Optically Induced Topological Phase Transition and a Triple Dirac-Cone State in Square Lattice Antiferromagnet

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The square lattice antiferromagnet with spin-orbit coupling and nonsymmorphic symmetry is recently found to be topological insulator (TI) with helical edge state. We found that the optical irradiation with circular or linear polarization could induce topological phase transition into quantum Anomalous Hall (QAH) phase with varying winding number or semi-metal (SM) phase with a pair of two Dirac cones, respectively. In the phase diagram, the SM and TI phase regimes overlap. At the phase boundary between TI/SM phase and SM phase, the pair of two Dirac cones of the SM phase coexist with another Dirac cone that induces topological phase transition into the TI phase. The bulk states that have three Dirac cones is designated as triple Dirac-cones states. The triple Dirac-cones state is found to have sizable Berry curvature dipole. In the SM phase regime, the flat edge states connecting the pair of two Dirac cones behave as chiral edge states. Near to the TI/SM phase boundary, the coexistence of the flat edge state and the helical edge state is controlled by the optical field. The optically controlled triple Dirac-cone state could be carrier of ternary valleytronic physics.

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I. INTRODUCTION

Periodic perturbations of electronic systems create many topological phases, including topological insulator (TI) [1–3], Chern insulator [4, 5] and Weyl semi-metal [6]. The perturbation could be optical irradiation [7–9] or mechanical vibration [10, 11]. For optical driven system, the topological phase depends on the polarization and amplitude of the optical field. The optical control of the topological phase offer vast candidates for opto-electronic and opto-spintronic application. For example, graphene under optical irradiation has Floquet chiral edge states with edge dependent transport [12–16], or Floquet zigzag edge states with one-way transport [17]. Similar Floquet states exist in the other two dimensional materials described by the honeycomb lattice model [18–20]. The Floquet systems in square lattice models have been studied to demonstrate the topological properties as well, which can be realized in condensate materials [16, 21, 22] or cold atomic gas in optical lattice [23–25]. The search for a realistic condensate materials that realized the Floquet states become important for the development of the spintronic applications.

Floquet states found major role for the applications in valleytronic physics. The driven of graphene by combination of the fundamental and third harmonic frequency optical field could selectively gap one of the two Dirac cones [26]. The combination of the optical driven with spin-orbit coupling (SOC) could also selectively gap the Dirac cone, and induce one Dirac-cone state in silicone [27]. By controlling the status of each band valley, the information could be encoded into the pseudospin as the valleytronic physics proposes.

The recently proposed antiferromagnetic topological insulator in two dimensional square lattice has gapless helical edge states, because of the protection by the nonsymmorphic symmetry. The materials realization is found in intrinsic antiferromagnetic XMnY (X=Sr and Ba, Y=Sn and Pb) quintuple layers [28]. Because of the weak interlayer van der Waals interaction, the two dimensional system could be obtained by exfoliation. The systems could be theoretically described by the four band model in the checkerboard square lattice with intrinsic and Rashba spin-orbit coupling (SOC).

In this article, we studied the Floquet state of the antiferromagnetic XMnY. We found that the normally incidence circular polarized optical field could induce phase transition into the quantum Anomalous Hall (QAH) phase with varying winding number; the linear polarized optical field could induce phase transition to semi-metal (SM) phase, which has two Dirac cones at the Y–M line. At the phase boundary, the bulk gap close at the high symmetric points, such as Γ, X, Y, or M. Entering the SM phase regime, the gap closing point is not gapped, but split into two Dirac cones. Because the phase regime of TI and SM overlap, part of the phase boundary of the TI phase is within the phase regime of the SM phase, where the bulk state have three Dirac cones. Application of the triple Dirac-cone state for the valleytronic physics could enhance performance, because the system with three valleys could encode ternary information [29].
II. MODEL

