Searching for topological density wave insulators in multi-orbital square lattice systems

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We study topological properties of density wave states with broken translational symmetry in two-dimensional multi-orbital systems with a particular focus on \(t_{2g}\) orbitals in square lattice. Due to distinct symmetry properties of \(d\)-orbitals, a nodal charge or spin density wave state with Dirac points protected by lattice symmetries can be achieved. When an additional order parameter with opposite reflection symmetry is introduced to a nodal density wave state, the system can be fully gapped leading to a band insulator. Among those, topological density wave (TDW) insulators can be realized, when an effective staggered on-site potential generates a gap to a pair of Dirac points connected by the inversion symmetry which have the same topological winding numbers. We also present a mean-field phase diagram for various density wave states, and discuss experimental implications of our results.

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I. INTRODUCTION

Identifying topological insulators has been one of the most fascinating research fields in contemporary condensed matter physics.\(^1,2\) Topological insulators have a bulk gap like band insulators, but are distinguished by topologically protected conducting edge states preserving time-reversal invariance. In particular, two-dimensional topological insulators are known as quantum spin Hall insulators with finite counter-propagating edge modes which carry opposite spin quantum numbers result in quantum spin Hall insulators. It was shown that these modes are protected by time reversal symmetry even in the absence of spin rotational invariance.\(^3\) It was further pointed out that an effective spin-orbit coupling term can be generated by spontaneous spin rotational symmetry breaking in an extended Hubbard model on the honeycomb lattice.\(^4\) In these studies, the structure of the honeycomb lattice plays an important role, as the tight binding model on this lattice possesses two Dirac points at the Brillouin zone corners. Therefore in low energy description, various gapped insulating phases proximate to the Dirac semi-metal can be understood in terms of mass perturbations to gapless Dirac particles. For instance, the fictitious magnetic fluxes introduced by Haldane generate a mass term that has the opposite signs at the two Dirac points leading to an insulator with finite quantized Hall conductivity. The Dirac Hamiltonian approach further provides a framework to understand the time-reversal invariant \(Z_2\) topological insulators.\(^5\)

While systems on the honeycomb lattice such as graphene naturally support two-dimensional massless Dirac particles in the bare band structures, this is not the case in a simple square lattice system which is an effective model for abundant layered perovskite materials in nature. In this respect, it is interesting to note that the recent proposed nodal density wave state\(^6\) exhibits gapless Dirac particles via broken translational symmetry. This proposal was made in the context of iron pnictide systems, where \(d\)-orbitals of \(t_{2g}\) bands in an effectively two-dimensional square lattice give rise to several Fermi pockets with interesting topological properties. In this system, the spin density wave instability with the finite ordering wave vector \(Q = (\pi, 0)\) (or \((0, \pi)\)) leads to band touchings between the \(k\) states with the momentum difference of \(Q\). In general, the degeneracies at the band touching points disappear because of the finite overlap matrix between the degenerate states induced by the density wave order parameter. However, in multi-orbital systems, because of the distinct symmetry properties of orbitals, the degeneracies at some band touching points are protected leading to nodal density wave states, which is generally valid for any density wave orders.

In this work, we ask if topological insulators can be emerged by gapping nodal points turning the system from nodal density wave states to topological density wave (TDW) insulators. To find such a TDW insulator, we first investigate the properties of the nodal density wave states. We find that one general and important characteristic of the Dirac particles in nodal density wave states is that a pair of Dirac Hamiltonians connected by the inversion symmetry have the same topological winding numbers. Thus an effective staggered on-site potential generating a mass term, which has the same signs at the inversion symmetric nodal points, induces TDW insulators. This can be contrasted with the topological properties of the Dirac particles in the honeycomb lattice where the Dirac Hamiltonians at the two inversion symmetric nodal points have the opposite winding directions.\(^7\)
the mass term induced by, for example, a staggered sublattice chemical potential, which has the same signs at the two Dirac points would generate a topologically trivial band insulator as shown in graphene system.\textsuperscript{3,15}

The rest of the paper is organized as follows. In Sec. II, we first consider a simple two-band model Hamiltonian composed of $d_{xz}$ and $d_{yz}$ orbitals on the square lattice. After classifying all possible charge and spin density wave order parameters with the ordering wave vector $Q = (\pi, 0)$ based on their transformation properties under lattice symmetries, we establish general relations between the locations of Dirac nodes and order parameter symmetries in Sec. III. The fact that $d_{xz}$ and $d_{yz}$ orbitals have the opposite eigenvalues under reflection symmetries along high symmetry directions in the momentum space, plays the key role for the emergence of Dirac points. In addition to the Dirac points coming from the Brillouin zone folding, additional contributions from quadratic band degeneracy splitting are also discussed. In Sec. IV, topological properties of gapped density wave phases with two or parameters with the opposite reflection symmetries are studied. Fully-gapped insulating phases can be obtained by introducing two density wave order parameters which have the opposite eigenvalues under reflection symmetries. Among them, a certain combination turns the system to a TDW insulator. In Sec. V, the mean field phase diagram including the TDW phase is presented, which is obtained by solving an extended Hubbard model Hamiltonian with orbital degeneracy. Topological density wave states in three orbital systems are discussed in Sec. VI. Straightforward extension to three-orbital systems shows the general applicability of the idea we pursue in this work to obtain topological insulators in multi-orbital systems. Finally, we conclude in Sec. VII.

II. TWO BAND HAMILTONIAN AND SYMMETRIES OF ORDER-PARAMETERS

A. Tight-binding Hamiltonian

We consider a tight binding Hamiltonian on the square lattice with two orbital ($d_{xz}$, $d_{yz}$) degrees of freedom at each site. A generic Hamiltonian which contains all possible hopping processes allowed by lattice symmetries is given by

$$H_0 = \sum_{\mathbf{k}, \sigma} \psi_{\mathbf{k}, \sigma}^\dagger H(\mathbf{k}) \psi_{\mathbf{k}, \sigma},$$

(1)

where

$$H(\mathbf{k}) = (\varepsilon_{+}(\mathbf{k}) - \mu) 1 + \varepsilon_{-}(\mathbf{k}) \tau_3 + \varepsilon_{xy}(\mathbf{k}) \tau_1.$$  

(2)

Here a two-component field $\psi_{\mathbf{k}, \sigma}^\dagger = \begin{bmatrix} d_{xz, \sigma}(\mathbf{k})^\dagger \end{bmatrix}$ describes the creation of particles with $d_{xz}$ orbital flavors with spin $\sigma$, and the Pauli matrix $\tau$ connects these two orbital states. In the above,

$$\varepsilon_{+}(\mathbf{k}) = -(t_1 + t_2)(\cos k_x + \cos k_y) - 4t_3 \cos k_x \cos k_y,$$

$$\varepsilon_{-}(\mathbf{k}) = -(t_1 - t_2)(\cos k_x - \cos k_y),$$

$$\varepsilon_{xy}(\mathbf{k}) = -4t_4 \sin k_x \sin k_y.$$  

(3)

