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Three-dimensional topological insulators in the supercubane-like lattice: Phase diagram, surface state and spin texture

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ABSTRACT

We study a tight-binding model of the supercubane-like lattice with spin–orbit coupling. By evaluating the Z_2 topological indices, we find that the supercubane-like lattice can support strong topological insulator and the phase diagrams of the lattice with different filling fractions are present. Strong topological insulators with Z_2 invariants $(1; 000)$ and $(1; 111)$ can be realized for 1/8 filling fraction and semimetals can be obtained for 1/8, quarter and half filling fractions. We analyze and discuss the characteristics of these topological insulators and their surface states. Spin textures of surface states are also evaluated for $1\bar{1}1$ slab geometry.

1. Introduction

Many efforts have been devoted to study various topological phases of matter, since the integer quantum Hall state was discovered in 1980s. The integer quantum Hall state belongs to a topological class which breaks time reversal symmetry and can be identified with TKNN number [1]. The TKNN number is a topological invariant in the sense that it cannot change when the Hamiltonian varies continuously. Recently, a new class of topological states, called topological insulator [2,3], emerges with the presence of time reversal symmetry. Besides bulk gaps, these materials have gapless edge or surface states that are topologically protected by time reversal symmetry [2], which is different from conventional band insulators. In contrast to the integer quantum Hall states, the topological insulators are characterized by the so-called Z_2 topological invariants [4,5].

In two dimensions, quantum spin Hall phase [3] is characterized by a single Z_2 invariant [4] which was first predicted to be achieved in graphene but the spin–orbit coupling opens an unobservably small gap at the Dirac points [6,7]. In experiment quantum spin Hall state was observed in HgTe/CdTe quantum well structures at large well thickness [8,9]. Other two dimensional topological insulators have also been proposed owing to a surge of researches [10–16]. Soon the topological insulators are extended to three dimensions (3D) [5,17,18]. For 3D case, according to four Z_2 topological indices $(\nu_0; \nu_1, \nu_2, \nu_3)$ with $\nu_i = 0, 1$, all the band insulators with time-reversal invariant can be classified into 16 topological classes [18]. When $\nu_0 = 1$, there is an odd number of surface states on all surfaces, which behaves as a perfect metal, robust with weak nonmagnetic disorder and predicted to exhibit unusual properties [19–21]. This is called a strong topological insulator (STI). If $\nu_0 = 0$ and any of ν_i $(i = 1, 2, 3) \neq 0$, we get a weak topological insulator (WTI) which exhibits an even number of surface states on at least some of its surfaces. An ordinary trivial band insulator has an index $(0; 000)$ with no robust surface states.

Theoretically Fu and Kane predicted that the alloy $Bi_{1-x}Sb_x$ be a 3D topological insulator in a special range of x [17], which was later verified experimentally [22]. Following the verification of alloy $Bi_{1-x}Sb_x$, other materials, such as Bi_2Te_3 [23–25], Bi_2Se_3 [26] and Sb_2Te_3 [27], are discovered to support 3D topological insulators benefiting from the band inversion theory. Among them, the most promising one is Bi_2Se_3 which has a large band gap and a single surface Dirac cone [26]. Vigorous search for new topological materials is ongoing and several more have been predicted as candidates [28–33].

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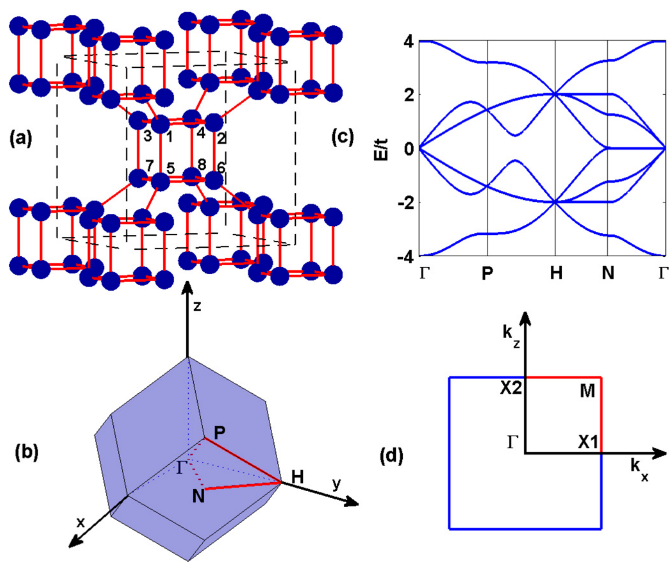

Fig. 1. (a) The lattice structure of supercubane-like lattice. (b) The first Brillouin zone with time-reversal invariant momenta and high symmetry lines. (c) Band structure of the Hamiltonian $H^0_{\mathbf{k}}$ with $t_1/t = 1$. (d) The two dimensional Brillouin zone of $1\bar{1}1$ surface with high symmetry points.