The lattice structure is plotted in Fig. 1(a). The two sublattices are arranged in the checkerboard square lattice. In each lattice site, one atomic orbit with both spin are included into the tight binding model. The Hamiltonian model is given as

\[
H = t_1 \sum_{(\mathbf{r}_A, \mathbf{r}_B)} c_{\mathbf{r}_A, s}^\dagger c_{\mathbf{r}_B, s} + t_2 \sum_{(\mathbf{r}_A, \mathbf{r}_B) \neq (\mathbf{r}_A, \mathbf{r}_B)} c_{\mathbf{r}_A, s}^\dagger c_{\mathbf{r}_B, s} + t_i \sum_{\mathbf{r}_r, \mathbf{s}, n} \tau \sigma^z_{\mathbf{r}_r, \mathbf{s}} c_{\mathbf{r}_r, \mathbf{s}}^\dagger c_{\mathbf{r}_r + n, \mathbf{s}}^\dagger + t_R \sum_{\mathbf{r}_r, \mathbf{s}, s'} n = \pm 1 \tau \sigma^y_{\mathbf{r}_r, \mathbf{s}} c_{\mathbf{r}_r, \mathbf{s}}^\dagger c_{\mathbf{r}_r + \mathbf{n}_a \mathbf{\hat{e}}, \mathbf{s}}^\dagger + t_R \sum_{\mathbf{r}_r, \mathbf{s}, s'} n = \pm 1 \tau \sigma^y_{\mathbf{r}_r, \mathbf{s}} c_{\mathbf{r}_r, \mathbf{s}}^\dagger c_{\mathbf{r}_r + \mathbf{n}_a \mathbf{\hat{e}}, \mathbf{s}}^\dagger + \lambda_{\text{AF}} \sum_{\mathbf{r}_r, \mathbf{s}, s'} \tau \sigma^z_{\mathbf{r}_r, \mathbf{s}} c_{\mathbf{r}_r, \mathbf{s}}^\dagger c_{\mathbf{r}_r, \mathbf{s'}}^\dagger \quad (1)
\]

where \( \tau = \pm 1 \) and \( s = \pm 1 \) represent A(B) sublattice and spin up(down), \( \sigma^{x,y,z} \) are the three Pauli matrix of spin, \( a \) is the lattice constant, and \( c_{\mathbf{r}}^{(f)}\) is the annihilation (creation) operator of the orbit at site \( \mathbf{r} \) with spin \( s \). The first two summations cover \( (\mathbf{r}_A, \mathbf{r}_B) \), which include the nearest neighbor sites between A and B sublattice marked as red dashed (blue solid) lines in Fig. 1(a). In our numerical simulation, \( t_1 \) and \( t_2 \) are assumed to be 0.7 eV and 0.4 eV, respectively; \( t_i \) and \( t_R \) are the strength of intrinsic and Rashba SOC, which are assumed to be 0.7 eV and 1 eV. The strength of the antiferromagnetic exchange field \( \lambda_{\text{AF}} \) is a varying parameter in the phase diagram. With \( \lambda_{\text{AF}} < 0 \) (\( \lambda_{\text{AF}} > 0 \)), the system is in the antiferromagnetic topological insulator (topologically trivial band insulator) phase.

In the present of the optical field, the quantum states under periodic drive are described by the Floquet theory. The hopping parameters contain a time-dependent Peierls phases due to the irradiation. We consider normally incident optical field with frequency being \( \Omega \). With circular polarization, the vector potential of the optical field is \( \mathbf{A}(t) = \mathbf{A}(t) + \eta \mathbf{\hat{y}} \sin(\Omega t) \), with \( \eta = \pm 1 \) for left or right circular polarization. With linear polarization along \( \mathbf{\hat{y}} \) direction, the vector potential of the optical field is \( \mathbf{A}(t) = \eta \mathbf{\hat{y}} \cos(\Omega t) \). Since the linearly \( \mathbf{\hat{x}} \) polarized optical field does not induce significant topological phase transition, the article only present the result with linearly \( \mathbf{\hat{y}} \) polarized optical field.