Diagonalization of $H(\mathbf{k})$ gives rise to the following two band dispersions,

$$E_{\pm}(\mathbf{k}) = \varepsilon_{+}(\mathbf{k}) - \mu \pm \sqrt{\varepsilon_{-}^2(\mathbf{k}) + \varepsilon_{xy}^2(\mathbf{k})}.$$  

(4)

In addition to time-reversal symmetry $T$, the Hamiltonian $H_0$ has the $C_4$ point group symmetry, which consists of the four-fold rotation $C_\pi$, the inversion $I$, and the two reflections $P_x$ and $P_y$ mapping $x$ to $-x$ and $y$ to $-y$, respectively. Each symmetry operation transforms a two-component field $\psi_\sigma(k_x, k_y)$ in the following way.

$$C_\pi : \psi_\sigma(k_x, k_y) \rightarrow i\tau_2 \psi_\sigma(-k_y, k_x),$$

$$P_x : \psi_\sigma(k_x, k_y) \rightarrow -\tau_3 \psi_\sigma(-k_x, k_y),$$

$$P_y : \psi_\sigma(k_x, k_y) \rightarrow \tau_3 \psi_\sigma(k_x, -k_y),$$

$$I : \psi_\sigma(k_x, k_y) \rightarrow -\tau_0 \psi_\sigma(-k_x, -k_y).$$  

(5)

If we choose the hopping parameters in such a way as $t_2$=1.0, $t_2$=1.3, $t_3 = t_4 = -0.85$, the $H_0$ works as an effective two-band Hamiltonian describing the Fe-pnictide systems.\textsuperscript{16} Given the hopping parameters above, the Fermi surface consists of two hole pockets and two electron pockets when the system is near half-filling.\textsuperscript{14,16} A pair of electron and hole pockets are connected by a nesting wave vector $Q = (\pi, 0)$ (or $(0, \pi)$), which drives various density wave instabilities.\textsuperscript{17} Here we choose $Q = (\pi, 0)$ and perform a detailed study about the band structures of density wave ground states considering all possible density wave order parameters.

B. Symmetry of order parameters

We consider various on-site density wave order parameters and investigate their symmetry properties. Since we have two orbitals per site, there are 4 different on-site charge density wave (CDW) states with the ordering wave vector $Q = (\pi, 0)$, which are given by

$$\hat{D}_a = \frac{1}{N} \sum_{\mathbf{k}} \sum_{a, b = 1}^{2} d_{a, \sigma}^\dagger(\mathbf{k}) [\tau_a]_{\sigma b} d_{b, \sigma}(\mathbf{k} + \mathbf{Q}),$$  

(6)

where $a, b$ are indices describing the $d_{xz}$ ($a=1$) or $d_{yz}$ ($a=2$) orbital states. $N$ counts the number of unit cells in the system. Similarly, we also define spin density wave (SDW) states choosing the spin ordering direction along the $z$-axis,
Table I: Symmetry of density wave order parameters. Here ‘+’ (‘-’) indicates ‘even’ (‘odd’) symmetry of the order parameters under the corresponding symmetry operation.

| $D_0$ | $D_1$ | $D_2$ | $D_3$ | $M_0$ | $M_1$ | $M_2$ | $M_3$ |
|-------|-------|-------|-------|-------|-------|-------|-------|
| +     | +     | -     | +     | +     | -     | +     | -     |
| -     | +     | -     | +     | +     | -     | +     | -     |
| $I$   | +     | +     | +     | +     | +     | +     | +     |
| $T$   | +     | +     | -     | -     | +     | +     | -     |

These symmetry properties of density wave order parameters strongly constrain the location of Dirac nodes generated by the Brillouin zone folding and the winding numbers around Dirac nodes in the momentum space, which are discussed in detail in the following section.

### III. NODAL DENSITY WAVE PHASES

One intriguing property of the $\mathbf{Q} = (\pi, 0)$ density wave ground states is that a large number of Dirac nodes emerge in the band structure. The numbers and locations of the nodal points depend on band dispersions and the symmetries of the order parameters.

There are two different sources generating nodal points in general. One way is via introducing a density wave order parameter carrying a finite momentum. This induces a Brillouin zone folding which generates several band touching points. In most cases, the degeneracy at the band touching point is lifted because the density wave order parameter induces a finite overlap between the pair of states touching at a point. Henceforth a band gap opens up. However, when the band touching occurs at a high symmetry point in the Brillouin zone, the overlap matrix vanishes due to the lattice symmetries, generating symmetry protected nodal points.

The second group of nodal points come from the splitting of quadratic band touching points, which exist in the bare band-structure. Because of the underlying four-fold rotational symmetry, the original hopping Hamiltonian in Eq. (1) supports quadratic band crossing points. The introduction of the density wave order parameter carrying a finite momentum splits a quadratic band touching point into two Dirac points along high symmetry directions in the momentum space. In the following, we discuss in detail the relation between the order parameter symmetry and the locations of Dirac points derived from these two different sources in separate subsections.

#### A. Dirac nodes generated by Brillouin zone folding

We first focus on the generation of Dirac nodes along the $k_y$-axis. In Fig. 2(a) (Fig. 2(b)), we plot the energy dispersion of the two bands given in Eq. (4) along the $k_x = 0$ ($k_x = \pi$) direction. Since the $\varepsilon_{xy}$ term in Eq. (3), which describes the hybridization between $d_{xz}$ and $d_{yz}$ orbitals, vanishes along the $k_x = 0$ axis, the upper and lower bands in Fig. 2(a) are...
just $d_{yz}$ and $d_{xz}$ bands, respectively. For $k_x = 0$, $H(k)$ is invariant under the $P_x$ reflection symmetry which transforms a momentum $k_x$ to $-k_x$. Therefore each band is an eigenstate of $P_x$ with eigenvalues of $\pm 1$. This is consistent with the fact that $d_{yz}$ ($d_{xz}$) orbital is odd (even) under $P_x$. Similar analysis can also be applied to the two bands dispersing along the $k_x = \pi$ direction. Since $H(k)$ has $P_x$ symmetry along $k_x = \pi$, the two bands also have definite $P_x$ eigenvalues. In Fig. 2 the $P_x$ even (odd) bands are represented by blue dotted (red solid) lines.

Once we introduce a density wave order parameter with the ordering wave vector $Q = (\pi, 0)$, the unit cell doubles along the $x$-direction, which leads to the Brillouin zone folding in the momentum space. Thus within the reduced Brillouin zone, we have four bands dispersing along the $k_y$-axis. Note that the zone folding generates 8 band touching points, which are indicated by circles in Fig. 2(c). Here the band touching point between two bands with the same (opposite) $P_x$ eigenvalues is encircled by a solid (dotted) circle.

The degeneracy between two states, $|\psi_1(k)\rangle$ and $|\psi_2(k + Q)\rangle$, touching at the momentum $k$ after the Brillouin zone folding, is lifted when the matrix element of the density wave order parameter $D_1$ between these two states is finite, that is, $\langle \psi_1(k)|D_1|\psi_2(k + Q)\rangle \neq 0$. Therefore if the order parameter $D_1$ (or $M_1$) is $P_x$ even, the degeneracy is lifted when the two degenerate bands have the same $P_x$ eigenvalues. Hence, the nodal point remains gapless if the two degenerate bands have the opposite $P_x$ eigenvalues.

