Tunable topological Weyl semimetal from simple cubic lattices with staggered fluxes

Jian-Hua Jiang

1Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel
(Dated: April 2, 2012)

Three-dimensional Weyl fermions are found to emerge from simple cubic lattices with staggered fluxes. The mechanism is to gap the quadratic band touching by time-reversal-symmetry-breaking hoppings. The system exhibits rich phase diagrams where the number of Weyl fermions and their topological charge are tunable via the plaquette fluxes. The Weyl semimetal state is shown to be the intermediate phase between non-topological semimetal and quantum anomalous Hall insulator. The transitions between those phases can be understood through the evolution of the Weyl points as Berry flux insertion processes. As the Weyl points move and split (or merge) through tuning the plaquette fluxes, the Fermi arcs and surface states undergo significant manipulation. We also propose a possible scheme to realize the model in ultracold fermions in optical lattices with artificial gauge fields.

PACS numbers: 71.10.Fd, 03.75.Ss, 05.30.Fk, 03.65.Vf

I. INTRODUCTION

Massless Dirac fermions possess chiral symmetry and can be classified by their chirality \( \gamma \). For example, in three-dimension (3D), if the Hamiltonian is \( H = v_F \sigma \cdot q \) where \( \sigma \) is the Pauli matrices vector and \( q \) is the wavevector, then the chirality is \( \gamma = \text{sgn}(v_F) \). Such fermions (also called chiral or Weyl fermions) possess several peculiar behaviors such as Adler-Bell-Jackiw anomaly. Chiral fermions in two-dimension (2D) have been found in real condensed matter systems since the discovery of graphene. Many novel electronic properties of graphene, Klein tunneling, the peculiar integer quantum Hall effect, the transport properties such as the conductivity minimum, the weak (anti)localization, and edge states, originate from the chiral fermion nature. Recent studies also found the realizations of 2D chiral fermions in ultracold atomic gases optical lattices. A generic route to chiral fermions is to search systems with two-band touching. Around the band touching node, the Hamiltonian can generally be written as \( H = h(k) \cdot \sigma \) where Pauli matrices \( \sigma \) act on the space spanned by the two bands and \( |h| \to 0 \) at the node. For example, in graphene, around one of the node \( K \), \( h(k) = v_F(k - K) \). Thus chiral fermions emerge as topological defects (vortices) in k-space. They are generally classified by their vortex winding number \( N_w \). In the special cases when \( N_w = \pm 1 \), the winding number gives the chirality \( \gamma = N_w \). In general cases, \( N_w \) can be any integer. The total winding number in the system must be conserved under adiabatic transformation. The winding number can be defined by the Berry phase carried by the node, \( N_w = \frac{1}{\mathcal{S}} \oint_{\Gamma} d k \cdot (\Psi(k) i \nabla_k |\Psi(k)\rangle) \), where \( \Gamma \) is a contour enclosing the node and \( |\Psi(k)\rangle \) is the single-valued and continuous wavefunction of the eigenstates with \( H|\Psi(k)\rangle = \pm |h(k)||\Psi(k)\rangle \). By breaking the time-reversal symmetry, such two-band touching can be gapped, leading to a quantum anomalous Hall (QAH) insulator with Chern number \( C = \pm \frac{1}{2} N_w \).

3D Weyl fermions are more robust: they can not even be gapped by time-reversal symmetry breaking. In fact they can only be annihilated in pairs with the total winding number conserved under adiabatic transformations. The winding number of 3D Weyl fermion is defined as \( N_w = \frac{1}{2\pi \varepsilon} \oint_S dS^p \hat{n} \cdot (\partial_k \hat{n} \times \partial_h \hat{n}) \) (\( \nu, \delta, \rho = x, y, z \) and \( \varepsilon \) being the Levi-Civita tensor) where \( S \) is a surface enclosing the band touching node (Weyl point), \( dS^p \) is the surface area elements along \( p \) direction, and \( \hat{n} = h/|h| \). 3D Weyl fermions are monopoles of the Berry-phase gauge fields where the monopole charge is the topological charge \( N_w \). As a consequence, there is a step change in the Hall conductivity, e.g., \( \sigma_{xy}(k_z) \) and the Chern number \( C_{xy}(k_z) = \frac{1}{4\pi} \sigma_{xy}(k_z) \) as function of \( k_z \),

\[
\sigma_{xy}(k_z) = \text{sgn}(k_z - k_z^0) N_w \frac{e^2}{h} + ..., \tag{1}
\]
due to the monopole at \( k_z^0 \), while ... denotes other contributions to the Hall conductivity (Chern number). According to the Nielsen-Ninomiya theorem, Weyl points must appear in pairs with opposite \( N_w \) in a lattice system.