In general, the time dependent factor of a hopping parameter between lattice sites at \( \mathbf{r}_1 \) and \( \mathbf{r}_2 \) is \( \gamma (t) = e^{i \Omega (\mathbf{r}_1, \mathbf{r}_2)/\hbar} \), with \( \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j \) and \( \mathbf{\Phi} = \pi \hbar /e \) being the magnetic flux quantum. For example, for the circular polarization, the hopping parameters along \( \mathbf{\hat{x}} \) direction (\( t_i \) and \( t_R \) along \( \mathbf{\hat{x}} \) direction) have a time dependent factor given as \( \gamma (t) = e^{i \Omega \mathbf{r} /\hbar} e^{i \eta \pi /2} \). We denote the dimensionless parameter \( A_0 = 2 \pi a A_0 /\hbar \) to represent the amplitude of the optical field. The time dependent factor is expanded as \( e^{i A_0 \sin(\Omega t)} = \sum_{m=-\infty}^{\infty} i^m J_m (A_0) e^{-i m \pi /2} e^{i m \Omega t} \). For the hopping parameters along \( \mathbf{\hat{x}} + \mathbf{\hat{y}} \) direction (\( t_i \) and \( t_2 \)), the time dependent factor could be regrouped as \( e^{i A_0 \sin(\Omega t)} = \sum_{m=-\infty}^{\infty} \sum_{m'=0}^{\infty} i^m J_m (A_0) J_{m'} (A_0) e^{-i m \pi /2} e^{i m \Omega t} \).

As a result, the time dependent Hamiltonian could be expanded as \( \sum_{m=-\infty}^{\infty} H_m e^{i m \Omega t} \). The eigenstate of the time dependent Hamiltonian, which is denoted as Floquet states, are also expressed as \( |\Psi_\alpha (t)\rangle = e^{i \epsilon_\alpha t /h} \sum_m |u_m^\alpha\rangle e^{i m \Omega t} \), with \( \epsilon_\alpha \) being quasi-energy level of the \( \alpha \)-th eigenstate and \( |u_m^\alpha\rangle \) the corresponding eigenstate in the \( m \)-th Floquet replica. The Floquet state satisfies the eigenvalue problem, \( H_F |\Psi_\alpha (t)\rangle = \epsilon_\alpha |\Psi_\alpha (t)\rangle \), with \( H_F = H(t) - i \hbar \partial_t \) being the Floquet Hamiltonian. The Floquet states and the Floquet Hamiltonian can be represented by time-independent state \( |u_m^n\rangle \), \( m \in \mathbb{N} \) and time-independent operator \( \mathcal{H} \) in the Samb space, respectively. The Samb space is the direct product space of the Hilbert space of spatial wave functions and Fourier space of periodic functions in time. The diagonal and nondiagonal blocks of \( \mathcal{H} \) are given as \( \mathcal{H}^{(m_1, m_2)} = H_0 + m \hbar \mathbf{\Omega} \) and \( \mathcal{H}^{(m_1, m_2)} = H_{m_1, m_2} \), respectively. In the numerical calculation, the Floquet index is truncated at a maximum value as \( -m_{\text{max}} \leq m \leq m_{\text{max}} \). Thus, \( \mathcal{H} \) is a \((2m_{\text{max}} + 1) \times (2m_{\text{max}} + 1) \) block matrix, with each block having the same size as \( \mathcal{H} \). The eigen energies and eigen states are obtained by diagonalization of \( \mathcal{H} \). In this article, we consider the non-resonant condition with \( \hbar \mathbf{\Omega} = 6 \) eV, which is larger than the bandwidth of the unperturbed systems, so that \( m_{\text{max}} = 1 \) is sufficient.
III. RESULT AND DISCUSSION

