAKENHI, Grant num-
A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. 81, 109 (2009).

1 A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. 81, 109 (2009).

2 T. Kariyado and Y. Hatsugai, Sci. Rep. 5, 18107 (2015).

3 R. L. Chern, C. C. Chang, C. C. Chang, and R. R. Hwang, Phys. Rev. E 68, 026704 (2003).

4 H. Ajiki and T. Ando, J. Phys. Soc. Jpn. 64, 260 (1994).

5 M. Koshino, T. Morimoto, and M. Sato, Phys. Rev. B 90, 115207 (2014).

6 L.-H. Wu and X. Hu, Sci. Rep. 6, 24347 (2016).

7 T. Kariyado and X. Hu, Sci. Rep. 7, 16515 (2017).

8 E. Lee, A. Furusaki, and B.-J. Yang, arXiv:1903.02737.

9 L.-H. Wu and X. Hu, Phys. Rev. Lett. 114, 223901 (2015).

10 Y.-T. Yang, Y. F. Xu, T. Xu, H.-X. Wang, J.-H. Jiang, X. Hu, and Z. H. Hang, Phys. Rev. Lett. 120, 217401 (2018).

11 Y. Li, Y. Sun, W. Zhu, Z. Guo, J. Jiang, T. Kariyado, H. Chen, and X. Hu, Nat. Commun. 9, 4598 (2018).

12 W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Phys. Rev. B 96, 245115 (2017); Science 357, 61 (2017).

13 Z. Song, Z. Fang, and C. Fang, Phys. Rev. Lett. 119, 246402 (2017).

14 F. Schindler, A. M. Cook, M. G. Vergniory, Z. Wang, S. S. P. Parkin, B. A. Bernevig, and T. Neupert, Sci. Adv. 4, eaat0346 (2018).

15 M. Ezawa, Phys. Rev. Lett. 120, 026801 (2018).

16 F. K. Kunst, G. van Miert, and E. J. Bergholtz, Phys. Rev. B 97, 241405(R) (2018).

17 H. Araki, T. Mizoguchi, and Y. Hatsugai, arXiv:1906.00218.

18 Y. Hatsugai and I. Maruyama, Europhys. Lett. 95, 20003 (2011).

19 M. Ezawa, Phys. Rev. B 98, 045125 (2018).

20 Y. Hatsugai, J. Phys. Soc. Jpn. 75, 123601 (2006).

21 P. W. Brouwer, E. Racine, A. Furusaki, Y. Hatsugai, Y. Morita, and C. Mudry, Phys. Rev. B 66, 014204 (2002).

22 S. Sorella, K. Seki, O. O. Brovko, T. Shirakawa, S. Miyakoshi, S. Yunoki, and E. Tosatti, Phys. Rev. Lett. 121, 066402 (2018).

23 K. Kudo, T. Yoshida, and Y. Hatsugai, arXiv:1905.03484.