On the other hand, if the density wave order parameter $D_1$ (or $M_1$) is $P_x$ odd, the full Hamiltonian is not invariant under $P_x$ anymore. However, even in this case $\langle \psi_{1,s_1}(k)|D_1|\psi_{2,s_2}(k + Q)\rangle = 0$ in the weak coupling limit, if $s_1 = s_2$ or if $s$ refers to $P_x$ eigenvalues. Namely, the matrix element of $D_1$, which is odd under $P_x$, vanishes when the two degenerate eigenstates have the same $P_x$ eigenvalues.

To understand this point clearly, let us define the eigenvector $|\phi^{(0)}_{n,s}(k)\rangle$ of the hopping Hamiltonian $H_0$ with the even ($s = +$) or odd ($s = -$) $P_x$ eigenvalues. Here $n$ is a band index. Now we turn on a small density wave order parameter $D_1$ which is odd under $P_x$. Since $P_x$ eigenvalue is not a good quantum number, $|\phi^{(0)}_{n,s}(k)\rangle$ can be contaminated by the states with the opposite $P_x$ eigenvalue $|\phi^{(0)}_{n,s}(k+Q)\rangle$, leading to

$$|\phi^{(0)}_{n,s}(k)\rangle \xrightarrow{D_1} |\phi_{n,s}(k)\rangle + |\phi_{n,s}(k+Q)\rangle,$$

where $|\phi_{n,s}(k)\rangle = \sum_n c_n|\phi^{(0)}_{n,s}(k)\rangle$ is a linear combination of the states with the $P_x$ eigenvalue of $s$, while $|\phi_{n,s}(k+Q)\rangle = \sum_n c_n|\phi^{(0)}_{n,s}(k+Q)\rangle$ is a linear combination of the states with the opposite $P_x$ eigenvalue of $s$. Notice that $|\phi_{n,s}(k)\rangle$ and $|\phi_{n,s}(k+Q)\rangle$ have a momentum difference given by the ordering wave vector $Q$ carried by the density wave order parameter $D_1$. Because of the fact that the two components of the wave function with the opposite $P_x$ eigenvalues have the momentum difference given by $Q$, it is straightforward to show that $\langle \psi_{1,s_1}(k)|D_1|\psi_{2,s_2}(k + Q)\rangle = 0$ if $s_1 = s_2$.

Therefore the nodal point remains gapless if the order parameter $D_1$ is $P_x$ even ($P_x$ odd) while the two generated bands have the opposite (same) $P_x$ eigenvalues. It means that 4 nodal points among the 8 band touching points remain gapless.

FIG. 2: (Color online) (a) Band dispersion along $k_x = 0$ for the hopping Hamiltonian in Eq. [1]. Here we use a red solid (blue dotted) line to indicate a band which is odd (even) under the $P_x$ reflection symmetry. (b) Band dispersion along the $k_x = \pi$ direction. (c) Band structure along $k_x = 0$ after the unit cell doubling due to the $Q = (\pi, 0)$ density wave ordering. Four bands in (a) and (b) meet and disperse together along $k_x = 0$ after the Brillouin zone folding. Note that the zone folding generates 8 band touching points. Black solid (dotted) circles indicate the band touching points between two bands having the same (opposite) $P_x$ eigenvalues.

FIG. 3: (Color online) The band structures of the $Q = (\pi, 0)$ density wave ground states along the $k_y$-axis. (a) For $P_x$ even density wave states. (b) For $P_x$ odd density wave states.
axes also show the opposite behaviors. In Fig. 4, we plot the dispersion of the two bands in Fig. 4(a) and (b). In Fig. 4(c), we plot the bandstructure of the bands in Fig. 4(a) and (b) meet and disperse together along the $k_y$-axis. In this case we have the following low energy effective Hamiltonian, 

$$H_{\text{eff}} = \int d^2k \psi^\dagger(k) H_{\text{quad}}(k) \psi(k),$$

where the $H_{\text{quad}}(k)$ is a Bloch wave function corresponding to one of the bands involved in the band touching and $C$ is a closed loop in the momentum space encircling the band crossing point. A quadratic band crossing point contributes $N_W = \pm 2$, which is twice larger than the winding number around a Dirac point.

Adding a generic perturbation given by $V = \sum_{i=1}^3 m_i \hat{\tau}_i$, the degeneracy at the quadratic band crossing point can be lifted. $m_2$ term breaks time-reversal symmetry and the degeneracy is lifted by opening a gap. On the other hand, $m_1$ and $m_3$ terms that break 4-fold rotational symmetry, split the quadratic band touching point into two Dirac points.

Now we consider the effect of the $Q = (\pi, 0)$ density wave orderings on the degeneracy lifting at quadratic band crossing points. Since the density wave order parameters carry the momentum $Q = (\pi, 0)$, they cannot couple to the degenerate states at $k = (0, 0)$ or $k = (\pi, \pi)$ at first order. The lowest order contribution to degeneracy lifting at quadratic band touching points starts from the second order processes. We first consider charge density wave order parameters given by,

$$H_{\text{CTDW}} = \sum_{k,\sigma} \psi_k^{\dagger,\sigma} \hat{D} \psi_k + Q_{\sigma},$$

where $\hat{D} = \sum_{i=0}^3 D_i \hat{\tau}_i$. Treating the above $H_{\text{CTDW}}$ as a perturbation, the standard second order perturbation theory gives rise to the following effective Hamiltonian near the quadratic band touching point at $k = (0, 0)$,

$$H_{\text{eff}}^{\text{quad}} = H_{\text{quad}}(k) + H_{\text{mass}},$$

$$= H_{\text{quad}}(k) + \sum_{i=0}^3 m_i(\hat{\tau}_i),$$

B. Dirac nodes from quadratic band crossing

The band structure of the two-band hopping Hamiltonian $H_0$ in Eq. (1) supports two quadratic band crossing points at $k = (0, 0)$ and $k = (\pi, \pi)$. Splitting of these quadratic band crossing points generates additional Dirac points, which contribute additional Chern numbers for various insulating phases.

Expanding the Hamiltonian $H(k)$ in Eq. (2) near $k = (0, 0)$, we obtain the following low energy effective Hamiltonian,
FIG. 5: (Color online) Distribution of Dirac points for the $D_3$ (or $M_3$) density wave state. (a) Four bands within the reduced Brillouin zone. The energy eigenvalue $E_i(k)$ for a band $i$ satisfies $E_1(k) \geq E_2(k) \geq E_3(k) \geq E_4(k)$. (b) Dirac points between the band 1 and 2, (c) between band 2 and 3, (d) between band 3 and 4. Blue (Red) dots indicates Dirac points coming from the Brillouin zone folding (splitting quadratic band touching points).

where $\lambda = -1/[8(t_1 + 2t_2)(t_2 + 2t_3)]$. Note that as long as only one of the order parameters has finite magnitude while all the other order parameters are zero, $m_1^{(1)} = m_1^{(2)} = 0$. In other words, if $D_n \neq 0$ for a given $n$ while all the other $D_{i \neq n} = 0$, the quadratic band crossing point always splits into two Dirac points along the main axes.