By solving the Floquet Hamiltonian with Bloch periodic boundary condition of bulk or nanoribbon, the band structure can be calculated. The Berry curvature of the \(\alpha\) bulk band at a fixed time is given as

\[
B_{\alpha}(k) = -\sum_{\alpha' \neq \alpha} \frac{2Im(\langle \Psi_{\alpha}(t)|v_x|\Psi_{\alpha'}(t)\rangle\langle \Psi_{\alpha'}(t)|v_y|\Psi_{\alpha}(t)\rangle)}{\left(\varepsilon_{\alpha} - \varepsilon_{\alpha'}\right)^2}
\]

(2)

where \(v_{xy}(y) = \nabla_{k_{xy}} H_F(k)\) is the velocity operator. For bulk, integration of the Berry curvature across the first Brillouin zone gives the Chern number of each band [21, 27, 31]. Summation of the Chern number of all valence band gives the winding number of the insulator. For the insulating state that the winding number is nonzero, the system is in the QAH phase. With a zero winding number, the insulating state is either trivial band insulator (BI) or TI.

For the gapless SM phase, the winding number is zero. Because the mirror symmetric along the \(\hat{y}\) direction is broken by the linearly \(\hat{y}\) polarized optical field, the Berry curvature is not symmetric about the \(\hat{x}\) axis. As a result, the Berry curvature dipole along \(\hat{y}\) direction is sizable, which induce nonlinear Hall effect [32]. The Berry curvature dipole along the \(\hat{y}\) direction is defined as

\[
D_y = \sum_{\alpha} \int_{BZ} dk \frac{\partial B_{\alpha}(k)}{\partial k_y} f_0[E(k)]
\]

(3)

where \(f_0\) is the Fermi-Dirac distribution. Room temperature is assumed in our numerical calculation. Because the Berry curvature dipole depend on the Fermi energy, we focus on the SM phase with pair of two Dirac cones, whose Fermi energy could be easily tuned.

The nanoribbon have two types of configuration, as shown in Fig. 1(b) and (c), which is designated as parallel and diagonal nanoribbon, respectively. The edge of the parallel (diagonal) nanoribbon preserves (breaks) the nonsymmorphic symmetry of the bulk, so that the helical edge state of the TI phase present (absent). For the QAH phase, the chiral edge state exist for both type of nanoribbon, but with different properties.

The numerical result of the driven systems by circular and linearly \(\hat{y}\) polarized optical field is given in the following.

A. Circular Polarization

In the presence of the optical field with circular polarization, the phase diagram is given in Fig. 2 which contains QAH phases with varying winding numbers. Before reaching the QAH phase, the system is in the BI or the TI phase, if the antiferromagnetic exchange field \(\lambda_{AF}\) is positive or negative, respectively. As \(A_0\) increases, the bulk gap close and reopen at \(X\) point of the first Brillouin zone, leading to a topological phase transition to the QAH phase with winding number being one. With \(A_0 = 0.58\) and \(\lambda_{AF} = 0\), the winding number is one; the band structures of the parallel and diagonal nanoribbon are plotted in Fig. 3(a) and (b), respectively. In parallel nanoribbon, there are one pair of gapless chiral edge states, as shown in Fig. 3(a). The forward and backward moving edge states are localized at the left and right edges, where the forward (backward) direction is defined as \(+\hat{x} (-\hat{x})\) direction, and the left (right) edge is defined at the \(+\hat{y} (-\hat{y})\) side of the nanoribbon. In diagonal nanoribbon, the dispersion of each chiral edge state connect the conduction and valence bands with an extra round trip around the first Brillouin zone, as shown in Fig. 3(b). For example, the chiral edge state localized at the right edge (the red one) starts at the bottom of the conduction band and extends to the forward boundary of the first Brillouin zone; as the state periodically circles back to the backward boundary of the first Brillouin zone, it extends to the forward boundary of the first Brillouin zone within the bulk gap again and circle back to the backward boundary of the first Brillouin zone for the second time; and then the state merges into the top of the valence band. As \(A_0\) further increases, the bulk state is transited into the QAH phase with larger winding number, such as two, three or four. The number of pairs of chiral edge states is the same as the corresponding winding number, as shown in Fig. 3(c-f). For the phases with winding number larger than one, the edge states of the diagonal nanoribbon does not circle the first Brillouin zone as they connect the conduction and valence band.

