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Realizing type-II Weyl points in an optical lattice

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The recent discovery of the Lorentz symmetry-violating “type-II” Weyl semimetal phase has renewed interest in the study of Weyl physics in condensed-matter systems. However, tuning the exceptional properties of this novel state has remained a challenge. Optical lattices, created using standing laser beams, provide a convenient platform to tune tunneling parameters continuously in time. In this paper, we propose a generalized two level system exhibiting type-II Weyl points that can be realized using ultracold atoms in an optical lattice. The system is engineered using a three-dimensional lattice with complex π phase tunneling amplitudes. Various unique properties of the type-II Weyl semimetal such as open Fermi surface, anomalous chirality, and topological Fermi arcs can be probed using the proposed optical lattice scheme.

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I. INTRODUCTION

In spite of its theoretical proposal as early as 1929 [1], the Weyl fermion, one of the intriguing particles predicted in the development of quantum field theory, has not been observed as an elementary particle. However, these massless particles have been recently detected in condensed-matter experiments as low energy collective excitations, or quasiparticles, in a Weyl semimetal (WSM) that supports Fermi-arc topological surface states [2–4]. As described by quantum field theory that is intrinsically relativistic, Weyl fermions are Lorentz covariant. Nevertheless, Lorentz symmetry can be violated in condensed-matter systems, resulting in a “type-II” Weyl semimetal phase, which has no equivalent in quantum field theory. This newly proposed type-II WSM phase [5,6] has been experimentally observed in materials such as MoTe₂ [7], Mo_xW_{1-x}Te₂ [8], and Ta₃S₂ [9] and has been predicted to exist in other materials such as diphosphides of Mo and W [10]. Compared to the type-I WSM phase, the type-II phase exhibits many novel properties such as nonvanishing finite density of states at Fermi level [5] and anomalous chiral Landau levels [11–13]. These properties together with the topologically protected Fermi-arc surface states, apart from being interesting in fundamental physics, may be useful in the realization of quantum computation and high efficiency circuitry.

Tuning the WSM to explore its various properties has remained difficult in condensed-matter systems. Alternate systems such as those based on ultracold atoms and classical (electromagnetic [14] and acoustic) waves offer flexible platforms to realize and probe these WSM phases. In systems based on ultracold atoms, since the optical lattice is created using standing optical waves, parameters such as tunneling amplitude between lattice sites can be continuously modulated in time [15,16], thereby easily tuning the properties of WSM phases. This is in contrast to condensed-matter samples where tunneling amplitude is a fixed material property. There have been a number of proposals to construct type-I WSM using

ultracold atoms in optical lattices [17–23]. Of these, the proposals in Refs. [18,22] have proved promising because they are extensions of the experimentally realized Harper-Hofstadter Hamiltonian [24,25] and staggered flux lattice [26]. Moreover, type-I Weyl points (WPs) have been observed in photonic crystals [27], in photonic material based on magnetized plasma [28], and predicted to exist in acoustic structures [29,30].

The type-II WSM phase, on the other hand, is much less explored. Besides the recent condensed-matter realizations, this type-II WSM phase can be realized in a spin-orbit-coupled Bose-Einstein condensate [6], and can be constructed for electromagnetic waves in a metallic-helical-wire metamaterial system [31]. However, all these systems, once constructed, cannot be easily tuned. To fill this gap, we propose a model with type II-WP spectra that can be realized in optical lattices using ultracold atoms. This model consists of a three-dimensional (3D) square lattice with complex π phase tunneling amplitudes from one lattice site to another. We have chosen this model because nonzero phase tunneling amplitudes have already been implemented in two-dimensional (2D) ultracold atoms in optical lattices [15,32], thereby making it easily realizable using current know-how.