Combining the contributions both from the Brillouin zone folding and from the splitting of quadratic band crossing points, we show the distribution of Dirac points for a $D_3$ (or $M_3$) density wave ground state in Fig. 5. There are four bands within the reduced Brillouin zone as shown in Fig. 5a). We assign a band index $i$ such that the energy eigenvalue $E_i(k)$ of the band $i$ satisfies $E_1(k) \geq E_2(k) \geq E_3(k) \geq E_4(k)$.

The location of Dirac points between the upper two bands (band 1 and 2) are indicated in Fig. 5(b). Similarly, the Dirac points between the middle (bottom) two bands are described in Fig. 5(c) (Fig. 5(d)). Notice that there are many Dirac touching points between the bands. Blue dots indicate the nodal points coming from the Brillouin zone folding induced by the $Q = (\pi, 0)$ density wave states. On the other hand, red dots result from the splitting of quadratic band touching points. Two quadratic band touching points generate four Dirac points lying on the $y$-axis. With the understanding of the origin and locations of Dirac points, below we discuss how to achieve TDW insulators.

IV. TOPOLOGICAL PROPERTIES OF THE GAPPED DENSITY WAVE PHASES

A single density wave order parameter induces a metallic phase with many Dirac points. The locations of Dirac points are determined by the transformation properties of the order parameters under the reflection symmetries $P_x$ and $P_y$. Therefore to get an insulating phase, two coexisting density wave states, in which one is even and the other is odd under the $P_x$ and $P_y$ symmetries, are required. In addition, according to the order parameter symmetries summarized in Table I if time-reversal invariance is imposed, there are only four different ways of choosing a pair of density wave order parameters, which give rise to a gapped phase. The four pairs of time reversal invariant density wave order parameters with the opposite transformation properties under the reflections $P_x$ and $P_y$, are given by $(D_3, D_1), (D_3, M_2), (D_0, D_1)$, and $(D_0, M_2)$.

Since the $z$ component of the spin, $S_z$, is conserved, the Chern number $N_{C,\sigma}^{(n)}$ is well defined for each band in a fully gapped phase. Here $N_{C,\sigma}^{(n)}$ is the Chern number of the $n$th spin-up (spin-down) band. For every pair of the density wave order parameters generating a fully gapped phase, the four bands within the reduced Brillouin zone are well-separated from each other with a finite gap between any pairs of the bands. Each band is distinguished by the index $n$ ranging from 1 to 4 as the energy decreases. The Chern number $N_{C,\sigma}^{(n)}$ of the $n$th band with the spin $\sigma$ is defined as,

$$N_{C,\sigma}^{(n)} = \frac{1}{2\pi} \int_{RBZ} d^2k F(\sigma)^{(n)}(k),$$

where the momentum space Berry curvature $F(\sigma)^{(n)}(k)$ for the $n$th band with the spin $\sigma$ is defined as $F(\sigma)^{(n)}(k) = \partial_{k_y} A_{\mu,\sigma}^{(n)}(k) - \partial_{k_x} A_{\mu,\sigma}^{(n)}(k)$ in which the Berry potential $A_{\mu,\sigma}^{(n)}(k)$ is given by $A_{\mu,\sigma}^{(n)}(k) = -i \langle \Phi(\sigma)^{(n)}(k) | \partial_{k_{\mu,\sigma}} | \Phi(\sigma)^{(n)}(k) \rangle$. Here the Bloch wave function $| \Phi(\sigma)^{(n)}(k) \rangle$ is defined within the reduced Brillouin zone (RBZ).

Explicit computation of the Chern numbers using Eq. (14) shows that every band of the insulating density wave phase with finite $D_3$ and $M_2$, has a non-zero Chern number as shown in Table II. On the other hand, every band has zero Chern number for the other three gapped phases defined with a pair of non-zero order parameters given by $(D_3, D_1), (D_0, D_1)$, and $(D_0, M_2)$. 
TABLE II: The Chern number of each band for the gapped density wave ground state with finite $D_3$ and $M_2$.

| Band  | $N_{C,1}$ | $N_{C,2}$ |
|-------|-----------|-----------|
| 1     | 1         | -1        |
| 2     | -3        | 3         |
| 3     | 3         | -3        |
| 4     | -1        | 1         |

FIG. 6: (Color online) (a) Band structure of the $D_3$ nodal density wave state along the $k_y$ axis. (b) Band structure of the gapped density wave phase with finite $D_3$ and $M_2$.

A. Topological properties of the topological density wave ground state with finite $D_3$ and $M_2$

Nontrivial topological properties of the fully gapped density wave phase with nonzero $D_3$ and $M_2$ can be understood in the following way. We first consider the charge density wave state with the finite $D_3$ order parameter. The $D_3$ density wave phase supports many Dirac points whose distribution is described in Fig. 5. Now we turn on a small $M_2$ which induces gap opening at each nodal point, leading to the fully gapped insulating phase, which is described in Fig. 3. The degeneracy lifting at each nodal point can be understood as a result of the mass perturbation, induced by the finite $M_2$, to the gapless Dirac particles. The nonzero Chern number of each band is obtained by adding up the Chern number contributions of the massive Dirac particles derived from the corresponding band.

We first focus on the two Dirac nodes lying along the $k_y$ axis between the band 3 and 4 shown in Fig. 5(d). The effective Dirac Hamiltonian can be obtained by linearizing the Hamiltonian near the two nodal points sitting at the momentum $\mathbf{k}_\pm=\mathbf{k}_+$. To simplify the computational procedures, the hopping parameters $t_i$ are slightly shifted from the initial values given in Sec. II(A) to $t_1=−t_2=t_3=t_4=-1.0$. This small parameter change does not affect the topological properties of the gapped phase but shifts the nodal points to $\mathbf{k}_\pm=(0, \pm \pi/3)$ making analytical analysis simpler. The effective Hamiltonian describing the low energy fermions near these two nodal points is given by

$$H_{\text{eff}}^{\text{Dirac}} = \sum_{\mu=\pm} \int d^2q \Psi_{\mu,\sigma}^\dagger (\mathbf{q}) H_{\mu,\sigma}^{\text{Dirac}} (\mathbf{q}) \Psi_{\mu,\sigma} (\mathbf{q}),$$

(15)

where

$$H_{\mu,\sigma}^{\text{Dirac}} (\mathbf{q}) = -\mu \{ (2 + \frac{8}{\sqrt{4+D_3^2}}) q_y \hat{\tau}_3 + \frac{4|D_3|}{\sqrt{4+D_3^2}} q_x \hat{\tau}_1 \}.$$

(16)

