Three-dimensional topological insulators in the octahedron-decorated cubic lattice

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(Dated: January 20, 2011)

We investigate a tight-binding model of the octahedron-decorated cubic lattice with spin-orbit coupling. We calculate the band structure of the lattice and evaluate the $Z_2$ topological indices. According to the $Z_2$ topological indices and the band structure, we present the phase diagrams of the lattice with different filling fractions. We find that the $(1; 111)$ and $(1; 000)$ strong topological insulators occur in some range of parameters at $1/6, 1/2$ and $2/3$ filling fractions. Additionally, the $(0; 111)$ weak topological insulator is found at $1/6$ and $2/3$ filling fractions. We analyze and discuss the characteristics of these topological insulators and their surfaces states.

PACS numbers: 73.43.-f, 71.10.Fd, 73.20.-r, 72.25.-b

I. INTRODUCTION

Usually, different phases of matter can be classified using Landau’s approach according to their underlying symmetries[1]. In 1980s, the discovery of the quantum Hall effect changed physicists’ viewpoint on the classification of matter[2]. The quantum Hall states can be classified by a topological invariant, now named the TKNN number[3] (equivalent to the first Chern number), which is directly connected to the quantized Hall conductivity, but they have the same symmetry. Since the Hall conductivity is odd under time reversal, the topological non-trivial quantum Hall states can only occur when time reversal symmetry is broken, which is performed by a magnetic field. In 1988, Haldane also proposed a time reversal symmetry broken toy model without a magnetic field to realize quantum Hall states[4]. All the quantum Hall states have a gapped band structure in bulk and chiral gapless edge states that are topologically protected.

Recently, the promising prospect of spintronics in technology stimulates physicists to generate spin current. Quantum spin Hall effect was proposed to create spin current[5, 6]. The quantum spin Hall states are non-trivial topological phases with time reversal symmetry, which have a bulk gap and topologically protected gapless helical edge states. For the above reason, the quantum spin Hall states also called topological insulators. Two-dimensional topological insulators are characterized by a $Z_2$ topological index $\nu = 0, 1[7]$. For a non-trivial topological insulator the topological index has a value $\nu = 1$ while $\nu = 0$ for a trivial band insulator. Therefore, a topological insulator always has a metallic boundary when placed next to a vacuum or an ordinary band insulator because topological invariants cannot change as long as a material remains insulating. The remarkable metallic boundaries of topological insulators may result in new spintronic or magnetoelectric devices and a new architecture for topological quantum bits. In quantum spin Hall phases, the spin-orbit coupling plays the role of the spin-dependent effective magnetic field. The first real material, a HgTe quantum well, supporting two-dimensional topological insulators was predicted by Bernevig, et al.[8] and experimentally conformed by König et al.[9].

FIG. 1: (Color online). (a) The octahedron-decorated cubic lattice which can be obtained by replacing every lattice site of a cubic lattice with an octahedral cluster as shown in (b). (c) The three-dimensional Brillouin zone and high symmetry points. (d) The two-dimensional Brillouin zone of a slab with two 001 surfaces.

Soon after the quantum spin Hall insulator was discovered, time-reversal invariant topological insulators were generalized to three dimensions[10–12]. Three-dimensional time-reversal invariant band insulators are classified according to four $Z_2$ topological indices $(\nu_0; \nu_1 \nu_2 \nu_3)$ with $\nu_i = 0, 1[11]$. In three dimensions, the time-reversal invariant band insulators can be classified into 16 phases according to the four $Z_2$ topological indices. A band insulator with $\nu_0 = 1$ is called a strong topological insulator(STI), a band insulator with
\[ H_0 = -t \sum_{(i,j),\sigma} c^\dagger_{i\sigma} c_{j\sigma} - t_1 \sum_{[i,j],\sigma} c^\dagger_{i\sigma} c_{j\sigma} \]

where \( c_{\sigma} \) is the annihilation operator destroying an electron with spin \( \sigma \) on the site \( r_i \) of the octahedron-decorated cubic lattice, \((i, j)\) represents nearest-neighbor hopping in the same octahedral cluster with amplitude \( t \) and \([i, j]\) denotes nearest-neighbor hopping between two different octahedral clusters with amplitude \( t_1 \).

To help experimental physicists find more topological insulator materials, theoretical physicists have investigated several models that support non-trivial topological insulators. Theoretical studies have demonstrated that, within the tight-binding approximation and with the spin-orbit coupling, the honeycomb, kagome, checkerboard, decorated honeycomb, Lieb, and square-octagon lattices support two-dimensional topological insulators, and the diamond, pyrochlore, and perovskite lattices support three-dimensional topological insulators.