B. Linear Polarization along \(\hat{y}\)

In the presence of the optical field with linear polarization along \(\hat{y}\) direction, the phase diagram is shown in
FIG. 3: The band structure of the parallel and diagonal nanoribbons driven by the optical field with circular polarization in (a,c,e) and (b,d,f), respectively. The number of unit cells along the width direction is 40. The system parameters are $A_0 = 0.58$, $\lambda_{AF} = 0$ in (a,b) [in the $C_1$ phase regime in Fig. 2], $A_0 = 1.11$, $\lambda_{AF} = 0$ in (c,d) [in the $C_c$ phase regime in Fig. 2], $A_0 = 1.48$, $\lambda_{AF} = -0.4$ in (e,f) [in the $C_3$ phase regime in Fig. 2]. The edge states that are localized at the left and right edges are marked by blue (solid) and red (empty) dots, respectively.

FIG. 4: The phase diagram of the systems that are driven by the optical field with linear polarization along $\hat{y}$. For the convenience of discussion, six typical SM states are marked in Fig. 4 and designated as SM state-(i-vi). As $A_0$ increases and reach the black solid line in Fig. 4 the gap closes at $Y$ point [the SM state-(i)]. At the gap closing point, the band dispersion is anisotropic: linear along the $Y - \Gamma$ direction, and quadratic along the $Y - M$ direction. As $A_0$ further increases, the gap closing point split into a pair of two Dirac cones, which move along $Y - M$ line in opposite directions. Thus, the regime to the right of the black solid line in Fig. 4 is SM phase with one pair of two Dirac cones at the $Y - M$ line. The bulk band structure of the SM state-(ii) is plotted in Fig. 5(a). The separation between the two Dirac cones is controlled by the amplitude of the optical field. On the other hand, the phase transition between TI and non-TI phases is induced by the gap closing at the $X$ point along the blue dashed line in Fig. 4. The phase regime below the blue dashed line is TI phase. The TI and SM phase regimes overlap, as shown by the TI/SM phase regime in Fig. 4. At the blue dashed line within the SM phase regime, the pair of two Dirac cones of the SM phase coexist with the second order degenerated Dirac cone at $X$ point, so that the state includes three Dirac cones. This state is designated as triple Dirac-cones state. The band structure of a typical triple Dirac-cones state, i.e. the SM state-(iv), is plotted in Fig. 5(b). The valleytronic based on the optically manipulated band structure with three Dirac cones could outperform the valleytronic based on graphene with two valleys.

The band structure of the first conduction bulk band...
of the SM phase has three saddle points (SPs): SP$_Y$ at the Y point, SP$_{Y+}$ (SP$_{Y-}$) at the $\Gamma - Y$ line with $k_x > 0$ ($k_x < 0$), which can be visualized in the contour plot in Fig. 5(c). The Berry curvature has two peaks at the $\Gamma - Y$ line between SP$_Y$ and SP$_{Y\pm}$, as shown in Fig. 5(c). The signs of the two peaks are opposite to each other. The first valence band has the same SPs and Berry curvature distribution. As a result, the partially filled conduction or valence band has sizable Berry curvature dipole. The Berry curvature dipole $D_y$ versus the Fermi energy $E_F$ of the SM state-(i-iv) are plotted in Fig. 6. For the SM states-(ii), the Berry curvature is small around the pair of two Dirac cones; the peak of the Berry curvature is narrow, as shown in Fig. 5(c). As a result, $D_y$ is nearly zero when $E_F$ is near to 0 eV, and has large peaks when $|E_F|$ is near to 1 eV, as shown by the blue dashed line in Fig. 6. Decreasing $A_0$ pull the distance between the pair of two Dirac cones closer to each other. The peaks of the Berry curvature within the regions between SP$_Y$ and SP$_{Y\pm}$ become wider (narrower) along $\Gamma - Y$ ($\Gamma - X$) direction. Consequently, $D_y$ becomes sizable when $E_F$ is near to 0 eV, and has smaller peaks when $|E_F|$ is near to 1 eV. As $A_0$ reaches the phase boundary [the SM state-(i)], $D_y$ has nearly linear slope versus $E_F$, as shown by the black solid line in Fig. 6. Further decreasing $A_0$ opens finite gap, so that $D_y$ is zero with $E_F$ within the bulk gap. The SM state-(iii) and SM state-(iv) is at phase boundary of the TI phase with a Dirac cone at X point. Since the Berry curvature near to the Dirac cone at the X point is small, the $D_y$ of the SM state-(iii) and SM state-(iv) have similar behaviors as that of the SM state-(i) and SM state-(ii).