Here the momentum $\mathbf{q}$ of the Hamiltonian $H_{\mu,\sigma}^{\text{Dirac}} (\mathbf{q})$ is measured with respect to the degeneracy point at $\mathbf{k}_\mu = \mathbf{k}_\mu (\mu = +, -)$. The two-component fermion field $\Psi_{\mu,\sigma} (\mathbf{q})$ is given by

$$\Psi_{\mu,\sigma} (\mathbf{q}) = \left( \begin{array}{c} \alpha_1 d_{y,z,\sigma} (\mathbf{k}_\mu + \mathbf{q}) + \alpha_2 d_{y,z,\sigma} (\mathbf{k}_\mu + \mathbf{Q} + \mathbf{q}) \\ \beta_1 d_{x,z,\sigma} (\mathbf{k}_\mu + \mathbf{q}) + \beta_2 d_{x,z,\sigma} (\mathbf{k}_\mu + \mathbf{Q} + \mathbf{q}) \end{array} \right),$$

(17)

where the constant coefficients $\alpha_i$ and $\beta_i$ satisfy $\alpha_1^2 + \alpha_2^2 = \beta_1^2 + \beta_2^2 = 1$. Explicitly, $\alpha_i$ and $\beta_i$ ($i=1,2$) are given by

$$\alpha_1 = (2 + \sqrt{4+D_3^2})/\sqrt{8+2D_3^2+4\sqrt{4+D_3^2}},$$

$$\alpha_2 = D_3/\sqrt{8+2D_3^2+4\sqrt{4+D_3^2}},$$

$$\beta_1 = (2 - \sqrt{4+D_3^2})/\sqrt{8+2D_3^2-4\sqrt{4+D_3^2}},$$

$$\beta_2 = D_3/\sqrt{8+2D_3^2-4\sqrt{4+D_3^2}}.$$

Notice that the first (second) component of $\Psi_{\mu,\sigma} (\mathbf{q})$ is derived entirely from the $d_{y,z}$ ($d_{x,z}$) orbital.

Now we include the $M_2$ spin density wave order parameter which generates a mass term in the low energy limit given by

$$H_{M_2}^{\text{mass}} = \sum_{\mu=\pm} \int d^2q \Psi_{\mu,\sigma}^\dagger (\mathbf{q}) \{ -\frac{2|D_3|M_2\sigma}{D_3\sqrt{4+D_3^2}} \hat{\tau}_2 \} \Psi_{\mu,\sigma} (\mathbf{q}).$$

(18)

For the given spin $\sigma$, the mass term has the same magnitude and sign at the two Dirac points. At each Dirac point, this mass term opens a gap and contributes to the Chern number $N_{C,\sigma} = \pm M_2\sigma/2|M_2|$ for the upper band (band 3) and $N_{C,\sigma} = -M_2\sigma/2|M_2|$ for the lower band (band 4). Adding the Chern number contributions from the two Dirac points, the total Chern number of the band 4 with the spin $\sigma$ is given by $N_{C,\sigma}^{(4)} = -\text{sgn}(M_2)\sigma$, which is consistent with the result obtained from the integration of the Berry curvature over the reduced Brillouin zone using Eq. (13). (See Table II.) In the case of the band 3, the Chern number is determined after including the additional contributions from the nodal points between the band 2 and band 3.

Similarly, the trivial topological property of the gapped phase with finite $D_3$ and $D_1$ can also be understood by applying the same analysis. For the $D_3$ nodal density wave state, the small $D_1$ charge density wave order parameter generates mass perturbations to Dirac particles, which can be described by the following Hamiltonian,

$$H_{D_1}^{\text{mass}} = \sum_{\mu=\pm} \int d^2q \Psi_{\mu,\sigma}^\dagger (\mathbf{q}) \{ \frac{2|D_3|D_1}{D_3\sqrt{4+D_3^2}} \hat{\tau}_1 \} \Psi_{\mu,\sigma} (\mathbf{q}).$$

(19)
Notice that this term just induces the shifting of the nodal points away from the \( k_y \)-axis. Once a Dirac point moves away from the reflection symmetry axis, the degeneracy at the band touching point is no longer protected by the symmetry and a gap opens, because the density wave order parameters support finite matrix elements between the two bands touching at the nodal point. Since the \( D_1 \) charge density wave order parameter does not generate a mass term to the Dirac Hamiltonian, it has no contribution to the Chern number leading to the zero Chern numbers of all bands.

We apply similar analysis to every Dirac point derived from the Brillouin zone folding for all pairs of density wave order parameters generating fully gapped phases. In all cases, it is confirmed that the Chern number of each band obtained by summing up the Chern number contributions from the Dirac points is identical to the result obtained by the integration of the Berry curvature in the momentum space.

In addition, the coexisting \( D_3 \) and \( M_2 \) density wave order parameters also lift the degeneracies of the two quadratic band touching points at \( k = (0, 0) \) and \( (0, \pi) \) leading to a fully gapped bandstructure. In contrast to the case of Dirac points, the Chern number obtained by lifting a quadratic band degeneracy is two times larger than the contribution from a single Dirac point. However, since the two quadratic band crossing points lead to the Chern number contributions with the opposite signs, the net effect of the two quadratic band touching points vanishes.

Since the four bands are well separated from each other for the topological density wave phase with \( D_3 \neq 0 \) and \( M_2 \neq 0 \), if the magnitude of the order parameter \( M_2 \) is large enough, an insulating ground state is obtained whenever the Fermi level lies in the gap between two neighboring bands. Therefore there are three different insulating phases, in principle, whenever the Fermi level lies between the band \( n \) and \( n+1 \) \( (n=1, 2, 3) \) corresponding to the band filling factor \( N_{\text{filling}} = (4-n)/4 \). The topological property of the insulating phase can be explicitly characterized by computing topological invariants. We first consider the spin Chern number \( C_S \) which is defined in the following way:

\[
C_S = \sum_{n \in \text{ooc}} \{ N_{C, \uparrow}^{(n)} - N_{C, \downarrow}^{(n)} \},
\]

where the summation includes all the occupied bands. When the \( S_z \) is conserved, the spin Chern number \( C_S \) is quantized and characterizes the two dimensional topological insulators. In Table III we show the spin Chern numbers for the insulating phases. It is interesting that the spin Chern numbers are nonzero for all cases. Therefore as long as the \( z \) component of the spin is conserved, we can obtain the topological insulator with finite spin hall conductivity for every quarter filling. However, in the presence of spin non-conserving perturbations and disorders, the spin Chern number is not well-defined and conserved only modulo 4. In other words, when the \( S_z \) is not conserved, the half-filled system is equivalent to the phase with zero spin Chern number, which is nothing but a topologically trivial band insulator. However, it is important to notice that even in this case the system remains as a topological insulator with nonzero \( Z_2 \) topological invariant for 1/4 and 3/4 fillings.

We also compute the \( Z_2 \) topological invariant \( \nu \) shown in Table III which can be used to distinguish topological insulators \( (\nu = 1) \) from trivial band insulators \( (\nu = 0) \) for generic time-reversal invariant systems. Since the system has the inversion symmetry, the \( Z_2 \) invariant can be obtained from the parity eigenvalues \( \xi_m(\Gamma_l) \) of the occupied bands with the band indices \( m \) at the time-reversal invariant momenta \( \Gamma_l \). Using the reciprocal lattice vectors \( G_i \), the four time reversal invariant momenta can be written as \( \Gamma_l = n_1 G_1 + n_2 G_2 \) with \( n_{1,2} = 0, 1 \). Explicitly the \( Z_2 \) topological invariant \( \nu \) is given by

\[
(-1)^\nu = \prod_{n_1=0,1} \prod_m \xi_m(\Gamma_{n_1 n_2}),
\]

where the parity eigenvalues of the occupied bands at the four time reversal invariant momenta are multiplied. Because of the time reversal symmetry, each band is doubly degenerate at the time reversal invariant momentum and every Kramers doublet share the same inversion parity. The \( Z_2 \) topological invariant counts the parity of one state for each Kramers pair.