Weyl semimetal (system with 3D Weyl fermions) possesses very special properties such as chiral surface states with open Fermi surfaces (Fermi arcs) terminating at the projection of the Weyl points and thickness dependent quantized anomalous Hall conductivity in thin films, which are first found in the studies of \(^3\text{He}-\Lambda\). After that Murakami showed that a Weyl semimetal phase can appear as intermediate phase between normal insulator and topological insulator. Recent studies demonstrate that Weyl semimetal can also be realized in other condense matter systems: some pyrochlore iridates (such as \( Y_2\text{Ir}_2\text{O}_7\) ), superlattices made of topological insulator and non-topological insulator thin films with broken time-reversal\(^{13, 14}\) or inversion\(^{15}\) sym-
metry, the ferromagnetic compound HgCr$_2$Se$_4$[16, 17], and bulk magnetically doped Bi$_2$Se$_3$[18]. It is also found that in some situations the number and type of the Weyl points are determined and protected by the lattice symmetries[14, 15]. A topological nodal semimetals where the bulk spectrum exists nodal lines are also proposed and studied in Ref. [14]. There are also some lattice models where Weyl fermions are found[20].

In this work we show that Weyl fermions can emerge from simple cubic lattices with staggered fluxes through plaquettes [see Fig. 1]. Differing from previous studies where the Weyl semimetal phases emerge due to inverted bands with spin-orbit interactions[10, 15–17] or gapping Dirac cones by various mass terms[13, 14, 18], here the mechanism is to gap the quadratic band touching via time-reversal-symmetry-breaking hoppings due to the staggered fluxes. A direct distinction is that such scenarios do not need to invoke spin degeneracy breaking (i.e., spin-orbit coupling). The system exhibits rich phase diagrams where the number of Weyl fermions and their topological charge are tunable via the fluxes per plaquette[see Fig. 1(a)]. Differing from previous studies where Weyl fermions are found[20], we propose a realistic scenario does not need to invoke spin degeneracy breaking true-spin splitting, we keep the true-spin states here the mechanism is to gap the quadratic band touching via time-reversal-symmetry-breaking hoppings due to the staggered fluxes. A direct distinction is that such scenarios do not need to invoke spin degeneracy breaking (i.e., spin-orbit coupling). The system exhibits rich phase diagrams where the number of Weyl fermions and their topological charge are tunable via the fluxes per plaquettes. The Weyl semimetal state is demonstrated as the intermediate phase between non-topological semimetal and quantum anomalous Hall insulator. The transitions between those phases can be understood via the evolution of the Weyl points as Berry flux insertion processes [see Sec. IV and Summary section]. As the Weyl points move and split (or merge) through tuning the plaquette fluxes, the Fermi arcs and surface states undergo significant change, because the Fermi arcs act as Dirac strings which have to connect the monopoles with opposite charges. Finally, we propose a possible scheme to realize such model in ultracold fermionic gases in optical lattices with artificial gauge fields.

II. LATTICE AND HAMILTONIAN

We consider a simple cubic lattice system, which can be viewed as stacking of layers of 2D lattices with checkerboard-patterned staggered fluxes [see Fig. 1][21–24]. The 2D checkerboard lattice is designed in such a way that the hopping between the nearest-neighbor A-type sites along the x and y directions are $t_x$ and $t_y$ respectively, whereas those for B-type sites are $t_y$ and $t_x$ respectively [see Fig. 1(a)]. The hopping from A-type site to the nearest B-type ones are $t_{2x}e^{-i\phi_1}$ as indicated in Fig. 1(a). The flux per plaquette is $\pm \Phi_1 = \pm \Phi_0$[Fig. 1(a)]. Recently Sun et al. proposed a realistic optical lattice system to realize such model[21]. Besides it can be realized in ultracold fermions in optical lattices and in condensed matter systems with artificial gauge fields[22, 23, 24] or “emergent” gauge fields. The Hamiltonian for each layer is $H_{2D} = h_0(k)\sigma_0 + h_1(k)\cdot \sigma$ where $\sigma$ is the Pauli matrix vector acting on A/B (pseudo-spin up/down) site space and $\sigma_0$ is the $2 \times 2$ identity matrix. As it is no need to invoke true-spin splitting, we keep the true-spin states as degenerate. $h_0(k) = 2t_0(\cos k_x + \cos k_y)$, $h_1z(k) = 2t_1(\cos k_x - \cos k_y)$, $h_{1y}(k) = 4t_2 \sin \phi_1 \sin \frac{k_x}{2} \sin \frac{k_y}{2}$ where $t_0 = (t_x + t_y)/2$, $t_1 = (t_x - t_y)/2$ [Note that throughout this paper, we set the lattice constant $a = 1$.]. The two bands touches quadratically at $(\pi, \pi)$ when $\sin \phi_1 = 0$. This band touching is nontrivial as it carries a nonzero winding number $N_w = 2\text{sgn}(t_1 t_2 \sin \phi_1) = \pm 2$. At finite $\sin \phi_1$ (broken time-reversal symmetry) the quadratic band touching is gapped and the system becomes a QAH insulator with Chern number $C = \frac{1}{2}\text{sgn}(t_2 \sin \phi_1)N_w$[22, 23].