II. MODEL

Consider a two-dimensional lattice in the xy plane, under a perpendicular magnetic flux of strength ϕ in each plaquette. Assuming the lattice to be deep, the system is described by the time independent Harper-Hofstadter Hamiltonian [33,34] for $\alpha = \phi/2\pi$ flux quantum per plaquette,

$$H = \sum_{\mathbf{r}} -J_x e^{-i\Phi(\mathbf{r})} a_{\mathbf{r}}^{\dagger} a_{\mathbf{r}+\mathbf{e}_x} - J_y a_{\mathbf{r}}^{\dagger} a_{\mathbf{r}+\mathbf{e}_y} + \text{H.c.} \quad (1)$$

Here $a_{\mathbf{r}}^{\dagger}$ and $a_{\mathbf{r}}$ are creation and annihilation operators at site $\mathbf{r}$ and J_x (J_y) are the tunneling amplitudes in the x (y) direction. $\Phi(\mathbf{r})$ is the position dependent complex tunneling phase at site $\mathbf{r}$. The phase acquired by a particle while moving along a closed plaquette in this lattice is analogous to the Aharonov-Bohm phase gathered by the wave function of particles moving in circular trajectories under the influence

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FIG. 1. Structure of 3D lattice proposed to realize type-II Weyl points. Tunneling amplitude along the x direction alternately carries a complex phase of π (depicted using dashed lines) and 0 (solid). The lattice can be constructed using two dissimilar sites depicted in red and blue. Tunneling along the z direction has a constant phase of 0 (π) along the red (blue) sites and is shifted from 0 by a constant value J_z . Inset: A part of the lattice depicting the complex tunneling amplitudes in the x , y , and z directions.

of an external magnetic field, thereby simulating a synthetic magnetic field. Since the lattice is discrete, we can use integral indices (m, n) to represent the position vector as $\mathbf{r} = a(m\mathbf{e}_x + n\mathbf{e}_y)$, where a is the lattice constant and $\mathbf{e}_x$ and $\mathbf{e}_y$ are unit vectors along the x and y direction, respectively. In our model we set $\phi = \pi$ using complex hopping phases in the x direction $\Phi(m, n) = \pi(m + n)$. In cold atom lattices, this system has been experimentally demonstrated in Ref. [25]. Note that this scheme preserves both the inversion and time-reversal symmetry.

Next, we extend the lattice along the z direction. To realize the type-II WPs we propose to modulate the tunneling amplitude along the z direction as $J_z + \delta J_z e^{-i(m+n)\pi}$, depending on the position along the x (m) and y (n), thereby breaking the inversion symmetry. Alternately, this can be also viewed as a potential offset $J_z \pm \delta J_z$ since $e^{-i(m+n)\pi} = (-1)^{(m+n)}$ for $m, n \in \mathbb{Z}$. A sketch of the proposed structure is given in Fig. 1.

The modified Hamiltonian describing this system is

$$H = \sum_{m,n,l} [-J_x e^{-i\pi(m+n)} a_{m,n,l}^\dagger a_{m+1,n,l} - J_y a_{m,n,l}^\dagger a_{m,n,l+1} - (J_z + \delta J_z e^{-i(m+n)\pi}) \times a_{m,n,l}^\dagger a_{m,n,l+1} + \text{H.c.}], \quad (2)$$

where integers (m, n, l) refer to the lattice positions along the (x, y, z) axes. For an infinite periodic optical lattice, we can take the Fourier transform and rewrite the Hamiltonian in quasimomentum ($\mathbf{k}$) space as $\sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}^\dagger \mathcal{H}(\mathbf{k}) \mathbf{a}_{\mathbf{k}}$. Here $\mathcal{H}(\mathbf{k})$, known as Bloch Hamiltonian, is given by

$$\mathcal{H}(\mathbf{k}) = -2J_z \cos(k_z a) \mathbf{1} - 2J_y \cos(k_y a) \sigma_x - 2J_x \sin(k_x a) \sigma_y - 2\delta J_z \cos(k_z a) \sigma_z. \quad (3)$$

In this equation, $\sigma_x, \sigma_y, \sigma_z$ are Pauli matrices. We can confirm that the system is symmetric under time reversal by noting $\mathcal{T}\mathcal{H}(\mathbf{k})\mathcal{T}^{-1} = \mathcal{H}(\mathbf{k})^* = \mathcal{H}(-\mathbf{k})$, but not under inversion symmetry since $\mathcal{I}\mathcal{H}(\mathbf{k})\mathcal{I}^{-1} \neq \mathcal{H}(-\mathbf{k})$, where $\mathcal{T}$ and $\mathcal{I}$ are the canonical time-reversal and inversion operators [35]. Note that in our model, type-I WSM can be realized by setting $J_z < \delta J_z$ (as reported in [18] for $J_z = 0$), and type-II WSM can be realized by setting $J_z > \delta J_z$.