As shown in Table III the \( Z_2 \) topological insulators exist when the band filling is one-quarter or three-quarter. However, the 3/4 filled case requires unreasonably large \( M_2 \) to achieve an insulating phase. This is because, as shown in Fig. 6 the overall structures of the bands 1 and 2 are in parallel. To open a full gap between the upper two bands (band 1 and 2), the magnitude of the \( M_2 \) density wave order parameter should be as large as their bandwidth. Therefore the quarter-filled system is the most favorable for the realization of the \( Z_2 \) topological insulator.

To support further the nontrivial topological properties of the topological density wave phase with \( D_3 \neq 0 \) and \( M_2 \neq 0 \), we compute the edge state spectrum by considering the Hamiltonian on a strip geometry, which is infinite in the \( x \)-direction but finite in the \( y \)-direction with open boundaries at \( y=1 \) and \( y=N_y \). Here \( N_y \) indicates the number of lattice sites in the \( y \)-direction. The energy spectrum of the system with \( N_y = 40 \) is described in Fig. 7 which shows the existence of robust gapless edge states traversing between the lower two bands (band 3 and 4) and the middle two bands (band 2 and 3). The upper two bands (band 1 and 2) are not well separated for \( D_3 = 0.85 \) and \( M_2 = 0.75 \), which are used to obtain the energy spectrum. Each edge state represented by a red dotted line is doubly degenerate, one with spin-up and the other with spin-down. For the 1/4-filling with the chemical potential lying in the gap between the band 3 and 4, there are two gapless edges states on each boundary propagating in the

| Band filling | Spin Chern Number \((C_S)\) | \(Z_2\) invariant \((\nu)\) |
|--------------|-----------------|---------------------|
| 1/4          | -2              | 1                   |
| 3/4          | +4              | 0                   |
| 2            | -2              | 1                   |

TABLE III: Spin Chern numbers and topological \(Z_2\) invariants for the gapped density wave ground state with finite \( D_3 \) and \( M_2 \).
nodal density wave phase in the simple on-site order parameter, it is possible to realize the topological insulator by introducing a defect topological property of the Dirac particles in the potential gives rise to a trivial band insulator.ond neighbor hopping processes are required to obtain a topological insulator on the honeycomb lattice where complex second order parameter can generate insulating phases with nontrivial topological properties. This result can be contrasted with the topological property of the Dirac particles near the momentum \( k_x = k_y = 0 \), which conserves \( S_z \), there are robust gapless edge states for both the quarter-filled and half-filled systems.

B. Comparison to the honeycomb lattice

It is interesting that a simple on-site density wave order parameter can generate insulating phases with nontrivial topological properties. This result can be contrasted with the topological insulator on the honeycomb lattice where complex second neighbor hopping processes are required to obtain a topological insulator while the simple on-site staggered chemical potential gives rise to a trivial band insulator.\(^4\)\(^5\)\(^10\) It is the distinct topological properties of the Dirac particles in the \( D_3 \) nodal density wave phase in the \( d \)-orbital system, which make it possible to realize the topological insulator by introducing a simple on-site order parameter \( M_2 \).

In this subsection, we discuss the topological property of the Dirac particles in the \( D_3 \) nodal density wave state in detail and compare it with the topological property of the Dirac particles on the honeycomb lattice. In the forthcoming discussion we neglect the spin degrees of freedom and focus on the condition under which the insulating phase possesses a finite Chern number, which is nothing but a Chern insulator. Once we find the condition to obtain a Chern insulator, the time reversal invariant topological insulator can be realized by superposing two Chern insulators with spin-up and spin-down particles, respectively.

The topological property of the Dirac particles in the \( D_3 \) nodal density wave state can be understood in the following way. The low energy Hamiltonian \( H^\text{Dirac}_t \) in Eq. (16) for the Dirac particles near the momentum \( k = k_x \), where the band touching points between the band 3 and 4 locate, can be written as

\[
H^\text{Dirac}_t (\mathbf{q}) = h_{\pm, x}(\mathbf{q}) \hat{r}_1 + h_{\pm, y}(\mathbf{q}) \hat{r}_3. \quad (22)
\]

Since \( \sqrt{h^2_{\pm, x}(\mathbf{q}) + h^2_{\pm, y}(\mathbf{q})} \) is nonzero away from the degeneracy point, a two component vector \( \vec{d}_{\pm}(\mathbf{q}) \) with the unit length can be defined as

\[
\vec{d}_{\pm}(\mathbf{q}) = (d_{\pm, x}(\mathbf{q}), d_{\pm, y}(\mathbf{q})) \equiv \frac{(h_{\pm, x}(\mathbf{q}), h_{\pm, y}(\mathbf{q}))}{\sqrt{h^2_{\pm, x}(\mathbf{q}) + h^2_{\pm, y}(\mathbf{q})}}. \quad (23)
\]

Along the circle \( C_R \) satisfying \( q_x^2 + q_y^2 = R^2 \neq 0 \) with the degeneracy point at the center, the 2D unit vector \( \vec{d}_{\pm}(\mathbf{q}) \) defines a map from the circle \( C_R \) to the unit circle \( S^1 \). Since the fundamental group \( \pi_1(S^1) = Z \), the 2D unit vector \( \vec{d}_{\pm}(\mathbf{q}) \) has an integer-valued topological invariant, which is nothing but the winding number \( N_w \) defined in Eq. (10). In terms of the 2D unit vector \( \vec{d}_{\pm}(\mathbf{q}) \), the winding number \( N_w \) can be rewritten as,

\[
N_w = \frac{1}{2\pi} \oint_{C_R} d\theta \hat{z} \cdot (\vec{d} \times \frac{d\vec{d}}{d\theta}). \quad (24)
\]

where the loop integral is defined along the circle where the momentum \( \mathbf{q} = R e^{i\theta} \).\(^3\)^\(^5\)
In Fig. 8(a) we describe the directions of the two-component \( \vec{d} \) vector along the circular path around the Dirac points for the \( D_3 \) nodal density wave state. Notice that the \( \vec{d} \) vector has the same winding direction with the winding number of \( N_w = 1 \) around the two Dirac points. The two Dirac points share the same winding number because of the constraint imposed by lattice symmetries. Since the first (second) component of the two-component Dirac field \( \Psi_\mu(q) \) is given by the \( d_{yz} \) (\( d_{xz} \)) orbital state, \( \Psi_\mu(q) \) transforms to \( \hat{\Psi}_\mu(-q) \) under the inversion symmetry due to the odd parity of \( d_{xz} \) and \( d_{yz} \) orbitals. Here \( \hat{\mu} \) has the opposite sign of \( \mu \). This imposes the following constraint on the pair of Dirac Hamiltonians related by the inversion symmetry,

\[
H_{+}^{\text{Dirac}}(q) = H_{-}^{\text{Dirac}}(-q). \tag{25}
\]

This constraint guarantees the same winding numbers for the two Dirac Hamiltonians \( H_{+}^{\text{Dirac}} \) and \( H_{-}^{\text{Dirac}} \). It is important to notice that every pair of Dirac Hamiltonians related by the inversion symmetry satisfies the same constraint for nodal density wave phases.