FIG. 1. (Color online) Lattice structure in (a) (001) plane in an odd layer and (b)(110) plane. Red-dots and blue-squares represent type A and B sites respectively. Hoppings along (opposite) the green-solid and blue-dotted arrows are $t_{2x}e^{-i\phi_1}$ and $t_{1x}e^{-i\phi_2}$ ($t_{2x}e^{i\phi_1}$ and $t_{1x}e^{i\phi_2}$) separately. Those along red-dashed and blue-dotted lines are $t_y$ and $t_x$ respectively. $\pm \Phi_1$ and $\pm \Phi_2$ are the plaquette fluxes. Phase diagram at (c) $|t_2/t_1| = 0.95$ and (d) $|t_2/t_1| = 1.3$. Yellow region: Weyl semimetal; green region: QAH state with Chern number $C_{2x}(k_z) = -2\text{sgn}(t_1 t_2)$ for all $k_z$; brown region: QAH state with $C_{2x}(k_z) = 2\text{sgn}(t_1 t_2)$ for all $k_z$.

The 3D lattice is a stacking of the 2D layers in such a way that different types of sites are on top of each other [see Fig. 1(b)]. The hopping between those sites is $t_{1x}e^{i\phi_2}$. The staggered flux per plaquette in the (110) plane is $\pm \Phi_2 = \pm 2(\phi_1 + \phi_2)$ [in (110) plane, the plaquette flux is $\pm 2(\phi_1 - \phi_2)$]. The Hamiltonian of the system is then

$$H = [h_0(k)\sigma_0 + h(k) \cdot \sigma] \gamma_0 + g(k_z)(\cos \phi_2 \sigma_x + \sin \phi_2 \sigma_y) \tau_x$$

Here $\sigma$ and $\tau$ matrices act on the A/B sites and odd/even layers respectively. $g(k_z) = 2t_2 \cos \frac{k_y}{2}$. The Hamiltonian can be block diagonalized directly, giving

$$H_\pm = h_0(k)\sigma_0 + h_\pm(k) \cdot \sigma$$

(3)
in the two blocks where

\[ h_{\pm x}(k) = 4t_2 \cos \phi_1 \cos \frac{k_x}{2} \cos \frac{k_y}{2} \pm g(k_z) \cos \phi_2, \]
\[ h_{\pm y}(k) = 4t_2 \sin \phi_1 \sin \frac{k_x}{2} \sin \frac{k_y}{2} \pm g(k_z) \sin \phi_2, \]
\[ h_{\pm z}(k) = 2t_1 (\cos k_x - \cos k_y). \]  

(4)

For the sake of easier formulation, we set the first Bril-louin zone as \( k_x \in [0, 2\pi], k_y \in [0, 2\pi] \) and \( k_z \in [0, 2\pi] \). Finally, the system possesses a series inversion symmetries. It is invariant under the following inversion transformations: (i) \( z \rightarrow -z, \) (ii) \( (x, y) \rightarrow (-x, -y), \) and (iii) \( (x, y, z) \rightarrow (-x, -y, -z). \) At \( h_0 = 0, \) the system also has particle-hole symmetry.