The Hamiltonian can be briefly written as $\mathcal{H} = d_0 \mathbf{1} + \mathbf{d} \cdot \boldsymbol{\sigma}$ where we have introduced the vector $\mathbf{d}$ with components $d_x = -2J_y \cos(k_y a)$, $d_y = -2J_x \sin(k_x a)$, $d_z = -2\delta J_z \cos(k_z a)$, and $d_0 = -2J_z \cos(k_z a)$. The energy spectrum of the system consists of two bands given by $E = d_0 \pm |\mathbf{d}|$. The two bands touch at four points $(0, \pm \pi/2a, \pm \pi/2a)$ in the first Brillouin zone (Fig. 2). Around these points, if the magnitude of the kinetic term (d_0) in the energy spectrum exceeds the second term ($|\mathbf{d}|$) along any direction in momentum space, the Weyl cone is tilted along this direction and the points are called “type-II” WPs [5]. In our scheme δJ_z can be chosen to be less than J_z , thereby tilting the Weyl spectrum in the $\pm z$ directions and creating four type-II WPs at $(0, \pm \pi/2a, \pm \pi/2a)$ in the first Brillouin zone [Fig. 2(a)]. At $\delta J_z = J_z$ there is a transition between a type-I and a type-II WSM and the particle-hole pockets are straight lines connecting the touching points in momentum space.

FIG. 2. (a) Band structure of the lattice in the $k_x = 0$ plane. The electron (orange) and hole (blue) bands touch to form type-II WPs at $(k_y, k_z) = (\pm\pi/2a, \pm\pi/2a)$. Each node, labeled W1–W4, is tilted in the k_z direction. (b) Fermi surface ($E = 0$) is depicted as a function of the crystal momentum $\mathbf{k}$. The electron-hole pockets in the first Brillouin zone (shaded in gray) touch at WPs (W1–W4). (c) Berry curvature in the $k_x = 0$ plane. Arrows represent the direction of the vector field. Type-II WPs W2, W3 act as sources and W1, W4 act as sinks of Berry curvature. The color scale, indicating the magnitude of the vector field, has been logarithmically scaled. In all calculations the magnitude of tunneling amplitudes is normalized to 1 and δJ_z is assumed to be 1/2.

To further confirm that the four touching points of the particle and hole band are indeed type-II WPs, we plot the $E = 0$ Fermi surface (FS) in Fig. 2(b). It can be seen that the FS is open, consisting of particle pockets (for $\pi/2a < k_z < \pi/2a$) and hole pockets (for $k_z > \pm\pi/2a$) unlike the pointlike FS of type-I WSM [18]. The open FS is indicative of a finite density of states at Fermi level in contrast to the vanishing density of states for type-I WPs. The nodes at the intersection of the particle-hole pockets in the first Brillouin zone (marked W1–W4) correspond to the location of the type-II WPs in k space.

Weyl points, both types I and II, always occur in pairs with opposite chirality. One of each pair is a source and the other, a sink of Berry curvature. For each band with eigenfunction $|n(\mathbf{k})\rangle$, the Berry curvature is defined as the curl of the Berry connection $\mathbf{\Omega}_n(\mathbf{k}) = \nabla \times \langle n(\mathbf{k}) | \nabla | n(\mathbf{k}) \rangle$. For a two level system, the Berry curvature for the hole (lower) band ($E = d_0 - |d|$) is given by [36]

$$\Omega_{-ij}(\mathbf{k}) = \frac{1}{2|d|^3} \mathbf{d} \cdot \partial_i \mathbf{d} \times \partial_j \mathbf{d}, \quad (4)$$

where the components of $\mathbf{d}$ for our system are defined in the previous section. For the scheme under consideration, we calculate the Berry curvature field using Eq. (4). The field in the $k_x = 0$ plane is plotted in Fig. 2(c). Points W1–W4 correspond to the location of the type-II WPs with W2 and W3 acting as sources and W1 and W4 acting as sinks of Berry curvature. We can find the topological charge of each point by integrating the Berry curvature over a surface enclosing the point in k space. The calculated topological charge for W1 and W4 is -1 and W2, W3 is $+1$ thereby confirming their opposite chiralities.