The fact that a pair of Dirac Hamiltonians related by the inversion symmetry have the same winding numbers is the distinct topological property of the Dirac particles in the nodal density wave states, distinguishable from the topological properties of the Dirac particles in the honeycomb lattice. In this system, the two Dirac points at the corners of the first Brillouin zone have the opposite winding directions, which is described in Fig. 8(b). Since the inversion symmetry interchanges the two sublattices of the honeycomb lattice, each of which comprises one component of the Dirac fermion field \( \Psi_\mu(q) \), the Dirac fermion field \( \Psi_\mu(q) \) transforms, for example, to \( \hat{\tau}_x \Psi_\mu(-q) \) under the inversion symmetry. This imposes the following constraint to the two Dirac Hamiltonians related by the inversion symmetry,

\[
H_{+}^{\text{Dirac}}(q) = \hat{\tau}_x H_{-}^{\text{Dirac}}(-q) \hat{\tau}_x. \tag{26}
\]

The additional Pauli matrix reverses the winding direction of one of the \( \vec{d} \) vectors, leading to the two Dirac Hamiltonians with the opposite winding numbers. Therefore these two Dirac points can be pair-annihilated when they are brought together by perturbations.

The relative winding numbers of the pair of the Dirac Hamiltonians related by the inversion symmetry, strongly constrain the topological properties of the insulating phases obtained by mass perturbations to the Dirac particles. The introduction of a constant mass term \( H_{\text{mass}}^\pm = m \hat{\tau}_2 \) to the Dirac Hamiltonian in Eq. (22) gives rises to the third component \( d_3(q) \) of the corresponding \( \vec{d} \) vector. Explicitly, for the massive Dirac Hamiltonian given by

\[
H^{\text{Dirac}}(q) = h_{xy}(q) \hat{\tau}_1 + h_y(q) \hat{\tau}_3 + m \hat{\tau}_2, \tag{27}
\]

the 3D unit vector \( \vec{d}_{3\text{D}} \) is defined as

\[
\vec{d}_{3\text{D}}(q) = (d_x(q), d_y(q), d_z(q)) \equiv \frac{(h_{xy}(q), h_y(q), m)}{\sqrt{h_{xy}^2(q) + h_y^2(q) + m^2}}. \tag{28}
\]

If we introduce, for instance, a positive mass term to the two Dirac Hamiltonians corresponding to the \( D_3 \) nodal density wave phase described in Fig. 8(a), both of the \( \vec{d}_{3\text{D}} \) vectors, which have positive \( z \) components, move along the northern hemisphere as the momentum \( q \) sweeps over the two dimensional momentum space. The net solid angles subtended by these two \( \vec{d}_{3\text{D}} \) vectors over the entire momentum space are the same, each of which covers \( 2\pi \). At this point, it is useful to take into account the following relation between the Chern number of the valence band and the 3D unit vector \( \vec{d}_{3\text{D}} \) for the two band Hamiltonian in Eq. (27).

\[
N_C = \int \frac{d^2k}{4\pi} \vec{d}_{3\text{D}} \cdot (\partial_{k_x} \vec{d}_{3\text{D}} \times \partial_{k_y} \vec{d}_{3\text{D}}). \tag{29}
\]

The above identity implies that the Chern number counts the number of times the 3D unit vector \( \vec{d}_{3\text{D}} \) winding around the unit sphere over the Brillouin zone torus. Therefore when a constant mass term is added to the two Dirac points connected by the inversion symmetry, the Chern number \( N_C = \pm 1 \) if the two Dirac points have the same winding numbers, which is realized in the nodal density wave ground state.

In contrast, the net solid angles covered by the two \( \vec{d}_{3\text{D}} \) vectors in the honeycomb lattice have the same magnitudes but with the opposite signs. Therefore the total solid angle covered by these two \( \vec{d}_{3\text{D}} \) vectors vanishes. The vanishing Chern number contributions from the two Dirac points leads to the topologically trivial insulating phase when the simple mass term in Eq. (27) is introduced. This contrasting behavior of the pair of 3D unit vectors \( \vec{d}_{3\text{D}} \) in these two systems results in the distinct topological properties of the insulating phases, the topological insulator in the \( d \)-orbital system and the topologically trivial band insulator in the honeycomb lattice when constant mass terms with the same signs are added to the pair of Dirac points connected by the inversion symmetry. However, in graphene if we introduce mass terms with the opposite signs at the two Dirac points, a topological insulator with a finite Chern number can be obtained, which is realized by considering the complex second nearest neighbor hopping processes on the honeycomb lattice.

V. MEAN FIELD THEORY

Now we address the question whether the TDW insulator with finite \( D_3 \) and \( M_2 \) can be achieved in real systems. In particular, by taking into account the interactions between electrons, we investigate the conditions to realize the TDW insulator via spontaneous symmetry breaking. Previous mean field studies on the two-orbital Hubbard model with the hopping Hamiltonian \( H_0 \) in Eq. (11) show that the leading instability of the system is the uniform spin density wave phase (\( M_0\text{-SDW} \)) which is described by nonzero \( M_0 \). However, there exist another density wave order parameters including imaginary charge and spin density wave states, which are competing with the uniform spin density wave state (\( M_0\text{-SDW} \)) with small energy differences. Therefore if we include longer range interactions which are not included in the multi-orbital on-site
FIG. 9: (Color online) Mean field phase diagram. Here we set $U = 5$, $J_H = 0$ and plot the ground state phase diagram varying the inter-orbital on-site repulsion $U_2$ and the effective next nearest neighbor repulsion $V_{2,eff} = V_{2B} - 2V_{2A}$. There is a finite range between $D_3$ charge density wave phase ($D_3$-CDW) and $M_2$ spin density wave phase ($M_2$-SDW) where the topological density wave phase (TDW) becomes the ground state. Solid (dotted) lines indicate the first (second) order phase transitions.

Hubbard Hamiltonian, another competing ground states, for example, the topological density wave state (TDW), can become the ground state replacing the $M_2$-SDW state.