III. PHASE DIAGRAMS

The energy spectrum of the system is

\[ E_{\alpha \pm}(k) = h_0(k) \pm |h_\alpha(k)| \]  

with \( \alpha = \pm. \) The equations for the nodes (Weyl points) are \( h_{\alpha x} = h_{\alpha y} = h_{\alpha z} = 0. \) One finds that away from \( \phi_1, \) or \( \phi_2 = 0, \pm \pi/2, \pi \) [see Fig. 1 and discussions below], there are four Weyl points \( K_{+\beta} = (\beta k_x^c, \beta k_y^c, k_z^c) (\beta = \pm) \) in the + block and \( K_{-\beta} = (\beta k_x^c, \beta k_y^c, 2\pi - k_z^c) \) in the - block where

\[ k_y^c = \pi - 2 \arctan \left( \frac{\tan \phi_1}{\tan \phi_2} \right), \]
\[ k_x^c = \eta k_y^c \text{ with } \eta = \text{sgn} \left( \frac{\tan \phi_1}{\tan \phi_2} \right), \]
\[ k_z^c = 2 \arccos \left[ \frac{-2\eta t_2 \sin \phi_1}{t_1 \sin \phi_2} \left( 1 + \left| \frac{\tan \phi_1}{\tan \phi_2} \right| \right)^{-1} \right]. \]  

(6)

Note that the above equation holds only when

\[ \left| \frac{2t_2 \sin \phi_1}{t_1 \sin \phi_2} \left( 1 + \left| \frac{\tan \phi_1}{\tan \phi_2} \right| \right)^{-1} \right| \leq 1, \]  

(7)

which sets the phase boundaries of the Weyl semimetal. It is required that \( |h_0(k) - h_0(K_{\alpha \beta})| \leq |h_\alpha(k)| \) so that the system is an insulator wherever away from the nodes \( K_{\alpha \beta} \) (the definition of semimetal). Given this, the \( h_0(k)\sigma_0 \) term is irrelevant for the physics to be discussed and we hence take \( h_0 \equiv 0 \) hereafter.

In Fig. 1(c) and 1(d) we plot the phase diagram at two different \( |t_2/t_1| \). There are three phases: the Weyl semimetal, the QAH, and the non-topological semimetal. The last one refers to semimetals which have only nodes with \( N_{\nu} = 0. \) Such nodes are accidental band degeneracy points, which can be gapped by infinitesimal band mixing without breaking any symmetries. The QAH phase actually consists of two topologically distinct phases with opposite Chern number \( C_{xy}(k_z) = \pm 2\text{sgn}(t_1t_2) \) for all \( k_z \). Those two phases are separated by the Weyl semimetal and non-topological semimetal phases. In fact, the Weyl semimetals can be viewed as the intermediate phases between the non-topological semimetal (or insulator) phase and the QAH phase. In the former the Chern number is always zero, whereas in the latter it is always nonzero. In Weyl semimetals, there are two regions in the Brillouin zone: the Chern number is zero in one region while nonzero in another. Specifically in the current model \( C_{xy}(k_z) \) is nonzero only when \( k_z \in (k_{z_{\min}}, k_{z_{\max}}) \) with \( k_{z_{\min}} = \text{Min}(k_z^c, 2\pi - k_z^c) \) and \( k_{z_{\max}} = \text{Max}(k_z^c, 2\pi - k_z^c) \). The QAH and non-topological semimetal phases can be viewed as the limit \( k_{z_{\min}} \rightarrow 0 \) and \( k_{z_{\min}} \rightarrow 0 \) respectively. There are actually two Weyl semimetal phases in which the Chern number \( C_{xy}(k_z) \) is opposite at \( k_z \in (k_{z_{\min}}, k_{z_{\max}}) \). Those two phases are the intermediate states between the two QAH states (with opposite Chern number) and the non-topological semimetal state separately. The latter lies at the lines \( \phi_1 = 0, \pm \pi/2, \) and \( \pi \) in the phase diagrams, where \( k_{z_{\min}} = k_{z_{\max}} = \pi. \) We will show in next section that the evolution of the ground state and quantum phase transitions between those phases can be understood via the evolution of the Weyl points as Berry flux insertion processes.

We find that as \( |t_2/t_1| \) increases, the area of the Weyl semimetal phase in the phase diagram as functions of \( \phi_1 \) and \( \phi_2 \) shrinks. At \( |t_2/t_1| \rightarrow \infty, \) such area becomes zero. When \( |t_2/t_1| \leq 1/2 \) the system is always in the Weyl semimetal phase except at the special lines \( \phi_1 = 0, \pm \pi/2, \pi. \) Hence the region of the Weyl