III. CHIRAL LANDAU LEVELS

In the presence of a magnetic field the Landau level spectrum near a WP exhibits chiral (unpaired) zeroth level. In type-I WPs the sign of the group velocity of the chiral Landau level changes with chirality of the WP. However, in type-II WPs the sign of the group velocity is independent of the chirality of the WP [12,13]. Furthermore, Landau level quantization is possible only if the magnetic field is applied along the direction of tilt of the WPs [11–13]. To study these properties in the proposed structure, we first linearize the Bloch Hamiltonian [Eq. (3)] around the WPs $K = (0, \pm\pi/2a, \pm\pi/2a)$ to get

$$\begin{aligned} \mathcal{H}(\mathbf{K} + \mathbf{q}) = & \pm 2J_z q_z a \mathbf{1} \pm 2J_y q_y a \sigma_x \\ & - 2J_x q_x a \sigma_y \pm 2\delta J_z q_z a \sigma_z. \end{aligned} \quad (5)$$

In this condensed equation the sign of the q_y and q_z terms depends on the sign of k_y and k_z , respectively, corresponding to the location of the WP ($\mathbf{K}$) around which the Hamiltonian is linearized. Next, we consider the model Hamiltonian in the presence of a magnetic field of strength B along the z axis. The energy spectrum can be calculated by introducing the usual ladder operators $a^\pm = (q_x \pm iq_y)l_b/\sqrt{2}$, where magnetic length (l_b) is defined as $l_b = \sqrt{eB/\hbar}$. The calculated result for all four WPs with $l_B = 10$ and $\delta J_z = 0.5$ has been plotted in Figs. 3(a), 3(c), 3(e), and 3(g). Since k_z corresponds to the

FIG. 3. Energy spectra in the vicinity of WPs in the presence of a magnetic field ($l_B = 10$) directed along the z axis. First 50 Landau levels are plotted for type-II WPs ($\delta J_z = 0.5$ and $J_x = J_y = J_z = 1$) located at $(k_x a, k_y a, k_z a) = (0, \pi/2, \pi/2)$ in (a), $(0, \pi/2, -\pi/2)$ in (c), $(0, -\pi/2, \pi/2)$ in (e), and $(0, -\pi/2, -\pi/2)$ in (g). For comparison, spectra of corresponding type-I WPs ($\delta J_z = J_x = J_y = 1$ and $J_z = 0$) are plotted in (b), (d), (f), and (h). The group velocities of the chiral Landau level in type I WPs (b),(f) have opposite slopes reflecting their opposite chirality. However, chiral Landau levels in type-II WPs (a),(e) have positive group velocities in spite of their opposite chiralities; same for (c),(g) in contrast to (d),(h).

tilt direction of the WP in our energy spectrum [Fig. 2(a)], an asymmetric chiral Landau level can be seen at each WP. Instead, if the magnetic field is induced outside the so-called “magnetic” regime [12], say, along the x and y directions, no Landau levels will be observed. Also, in Figs. 3(b), 3(d), 3(f), and 3(h) the energy spectrum for $J_z = 0$ and $\delta J_z = 1$, corresponding to type-I WPs [18] has been plotted for comparison. It can be confirmed that the slope of the zeroth Landau level for WPs with opposite chirality does not change in the type-II WSM in contrast to type I.

IV. FERMI ARCS

One of the most exciting properties of the WSM is the existence of topologically protected surface states. In the energy spectrum these states are seen as Fermi arcs connecting WPs of opposite chirality. In order to explore the structure of Fermi arcs, in our model, we consider a lattice that is finite along the $x - y$ direction. We choose this direction

FIG. 4. Energy spectra for an optical lattice consisting of 25 unit cells in the $x - y$ direction and infinite along the $x + y$ and z directions (coordinates in Fig. 1). (a) Spectra plotted as a function of k_z and $k_p = (k_x + k_y)/\sqrt{2}$. Surface states have been depicted in orange. Fermi arcs connecting type-II WPs $W1$ ($W3$) and $W2$ ($W4$) are highlighted using black lines. (b) Left: spectra plotted as a function of k_p for $k_z = \pi/2a$. Fermi arc connecting $W1$ and $W2$ can be clearly seen. Right: spectra plotted as a function of k_z for $k_p = \pi/8a$. Two surface states corresponding to propagation along the two edges of the lattice are evident.