In this paper, we shall show that a new lattice, the octahedron-decorated cubic lattice as shown in Fig.1 (a), supports three-dimensional topological insulators with the spin-orbit coupling existing. This lattice can be regarded as a three-dimensional generalization of the square-octagon lattice. We find that this model supports STI and WTI phases for 1/6 and 2/3 filling and STI phases for 1/2 filling as well as ordinary band insulator and metal phases.

II. MODEL

We consider the octahedron-decorated cubic lattice as shown in Fig.1 (a), which can be obtained by replacing every lattice site of a cubic lattice with an octahedral cluster as shown in Fig.1(b). This lattice has a unit cell with six different lattice sites as denoted in Fig.1(b) so that it contains six sublattices. Here, we assume that the distance between the centers of two nearest-neighbor octahedral clusters is \( a \), which is the same with the lattice constant of all sublattices, the distance of every lattice site of an octahedral cluster from its center is \( a/4 \), and the distance of two nearest-neighbor lattice sites in different octahedral clusters is \( a/2 \). With the tight-binding approximation, we can write the second quantized Hamiltonian of the lattice as follows,

\[ H_0 = -t \sum_{(i,j),\sigma} c^\dagger_{i\sigma} c_{j\sigma} - t_1 \sum_{[i,j],\sigma} c^\dagger_{i\sigma} c_{j\sigma} \]

where \( c_{\sigma} \) is the annihilation operator destroying an electron with spin \( \sigma \) on the site \( r_i \) of the octahedron-decorated cubic lattice, \((i, j)\) represents nearest-neighbor hopping in the same octahedral cluster with amplitude \( t \) and \([i, j]\) denotes nearest-neighbor hopping between two different octahedral clusters with amplitude \( t_1 \).

\[ H_k^0 = \begin{pmatrix}
0 & t & t & t e^{ik_x} & t e^{ik_y} \\
t & 0 & t & t & t e^{ik_y} \\
t & t & 0 & t & t e^{ik_y} \\
t & t e^{-ik_x} & t & 0 & t \\
t e^{-ik_x} & t & t e^{-ik_y} & t & 0 \\
t & t & t e^{-ik_y} & t & 0 \\
t & t & t & t & 0
\end{pmatrix} \]

Since \( H_0 \) is spin-decoupling, \( H_k^0 \) is spin-independent, i.e. it is the same for both spin-up and spin-down electrons. Fig.1(c) shows the first Brillouin zone of the octahedron-decorated cubic lattice. The spectrum of Eq.2 with \( t_1 = t \) is calculated and shown in Fig.1(d). The spectrum contains six bands which come from the six sites in every unit cell. A gap exists between the first and second bands. The second, third and fourth bands touch
together at points \( \Gamma, R \) and \( M \). The third, fourth and fifth band touch at point \( X \), near which a Dirac cone occurs. Five bands including the second, third, fourth, fifth and sixth bands meet at point \( \Gamma \). Along the \( \Gamma \rightarrow R \) line in momentum space, the second and third bands are degenerate and the fifth and sixth bands are degenerate.

Now, in order to find non-trivial topological insulators in the octahedron-decorated cubic lattice, we proceed to introduce the spin-orbit interactions between next-nearest-neighbor sites as follows,

\[
H_{SO} = i \frac{8 \lambda_{SO}}{a^2} \sum_{\langle (i,j) \rangle \alpha \beta} \langle d_{ij}^\dagger \times d_{ij}^\dagger \rangle \cdot \sigma_{\alpha \beta} c_{i \alpha} c_{j \beta},
\]

where \( \langle (i,j) \rangle \) represents two next-nearest-neighbor sites \( i, j \), and \( \lambda_{SO} \) is the amplitude of spin-orbit coupling of the two next-nearest-neighbor sites. \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) is the vector of Pauli spin matrices. \( d_{ij}^{1,2} \) are the two nearest neighbor bond vectors traversed between sites \( i \) and \( j \) with \( 8|d_{ij}^{1,2}|^2/a^2 = 1 \). In momentum space, the Hamiltonian for spin-orbit coupling \( \sum_k \) can be expressed as \( H_{SO} = \sum_k \Psi_k^\dagger H_{SO} \Psi_k \) with \( \Psi_k = (c_{1k \uparrow}, c_{2k \uparrow}, c_{1k \downarrow}, c_{2k \downarrow}, c_{3k \downarrow}, c_{4k \downarrow}, c_{5k \downarrow}, c_{6k \downarrow}) \). Since \( H_{SO} \) does not decouple for the two spin projections, it is a 12 \( \times \) 12 matrix. In momentum space, the total single particle Hamiltonian is \( H_k = H_0 + H_{SO} \). The bands and eigenstates can be obtained by exactly diagonalizing \( H_k \).