FIG. 2. (Color online) (a) and (c) Illustration of the Weyl points when there are four in \( k_y-k_z \) plane. The arrows indicate the \( z \)-direction movement of the Weyl points as \( \phi_1 \) increases. Blue-squares (red-dots) denote Weyl points with \( N_{\nu} = -1 \)(\( N_{\nu} = 1 \)). The parameters are \( t_1 = 1, t_2 = 2, t_1 = 2, \) and \( \phi_2 = -0.25\pi. \) \( \phi_1 = -0.1\pi \) in (a), and \( \phi_1 = 0.1\pi \) in (c). (b) and (d) Chern number \( C_{xy}(k_z) \) as function of \( k_z \) for the cases in (a) and (c) respectively.
semimetal phases can be tuned by the ratio $|t_2/t_\perp|$. It is noted that the phase diagram exhibits some angle-shaped structures around the special points $(\phi_1, \phi_2) = (\phi_\alpha, \pm \phi_\alpha)$ with $\phi_\alpha = 0, \pm \pi/2, \pi$ as well as $(0, \pi)$ and $(\pi, 0)$ where Eq. (4) becomes ill-defined. The structure around, say, $(0, 0)$, can be understood via the following analysis. For $(\phi_1, \phi_2)$ close to $(0, 0)$, along the line $\phi_2 = \xi \phi_1$, $k_\alpha^R = 2 \arccos[-2t_2/t_\perp(\xi + 1)]$. Hence the Weyl semimetal phase is at $|\xi| > |2t_2/t_\perp| - 1$, which is angle-shaped. When $|t_2/t_\perp| < 1/2$, the system is in the Weyl semimetal phase for all parameters $(\phi_1, \phi_2)$ around $(0, 0)$.

It is benefit to point out some special regions in the phase diagram. First, when $\phi_2 = \pm \pi/2$, there are only two Weyl points: $K_+ = (\pi, \pi, k_\alpha^R)$ in the + block and $K_- = (\pi, \pi, 2\pi - k_\alpha^R)$ in the − block. Those Weyl points are quadratic band touchings with winding number $N_w = \pm 2$. Similarly, when $\phi_2 = 0, \pi$, there are two quadratic-band-touching Weyl points: $K_+ = (0, 0, k_\alpha^R)$ in the + block and $K_- = (0, 0, 2\pi - k_\alpha^R)$ in the − block. Besides, as pointed out before at the lines $\phi_1 = 0, \pm \pi/2, \pi$ the system is a non-topological semimetal.

\[ H_{\alpha\beta}(k) = \sigma \cdot \hat{\nu}_{\alpha\beta} \cdot q + O(q^2) \] (8)

where $q = k - K_{\alpha\beta}$. The velocity tensors of the Dirac cones are

\[
\hat{v}_{\alpha\beta} = \begin{pmatrix}
-\beta_1 t_2 \cos \phi_1 \sin k_y^c & -\beta_1 t_2 \cos \phi_1 \sin k_y^c \\
\beta_1 t_2 \sin \phi_1 \sin k_y^c & \beta_1 t_2 \sin \phi_1 \sin k_y^c \\
-2\beta_1 t_1 \sin k_y^c & 2\beta_1 t_1 \sin k_y^c \\
-\alpha t_{\perp} \cos \phi_2 \sin k_y^c & -\alpha t_{\perp} \cos \phi_2 \sin k_y^c \\
-\alpha t_{\perp} \sin \phi_2 \sin k_y^c & 0
\end{pmatrix}.
\] (9)

The winding number is the sign of the determinant of the velocity tensor $N_w(\alpha\beta) = \text{sgn}[\text{det}(\hat{v}_{\alpha\beta})]$. One finds

\[ N_w(\alpha\beta) = -\text{sgn}[t_1 t_2 t_\perp \sin(\phi_1 + \eta \phi_2)]. \] (10)

Note that Weyl points in the same block $\alpha$ have the same topological charge (independent of $\beta$), whereas Weyl points in different block have opposite topological charge. The positions and motions of the four Weyl points are illustrated in Fig. 2 for a specific case where $N_w = -\alpha$, $k_\alpha^c = -k_\alpha^R < \pi$, and $k_\alpha^R > \pi$. According to Eq. (11), the Chern number $C_{xy}(k_z)$ varies with $k_z$. The Chern number changes only when the gap is closed and re-opened, i.e., when $k_z$ passes through $k_\alpha^c$ and $2\pi - k_\alpha^c$. The Chern number is calculated as

\[ C_{xy} = \frac{1}{4\pi} \int_0^{2\pi} dk_x \int_0^{2\pi} dk_y \text{Re} \left( \text{tr} \left( \partial_{k_z} \mathbf{n}_\alpha \times \partial_{k_z} \mathbf{n}_\alpha \right) \right), \] (11)