The SM state have flat edge states that exhibit the properties of chiral edge state. The band structure of the parallel nanoribbon of the SM state-(ii) have a pair of two Dirac cones of the bulk states, and two edge states that are nearly flat and connect the two Dirac cones, as shown in Fig. 7(a). Similar band structure are found for the diagonal nanoribbon, as shown in Fig. 7(b). The Dirac cones are gapped by finite size effect. The edge states connect the conduction band of one of the two Dirac cones and the valence band of the other Dirac cone. The edge states localized at the opposite side of the nanoribbon have opposite dispersion, so that the edge states behave as chiral edge states. The chiral behavior of the edge state is determined by the property of the bulk band. The spin texture, which is the vector field of the expectation of spin $(\langle \sigma^x \rangle, \langle \sigma^y \rangle, \langle \sigma^z \rangle)$ in the Brilouin zone, near to the pair of two Dirac cones is plotted in Fig. 5(d) for the SM state-(ii). The spin texture of the conduction band of the Dirac cone at $k_x < 0$ region has the same pattern as that of the valence band of the Dirac cone at $k_x > 0$ region, and vice versa. This phenomenon could be comprehended as the band inversion in the reciprocal space along $Y - M$ direction, instead of the band inversion in energy degree of freedom for TI. The band inversion in the reciprocal space induces the chiral behavior of the edge states.

Near to the triple Dirac-cone state [the SM state-(iv)], the bulk band gap at the X point and the topological feature can be controlled by changing $A_0$. With a smaller $A_0$ [the SM state-(v)], the topological gap is opened at the X point. Thus, the band structure of the parallel nanoribbon has helical edge states, which coexist with the flat bands connecting the pair of two Dirac cones, as shown in Fig. 7(c). With a larger $A_0$ [the SM state-(vi)],
the trivial gap is opened at the X point, so that the helical edge states is absent in the nanoribbon, as shown in Fig. 7(d). If \( A_0 \) is smaller than the critical value at the SM phase boundary, the pair of two Dirac cones are annihilated and gapped, while the helical edge states remain robust. As a result, the nanoribbon can be tuned into three different conductive status by changing \( A_0 \): both helical edge states and chiral edge states conducting, only helical edge states conducting, and only chiral edge states conducting. The system could be applied to construct ternary information systems, instead of binary systems.

### IV. CONCLUSION

In conclusion, the Floquet states of the two dimensional antiferromagnet in square lattice with spin-orbit coupling and nonsymmorphic symmetry could be QAH phase or SM phase, depending on the polarization and amplitude of the optical field. The winding number of the QAH phase could be switched among one to four, so that the number of pairs of the chiral edge states in the nanoribbon is controlled by the optical field. The bulk band structure of the SM phase have one pair of Dirac cones. The pair of Dirac cones coexist with another Dirac cone at the TI phase boundary, forming a triple Dirac-cones state. The Berry curvature dipole of the SM phase is sizable. In the nanoribbon of the SM, two nearly flat bands that behave as chiral edge states connect the pairs of two Dirac cones.

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