### III. THREE-DIMENSIONAL TOPOLOGICAL INSULATORS

The classification of three-dimensional topological insulators is presented in Ref.\(^{10}\). For three-dimensional lattices there eight distinct time reversal invariant momenta (TRIM), which can be expressed in terms of primitive reciprocal lattice vectors as \( \Gamma = (n_1 b_1 + n_2 b_2 + n_3 b_3)/2 \) with \( n_j = 0, 1 \). Three-dimensional topological insulators are distinguished by four \( Z_2 \) topological invariants \( (\nu_0; \nu_1; \nu_2; \nu_3) \), which are defined as \( \nu_0 = \prod_{n_j=0,1} \delta_{n_1n_2n_3} \) and \( \nu_1 = 1/2 \). Here, the unitary matrix \( w \) is defined as \( w_{ij}(k) = (u_i(-k))^\dagger \theta u_j(k) \) with \( \theta \) being the time reversal operator and \( |u_j(k)\rangle \) being the Bloch wave functions for occupied bands. Fu and Kane have found a simple method to identify the \( Z_2 \) invariants for the system with the presence of inversion symmetry\(^{13}\). In this case, \( \delta_{n_1n_2n_3} \) can be calculated by \( \delta_{n_1n_2n_3} = \prod_{m=1}^N \xi_m \Gamma_{n_1n_2n_3} \), where \( N \) is the number of occupied bands and \( \xi_m = \pm 1 \) is the parity eigenvalue of the \( m \)th occupied band at \( \Gamma_{n_1n_2n_3} \). Our model is inversion symmetric so we will adopt this method to evaluate the \( Z_2 \) invariants \( \nu_1(t = 0, 1, 2, 3) \). We select the center of an octahedron in the lattice as the center of inversion, then the parity operator acts as \( P = \prod_{k} \delta_{k}^{\Lambda \rightarrow R} P_k e^{-ik \cdot \mathbf{r}} \). Then, in momentum space, we can obtain the equation \( P_k \) as \( \sum_k [\phi_1(k), \phi_2(k), \phi_3(k), \phi_4(k), \phi_5(k), \phi_6(k)] e^{ik \cdot \mathbf{r}} \) and the parity operator as \( P = \sum_k e^{ik \cdot \mathbf{r}} P_k e^{-ik \cdot \mathbf{r}} \).

![FIG. 3: (Color online). Band structures of the octahedron-decorated cubic lattice for various parameters \( t_1 \) and \( \lambda_{SO} \). Here, the horizontal axis represents the wave vectors along the path in the first Brillouin zone indicated by the red lines in Fig.1(c).](image)

(a) \( t_1 = t_2 = \lambda_{SO} = 0.5t \) (b) \( t_1 = t_2 = -\lambda_{SO} = 0.5t \) (c) \( t_1 = t_2 = \lambda_{SO} = t \) (d) \( t_1 = t_2 = \lambda_{SO} = 0 \) (e) \( t_1 = 3t_2, \lambda_{SO} = -0.4t \) (f) \( t_1 = -3t_2, \lambda_{SO} = 0.4t \) (g) \( t_1 = 3.2t, \lambda_{SO} = -0.2t \) (h) \( t_1 = t_2, \lambda_{SO} = 0.2t \) (i) \( t_1 = t_2, \lambda_{SO} = -0.2t \) (j) \( t_1 = t_2, \lambda_{SO} = 0.2t \) (k) \( t_1 = 2.5t, \lambda_{SO} = -0.2t \) and (l) \( t_1 = 0.5t, \lambda_{SO} = 0 \).
operator at the time reversal invariant momenta $\Gamma_{n_1n_2n_3}$ as follows,

$$\mathcal{P}_{\Gamma_{n_1n_2n_3}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$ (3)

where the $4 \times 4$ matrix is the unit matrix in spin space.

We diagonalize the total single-particle Hamiltonian $\mathcal{H}_{\mathbf{k}}$ and calculate the $Z_2$ topological invariants for different filling fractions. We find that non-trivial topological insulators exist for $1/6, 1/2$ and $2/3$ filling while only metal phase occurs for $1/3$ and $5/6$ filling. Thus, we will focus on and discuss the cases with $1/6, 1/2$ and $2/3$ filling fractions in the following part of the paper. We identify phases for different parameters $t_1$ and $\lambda_{SO}$ with $1/6, 1/2$ and $2/3$ filling fractions and draw phase diagrams as shown in Fig. 2. Figs. 2(a), 2(b) and 2(c) show the phase diagrams for $1/6, 1/2$ and $2/3$ filling, respectively.