where $\mathbf{n}_\alpha = \mathbf{h}_\alpha/|\mathbf{h}_\alpha|$. We find that $C_{xy}(k_z) = 2\text{sgn}[t_1 t_2 t_\perp \sin(2\phi_1)]$ when $k_z \in (k_{\text{min}}^c, k_{\text{max}}^c)$, otherwise $C_{xy}(k_z) = 0$. The relation between the quantum phase transitions and the evolution of the Weyl points is depicted in Fig. 2 where we consider a situation with $\phi_2 = -0.25\pi$ and $\phi_1$ varying from $-0.1\pi$ to $0.1\pi$. At $\phi_1 = -0.1\pi$, the Weyl points with $N_w < 0$ are in the $k_z < \pi$ region whereas those with $N_w > 0$ are in the $k_z > \pi$ region [Fig. 2(a)]. Consequently, the Chern number $C_{xy}(k_z)$ is negative at $k_z \in (k_{\text{min}}^c, k_{\text{max}}^c)$. As $\phi_1$ increases the Weyl points with $N_w < 0$ and those with $N_w > 0$ moves in opposite directions along $k_z$ and becomes closer. At $\phi_1 = 0$, Weyl points with opposite $N_w$ coincide and the system becomes a non-topological semimetal. After that their positions shift as $\phi_1$ increases [Fig. 2 (c)]: the Weyl points with $N_w < 0$ in the $k_z > \pi$ region whereas those with $N_w > 0$ move to the $k_z < \pi$. As a consequence the Chern number $C_{xy}(k_z)$ changes sign at $k_z \in (k_{\text{min}}^c, k_{\text{max}}^c)$. Further variation of $\phi_1$ will enlarge the region and finally the system becomes a QAH insulator after $k_z \rightarrow 0$ where pairs of monopoles with opposite topological charge ($N_w$) merge and annihilate each other. During those processes quantized Berry fluxes are inserted into each $k_z$-$k_y$ plane with fixed $k_z$, whenever the monopoles move across it, as there are quantized Berry fluxes flow between monopoles with opposite charge.

In addition, as $\phi_2 \rightarrow 0, \pm \pi/2$, and $\pi$, the two Dirac cones with same $k_z$ merge together and form a quadratic band touching as they have the same winding number. The $k_z$ dependence of $C_{xy}(k_z)$ in this situation is similar to the previous one. However, as we will show later, the Fermi arcs and surface states in those two situations are significantly different.

\section{Evolution of Fermi Arcs and Surface States}

The move and merge (or split) of the Weyl points have profound effects on the topologically protected surface states. In particular, we demonstrate the Fermi arcs on the surface for two situations where there are (i) four Dirac cones and (ii) two quadratic band touchings in Fig. 3 (a) and (b) respectively. The color represents the spectral function $A(E) = \frac{1}{\pi} \text{Im} G^\prime(E)$, $G^\prime(E)$ is the re-
FIG. 3. (Color online) Spectral function $A(E)$ of the surface states at zero energy ($E = 0$) in the case with (a) four Dirac cones and (b) two quadratic band touchings. Spectra of surface and bulk states as function of (c) $k_z$ (at $k_y = 0.8\pi$) and (d) $k_y$ (at $k_z = \pi$) respectively with the same parameters as in (a). The size of the system is 151 unit cell (due to the finite size effect the bulk bands are slight gapped at the node). Gray region represents bulk spectra, while red (green) curves denote the surface spectra at the left (right) boundary [Note that in (c) the surface spectra at the two boundaries coincide]. $t_1 = 1$, $t_2 = 2$, and $t_\perp = 2$. In (a), (c) and (d) $\phi_1 = 0.1\pi$, $\phi_2 = -0.25\pi$, whereas in (b) $\phi_1 = 0.15\pi$, $\phi_2 = -0.5\pi$. Correspondingly, $k_y^\ast = 0.8\pi$ and $k_y^\ast = 1.4\pi$ in (a), (c) and (d), whereas $k_y^\ast = \pi$ and $k_y^\ast = 1.5\pi$ in (b). The results are calculated via the iterative Green function method in Ref. [31]. An artificial spectral broadening 0.04 is taken for the sake of visibility.

FIG. 4. (Color online) Spectral functions of the surface states for two cases: (a) four Dirac cones (b) two quadratic band touchings. The energies of the surface states from left to right (in both the $k_y < \pi$ and $k_y > \pi$ regions) are -0.8, -0.4, 0, 0.4, and 0.8 respectively. E.g., both the leftmost arc in the $k_y < \pi$ region and the leftmost arc in the $k_y > \pi$ region are the arcs with energy -0.8. The parameters for (a) and (b) are the same as those in Fig.3 (a) and (b) respectively. An artificial spectral broadening 0.04 is taken for the sake of visibility.