to prevent WPs of opposite chirality from overlapping in momentum space. The energy spectrum of this finite lattice is calculated as a function of k_z and $k_p = (k_x + k_y)/\sqrt{2}$ (Fig. 4). Type-II WPs labeled $W1$ ($W3$) and $W2$ ($W4$), corresponding to opposite chiralities, are connected by Fermi arcs lying on the $k_z = \pm\pi/2a$ plane. The detailed structure of the Fermi arcs can be seen in the cross-sectional view [Fig. 4(b)] of the energy spectra. In Fig. 4(b) (left), k_z is set to $\pi/2a$, corresponding to the location of two type-II WPs ($W1, W2$). The Fermi arc lying on the $k_z = \pi/2a$ plane can be seen to connect the two WPs. Two distinct surface states can be noticed when momenta is away from the WPs but lying on the Fermi arc, as in $k_p = \pi/8a$ in Fig. 4(b) (right).

V. EXPERIMENTAL REALIZATION

In systems consisting of cold atoms in optical lattices many techniques can be applied [15] to realize complex tunneling amplitudes. Among these, the use of Raman lasers to drive resonant tunneling between neighboring sites has been widely used to achieve very high synthetic magnetic fields [24,25,37,38]. This technique, introduced in Refs. [39–42], is based on applying a linear energy tilt to the optical lattice

to inhibit bare tunneling and restoring the tunneling using spatially modulated Raman lasers with detuning frequency equal to the energy tilt. The model proposed here can be realized by extending the 2D optical lattice used to demonstrate the Harper-Hofstadter Hamiltonian [24,25]. Specifically, the 2D system in [25] corresponds exactly to our model in the xy plane. Bare tunneling in the x direction (J) is suppressed by tilting the lattice to ensure that $J \ll \Delta$, where Δ is the energy offset between neighboring sites due to the tilt. This is necessary to ensure that tunneling is due to the laser assisted hopping that impinges a position dependent phase ($J_x e^{-i\pi(m+n)}$) and not due to bare coupling between neighboring sites. The tunneling in z direction can be implemented using an additional pair of Raman lasers [18] to drive resonant tunneling with amplitude δJ_z and phase alternating between 0 and π along the x and y axes. In contrast to hopping in the x direction, along the z direction, a finite bare tunneling amplitude J_z can be implemented by changing the intensity of the lattice beams to achieve the desired hopping ($J_z + \delta J_z e^{-i\pi(m+n)}$). Type-II WPs are created if the bare tunneling amplitude is greater than the laser assisted tunneling amplitude $J_z > \delta J_z$ and type I if $J_z < \delta J_z$.

The type-II WPs obtained using this scheme can be detected using the conventional methods of time-of-flight imaging and Bragg spectroscopy [16]. Since the bare tunneling amplitude J_z can be easily tuned by changing the intensity of the lattice beam in the z direction, the topological phase transition between type-I ($J_z < \delta J_z$) and type-II ($J_z > \delta J_z$) WPs can be probed using this scheme. Furthermore, additional pairs of lasers can be used to create a synthetic magnetic field along the z direction to probe the anomalous zeroth Landau level. The proposed scheme inherits the advantages of Refs. [24,25], namely, not requiring a mixture of spin states and applicability to a wide class of particles. Note that engineering artificial gauge fields in ultracold atoms has an extremely rich literature [15] and the method outlined above is only one among the various ways to implement the proposed scheme.

Since we do not exploit the internal degrees of freedom such as spin, this concept can be extended to classical systems [14,43] like photonics using coupled optical resonators. Nonzero phase tunneling corresponding to large magnetic field has been experimentally implemented in these systems by changing the refractive index or optical length in a plaquette by placing the resonators asymmetrically [44,45]. Furthermore since all nonzero phase tunneling amplitudes in our model consist of a π phase, corresponding to a negative real coupling ($J e^{i\pi} = -J$), systems such as [46] can be implemented to realize the proposed structure.

To summarize, in this paper we have proposed a two band model to realize type-II WPs using π phase tunneling between adjacent lattice sites. The chosen model can be implemented using ultracold atoms in optical lattices. The proposed scheme can also be extended to other classical systems. Realization outside traditional condensed-matter systems will provide tunable control over the properties of the type-II WSM, thereby opening new avenues in its study.

Note added. We recently came across a preprint [47] proposing an alternative scheme to realize type-II WPs using spin-orbit coupling of alkali-metal atoms.

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