For $1/6$ and $2/3$ filling, there are $(1;111)$ and $(1;000)$ STI phases, $(0;111)$ WTI phase as well as trivial band insulator and metal phases. For $1/2$ filling, there are $(1;111)$ and $(1;000)$ STI phases, trivial band insulator and metal phases except $(0;111)$ WTI phase.

To clearly manifest the bulk band structure of different phases for various filling fractions, we calculate the bulk energy bands for several cases with different parameters $t_1$ and $\lambda_{SO}$, which are shown in Fig. 2. In order to investigate the characteristics of surface states for various phases, we evaluate the energy bands in a slab geometry with two 001 surfaces. The Brillouin zone of the slab is shown in Fig. 1(d). The energy bands are present along lines that connect the four surface TRIM as shown in Fig. 1. With the assistance of the bulk energy bands shown in Fig. 3 and the two-dimensional energy bands for a slab shown in Fig. 4 we will sequentially analyze various phases, identify three-dimensional topological insulators, and discuss their characteristics for $1/6, 1/2$ and $2/3$ filling.

### A. 1/6 filling

Fig. 2(a) shows the phase diagram of the octahedron-decorated cubic lattice for 1/6 filling. In this case, the $(1;111)$ and $(1;000)$ STI phases are discovered. The non-trivial STI phases have a gap between the first and second bands as shown in Fig. 2(a) and (b) corresponding to $(1;111)$ and $(1;000)$ STI phases, respectively. We note that for $1/6$ filling there is only one Dirac point on TRIM as shown in Fig. 4(a) and (b), that is, only a pair of robust spin-filtered states exists. We also find a $(0;111)$ WTI phase for 1/6 filling e.g., as shown in Fig. 4(c). Fig. 4(c) shows the surface states for a $(0;111)$ WTI phase that has two Dirac points between the first and second bands on TRIM. We note that trivial band insulators occur for smaller $t_1$ and smaller $\lambda_{SO}$ parameters, which is easily understood for when $t_1$ and $\lambda_{SO}$ approaches to zero the lattice becomes separated octahedral clusters. For a trivial band insulator there is a gap between the first and second bands as shown in Fig. 4(d), but there are not surface states as shown in Fig. 4(d). For a metal phase, the gap vanishes.

![Fig. 4: (Color online). Band structures of a slab with two 001 surfaces for various parameters $t_1$ and $\lambda_{SO}$. Here, the horizontal axis represents the wave vectors along the path in the surface Brillouin zone indicated by the red lines in Fig. 4(a).](image-url)
B. 1/2 filling

Fig.2(b) shows the phase diagram of the octahedron-decorated cubic lattice for 1/2 filling. For 1/2 filling, (1; 111) and (1; 000) STI phases, trivial band insulators, and metal phases occur, but WTI phases are not found. Figs.3(e) and 3(f) show the band structure for (1; 111) and (0; 111) STI phases, respectively. We can find from these diagrams that a gap opens between the third and fourth bands. For STI phases, there is only one Dirac point on TRIM as shown in Fig.4(e) and (f). For trivial band insulators, there is also a gap between the third and fourth bands as shown in Fig.4(g), but even number of Dirac points exist on TRIM as shown in Fig.4(j). For even number of surface states traversing the gap, for smaller $t_1$ and smaller $\lambda_{SO}$, the system for 2/3 filling is a trivial band insulator, which is feathered by a gap between the fourth and fifth bands combined with an even number of surface states traversing the gap as shown in Fig.3(i) and Fig.4(i), respectively.

IV. CONCLUSION

In summary, we have shown that the octahedron-decorated cubic lattice with spin-orbit coupling supports three-dimensional topological insulators at 1/6, 1/2 and 2/3 filling fractions. For 1/6 and 2/3 filling, (1; 111) and (1; 000) STI phases, (0; 111) WTI phase, trivial band insulator, and metal phase are found, while for 1/2 filling, (1; 111) and (1; 000) STI phases, trivial band insulator, and metal phase occur except (0; 111) WTI phase. We have calculated the band structure and surface band structure for the tight-binding model of the octahedron-decorated cubic lattice with spin-orbit coupling and evaluated the $Z_2$ topological invariants. We have analyzed and discussed the characters of the band structures and the surface states of different phases. Although the octahedron-decorated cubic lattice we considered is a toy model, our study points out an alternative path to search for real topological materials. On the other hand, it might as well be built from optical lattices due to their diversity and controllability.

Acknowledgments

This work was supported by the National Natural Science Foundation of China under Grant No. 11004028 and the Science and Technology Foundation of Southeast University under Grant No. KJ2010417

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