It is noted from Fig. 3(b) that in case (ii) the two Fermi arcs are actually connected together as $k_y^\ast = -k_y^\ast$, forming a closed Fermi surface. In the four Dirac cone case in Fig. 3(a), when $k_y^\ast \neq -k_y^\ast$, the Fermi surface is not closed. It seems that the Fermi arcs are also invariant under the inversion operation $k_y \to -k_y$. However, this is only a special property of zero energy surface states due to the particle-hole symmetry. For surface states with nonzero energy, the spectral function are not $k_y$-inversion symmetric as the boundary breaks the $(x, y) \to (-x, -y)$ inversion symmetry. To illustrate the surface states explicitly, we plot the spectral functions of the surface states in Fig. 4(a) and 4(b) for the two cases that correspond to Fig. 3(a) and 3(b) respectively. The selected energies of the surface states from left to right (in both the $k_y < \pi$ and $k_y > \pi$ regions) are -0.8, -0.4, 0, 0.4, and 0.8 respectively. For each energy there are two arcs: one in the $k_y < \pi$ region and another in the $k_y > \pi$ region. E.g., both the leftmost arc in the $k_y < \pi$ region and the leftmost arc in the $k_y > \pi$ region are the arcs with energy $E = -0.8$. It is clearly seen that the spectra are not invariant under $k_y$-inversion but invariant under the particle-hole transformation. Besides, only the arcs with zero energy links between the monopoles whereas other arcs merge into the bulk bands without going through the Weyl points. Finally, it is seen from Fig. 3(d) that the two Fermi arcs are assigned to two different chiral edge states at the left boundary which both have positive group velocity along the $z$-direction. It is found that the shape of the Fermi arcs can be tuned via $\phi_1$ and $\phi_2$ to be inner-curved (as in Fig. 3b), out-curved, or flat [as
in Fig. 3(a)]. Flat bands can be interesting in the context of elevated transition temperature in spontaneous symmetry broken [2], as the density of states are increased.

VI. A POSSIBLE SCHEME FOR EXPERIMENTAL REALIZATION

In this section we propose a possible scheme to realize the model in optical lattices. The required artificial gauge fields are generated by the spatial variation of the laser-atom interaction as suggested in Ref. [22]. Suppose that there is a excited states with energy much higher than the energy scale where the above model are defined. Impose standing waves of light to induce the following coupling between the ground and excited states in rotating wave approximation,

$$H_R(\mathbf{r}) = M[\cos 2\pi z \cos \pi(x+y) \hat{F}_x + \cos \pi(x-y) \hat{F}_y + \zeta \hat{F}_z],$$

where $\hat{F}_\nu (\nu = x,y,z)$ are the Pauli matrices acting on the (dressed-) ground and excited states. $M$ and $\zeta$ are parameters of the laser-atom coupling. It can be realized in a system with three standing wave Raman lasers with a detuning of $M\zeta$. The three laser wavevectors are $(\pi, \pi, \pm 2\pi)$ and $(\pi, -\pi, 0)$. When the kinetic energy is small compared to the energy splitting of the local dressed states [the eigenstates of the local Hamiltonian $H_R(\mathbf{r})$]. The emergent gauge fields can be obtained via the Berry-phase [22], $A = (\Psi_G(\mathbf{r})|i\nabla_r|\Psi_G(\mathbf{r}))$ with $\Psi_G(\mathbf{r})$ being the ground state of the local Hamiltonian $H_R(\mathbf{r})$. One can show that $A = \frac{i}{2}[\Theta \nabla_r \Pi]$, with $\Theta = 1 - \frac{|\zeta|}{\sqrt{\cos^2(2\pi z) \cos^2 \pi(x+y) + \cos^2 \pi(x-y) + \zeta^2}}$ and $\Pi = \text{Arg}[\cos(2\pi z) \cos \pi(x+y) + i \cos \pi(x-y)]$. The effective “magnetic field” (i.e., the Berry curvature, or the “magnetic flux density”) are written as $B_\nu = \varepsilon^{\nu\delta\rho} \partial_\delta A_\rho$, with $\nu, \delta, \rho = x,y,z$ and $\varepsilon$ being the Levi-Civita tensor. The plaquette flux for each plaquette is the “magnetic flux” through it. For example, for a plaquette in the $x$-$y$ plane, the plaquette flux is $\Phi = \int dxdy B_2$, where the integral is limited within the plaquette. We plot the effective “magnetic field” $B_2$ through the $x$-$y$ plane (in odd layer) and $B_{110}$ through the $(110)$ plane in Fig. 5(a) and 5(b) respectively. It is seen that the magnetic flux density has exactly the same checkerboard pattern as the plaquette fluxes in Fig. 1(a) and 1(b). This shows that the gauge fields generated by the Hamiltonian, Eq. (12), is exactly what is needed for the realization of the model. The magnetic flux density in (110) plane is zero everywhere, which is because the current scheme realizes the model with $\phi_1 = \phi_2$.