In this paper, we present a candidate of 3D topological insulator, the supercubane-like lattice. With the tight-binding model, we find that the supercubane-like lattice supports strong topological insulator in the presence of spin–orbit coupling. To identify our identification of topological classes, we evaluate the Z_2 topological indices and draw the phase diagram. We also solve the surface states in a slab geometry and calculate the spin textures of surface states.

2. Model

Supercubane-like lattice can be obtained by locating cubes of atoms at the nodes of the body-centered cubic lattice with eight sublattices, as shown in Fig. 1(a). The space group symmetry is $Im\ \bar{3}\ m$. Consider the tight-binding model

$$H^0 = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - t_1 \sum_{[i,j],\sigma} c^\dagger_{i\sigma} c_{j\sigma}, \tag{1}$$

where $c_{i\sigma}(c^\dagger_{i\sigma})$ annihilates (creates) an electron with spin σ on the site $\mathbf{r}_i$ of the supercubane-like lattice. $\langle i, j\rangle$ describes the nearest-neighbor hopping in the same cubic clusters and $[i, j]$ represents the nearest-neighbor hopping between neighboring cubic clusters. t and t_1 are the corresponding hopping amplitudes.

In momentum representation, Eq. (1) can be written as $H^0 = \sum_{\mathbf{k}\sigma} \Psi^\dagger_{\mathbf{k}\sigma} \mathcal{H}^0_{\mathbf{k}} \Psi_{\mathbf{k}\sigma}$ with $\Psi^\dagger_{\mathbf{k}\sigma} = (c^\dagger_{1\mathbf{k}\sigma}, c^\dagger_{2\mathbf{k}\sigma}, c^\dagger_{3\mathbf{k}\sigma}, c^\dagger_{4\mathbf{k}\sigma}, c^\dagger_{5\mathbf{k}\sigma}, c^\dagger_{6\mathbf{k}\sigma}, c^\dagger_{7\mathbf{k}\sigma}, c^\dagger_{8\mathbf{k}\sigma})$ and $\mathcal{H}^0_{\mathbf{k}}$ takes the following form:

$$\mathcal{H}^0_{\mathbf{k}} = -\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & t & t & 0 & t & 0 & 0 & t_1 e^{-ik_z} \\ t & 0 & 0 & t & 0 & t & t_1 e^{ik_y} & 0 \\ t & 0 & 0 & t & 0 & t_1 e^{ik_x} & t & 0 \\ 0 & t & t & 0 & t_1 e^{i(k_x+k_y+k_z)} & 0 & 0 & t \\ t & 0 & 0 & t_1 e^{-i(k_x+k_y+k_z)} & 0 & t & t & 0 \\ 0 & t & t_1 e^{-ik_x} & 0 & t & 0 & 0 & t \\ 0 & t_1 e^{-ik_y} & t & 0 & t & 0 & 0 & t \\ t_1 e^{ik_z} & 0 & 0 & t & 0 & t & t & 0 \end{pmatrix}. \tag{2}$$

Fig. 1(b) shows the first Brillouin zone of the supercubane-like lattice. The spectrum of $\mathcal{H}^0_{\mathbf{k}}$ along the direction of high symmetry in the Brillouin zone is shown in Fig. 1(c). The eight pairs of doubly degenerate bands come from the eight sites in every unit cell. An interesting feature is that at the momenta H two bands touch with each other with a locally flat band at a single Dirac point, which is similar to the case of the decorated honeycomb lattice [12] and the square–octagon lattice [13] model. And along N–Γ direction we can see four-fold degenerate flat band.

To open up a gap and find topologically nontrivial phases, we consider the spin–orbit coupling between next-nearest-neighbor sites [3,34], which does not break translational symmetry of H^0 and preserves time reversal symmetry. The Hamiltonian of the spin–orbit coupling takes the form

$$H^{so} = i\lambda_{so} \sum_{\langle\langle i,j\rangle\rangle} c^\dagger_{i\alpha} \boldsymbol{\sigma} \cdot \mathbf{e}_{ij} c_{j\beta}, \tag{3}$$

where λ_{so} is the spin–orbit coupling strength, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli spin matrices and the unit vector $\mathbf{e}_{ij}$ is defined as