The phase along a hopping path $l$ is given by $\phi_l = \int dr \cdot \mathbf{A}$. Combined with Figs. 1(a) and 1(b), one can show that the hopping phases $\phi_1$ and $\phi_2$ in Hamiltonian Eq. (11) are given by

$$\phi_1 = \phi_2 = g(\zeta)$$

whereas the phases of other hoppings are zero. The function $g(\zeta)$ is plotted in Fig. 6. $\phi_1 = \phi_2 \in [-\pi/4, 0]$. Due to the factor $\cos(2\pi z)$ the gauge phases are inverted from odd layer at $z = n$ to even layer at $z = n + 1/2$ with $n$ being integer. This exactly realizes the lattice structure in Fig. 1. The amplitudes and signs of the rest hoppings can, in principle, be tuned via various optical lattice techniques [32]. By manipulating the ratio $t_2/t_\perp$, the system can experience various phases in the phase diagram: (i) At finite $\phi_1$ when $|t_2/t_\perp| < 1$ it is a Weyl semimetal, (ii) otherwise it is a QAH insulator with $C_{xy}(k_z) = 2 \text{sgn}[t_1 t_2 t_\perp \sin(2\phi_1)]$ for all $k_z$; (iii) At $\phi_1 = 0$ the system is always a non-topological semimetal.

VII. SUMMARY

In summary, a model of simple cubic lattice with staggered fluxes which exhibits Weyl semimetal phase is proposed and studied. The model is simple and can act as a prototype to study the properties of Weyl semimetals. Due to its simplicity, the model is potentially achievable both in ultracold fermions in optical lattices and in condensed matter systems. In particular, we propose a possible scheme to realize the model in optical lattice system. Differing from previous works, here the mechanism to achieve the topological Weyl semimetal state is to gap the quadratic band touching by time-reversal-symmetry-breaking hoppings. The system exhibits rich

![FIG. 5. (Color online) The “magnetic flux density” through (a) (001) plane at an odd layer (b) (110) plane. $\tau = r \cdot (1,1,0)/2 = (x+y)/2$. The bright region has positive value, whereas the dark region has negative value.](Image)

![FIG. 6. The function $g(\zeta)$.](Image)
phase diagrams, where the number of Weyl fermions and their topological charges and positions are tunable via the plaquette fluxes (hopping phases). The Weyl semimetal state is demonstrated to be the intermediate phase between non-topological semimetal and quantum anomalous Hall insulator. The transitions between those phases can be understood via the evolution of the Weyl points [see below]. As the Weyl points move and split (or merge) via the manipulation of the hopping phases, the Fermi arcs and surface states undergo significant change, as the Fermi arcs have to be terminated at the Weyl points.

The relations between the non-topological insulators/semimetals, topological Weyl semimetals and QAH insulators demonstrated in this paper can be summarized in the following processes: (i) A non-topological insulator becomes non-topological semimetal via forming an accidental band-touching node with winding number \( N_w = 0 \). (ii) By splitting the node into pairs of Weyl fermions with opposite topological charges and moving the positively and negatively charged Weyl fermions in opposite directions in the \( k \)-space, a Weyl semimetal state is created. (iii) When the positively and negatively charged Weyl points are moved by half of the reciprocal lattice vector, they merge and annihilate each other in pairs, making the system transit into a QAH insulator.

The relations between the non-topological insulators/semimetals, topological Weyl semimetals and QAH semimetals, topological Weyl semimetals and the 3D quantum spin Hall insulator (i.e., the time-reversal invariant \( Z_2 \) topological insulators), where quantized non-Abelian Berry fluxes are inserted into the bulk states during the moving of the monopoles.

**ACKNOWLEDGMENTS**

Work at the Weizmann Institute was supported by the German Federal Ministry of Education and Research (BMBF) within the framework of the German-Israeli project cooperation (DIP) and by the Israel Science Foundation (ISF). I thank Zhong Fang, Xi Dai, Jonathan Ruhman, and Zohar Ringel for illuminating discussions and comments.

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