Including on-site and inter-site electron-electron interactions, the full Hamiltonian is given by

$$H_{\text{full}} = H_0 + H_{\text{onsite}} + H_{\text{intense}}$$

in which

$$H_{\text{onsite}} = U \sum_{i} \sum_{\alpha=1,2} n_{i,\alpha\uparrow} n_{i,\alpha\downarrow} + U_2 \sum_{i} n_{i,1} n_{i,2} + J_H \sum_{\sigma_1,\sigma_2} d_{i,1,\sigma_1}^{\dagger} d_{i,2,\sigma_2}^{\dagger} d_{i,1,\sigma_2} d_{i,2,\sigma_1} + J_H \sum_{(ij)} (d_{i,1,\uparrow}^{\dagger} d_{i,2,\downarrow}^{\dagger} d_{i,2,\uparrow} + \text{H.c.})$$

and

$$H_{\text{intense}} = V_{1A} \sum_{(ij)} \sum_{\alpha=1,2} n_{i,\alpha} n_{j,\alpha} + V_{1B} \sum_{(ij)} n_{i,1} n_{j,2} + V_{2A} \sum_{(ij)} n_{i,1} n_{j,2} + V_{2B} \sum_{(ij)} n_{i,1} n_{j,2}$$

where $H_0$ indicates the hopping Hamiltonian in Eq. (1). For the on-site interactions described by $H_{\text{onsite}}$, the intra-orbital repulsion $U$, the inter-orbital repulsion $U_2$, and the Hund’s coupling $J_H$ are considered. In the $H_{\text{intense}}$ describing the inter-site Coulomb interactions, $V_{1A}$ ($V_{1B}$) indicates the nearest-neighbor Coulomb repulsion between electrons in the same (different) kinds of orbitals. Finally, $V_{2A}$ ($V_{2B}$) indicates the next nearest-neighbor Coulomb repulsion between electrons in the same (different) kinds of orbitals.

To investigate the existence of the topological density wave state (TDW) with $D_3 \neq 0$ and $M_2 \neq 0$ and its competition with the uniform spin density wave phase ($M_0$-SDW), we apply a mean field approximation to the Hamiltonian $H_{\text{full}}$. The resulting mean-field Hamiltonian is given by

$$H_{\text{MF}} = H_0 + N \epsilon_0 + \sum_{\alpha=1,2} \sum_{\kappa \in \text{RBZ}} [A_{11,\sigma} \langle d_{1,\sigma}^{\dagger} d_{1,\sigma} (k + Q) + d_{1,\sigma}^{\dagger} (k + Q) d_{1,\sigma}(k) \} + A_{22,\sigma} \langle d_{2,\sigma}(k) d_{2,\sigma} (k + Q) + d_{2,\sigma}^{\dagger} (k + Q) d_{2,\sigma}(k) \} + A_{12,\sigma} \langle d_{1,\sigma}^{\dagger} (k) d_{2,\sigma} (k + Q) + d_{2,\sigma}^{\dagger} (k + Q) d_{1,\sigma}(k) \} + A_{21,\sigma} \langle d_{2,\sigma}^{\dagger}(k) d_{1,\sigma} (k + Q) + d_{1,\sigma}^{\dagger} (k + Q) d_{2,\sigma}(k) \}$$

in which

$$\epsilon_0 = \frac{U_0}{8} (M_0^2 - D_3^2) + \frac{U_2}{8} (M_2^2 + 2D_3^2) + \frac{J_H}{8} (M_0^2 - D_3^2 - M_2^2) + (V_{2A} - \frac{V_{2B}}{2}) D_3$$

and

$$A_{11,\sigma} = \frac{U}{4} (D_3 - \sigma M_0) - \frac{U_2}{2} D_3 - (2V_{2A} - V_{2B}) D_3 + \frac{J_H}{4} (-D_3 + \sigma M_0)$$

$$A_{22,\sigma} = -\frac{U}{4} (D_3 + \sigma M_0) + \frac{U_2}{2} D_3 + (2V_{2A} - V_{2B}) D_3 + \frac{J_H}{4} (D_3 + \sigma M_0)$$

$$A_{12,\sigma} = A_{21,\sigma} = \frac{U_2}{4} i \sigma M_2 - \frac{J_H}{4} i \sigma M_2$$

Note that the nearest neighbor Coulomb repulsions $V_{1A}$ and $V_{1B}$ do not contribute to the mean field Hamiltonian because the order parameters have the ordering wave vector $Q = (\pi, 0)$.

The order parameters $M_0$, $M_2$, $D_3$ are determined by solving the following self-consistent equations,

$$M_0 = \frac{1}{N} \sum_{r=(r_x, r_y)} \langle d_{r,1,\sigma}^{\dagger} d_{r,1,\sigma} + d_{r,2,\sigma}^{\dagger} d_{r,2,\sigma} \rangle$$

$$M_2 = \frac{1}{N} \sum_{r=(r_x, r_y)} \langle id_{r,1,\sigma}^{\dagger} d_{r,2,\sigma} - id_{r,2,\sigma}^{\dagger} d_{r,1,\sigma} \rangle$$

$$D_3 = \frac{1}{N} \sum_{r=(r_x, r_y)} \langle d_{r,1,\sigma}^{\dagger} d_{r,1,\sigma} - d_{r,2,\sigma}^{\dagger} d_{r,2,\sigma} \rangle$$

The chemical potential $\mu$ is also determined self-consistently to satisfy the half-filling condition.

The resulting mean field phase diagram is shown in Fig. 9. Here we choose $U = 5$, $J_H = 0$ and compute the ground
state phase diagram as a function of the inter-orbital on-site repulsion $U_2$ and effective next nearest neighbor repulsion $V_{2,eff} = V_{2B} - 2V_{2A}$. In the absence of the inter-site interactions $V_{2,eff} = 0$, the uniform spin density wave phase ($M_0$-SDW) dominates the phase diagram consistent with the previous studies. However, the inter-orbital on-site repulsion $U_2$ suppresses the uniform spin density wave states ($M_0$-SDW) which is diagonal in the orbital space, but promotes the $M_2$-SDW, which is off-diagonal in the orbital space, to the ground state. On the other hand, the $D_3$ charge density wave phase ($D_3$-CDW) is strongly affected by the next nearest neighbor Coulomb repulsions $V_{2A}$ and $V_{2B}$. In particular, the $V_{2A}$, the next nearest neighbor repulsion between the electrons in the same kinds of orbitals, strongly favors the $D_3$-CDW because the staggered orbital ordering described by $D_3$-CDW can avoid the energy cost coming from $V_{2A}$. Notice that there is a finite range in the parameter space where both $M_2$-SDW and $D_3$-CDW are nonzero realizing the topological density wave phase (TDW).

The above mean field phase diagram is obtained for the half filled case where the topological property of the TDW phase is not robust against perturbations breaking $S_z$ symmetry. On the other hand, the TDW insulator at 1/4 filling maintains its topological properties as long as time reversal symmetry is preserved. It was shown, in the study of the single orbital extended Hubbard model, that the next nearest neighbor interaction ($V_{2A}$ for our model) stabilizes a stripe pattern charge ordering with the momentum $Q = (π, 0)$. This occurs at 1/4 filling when the on-site Hubbard interaction $U$ is much stronger than the hopping amplitude $t$ satisfying $U >> t$, so that double occupancy is almost frozen. In our model, there are two orbitals of $d_{xz}$ and $d_{yz}$. Similar to the single orbital case, we find that the next nearest neighbor interaction stabilizes $D_3$ order. Therefore, when the on-site intra- and inter-orbital interactions satisfy $U, U_2 >> t$, the $D_3$-CDW ordering should be favored at 1/4 filling.

To get a TDW insulator, finite $M_2$ is required in addition to $D_3$. As shown in Sec. III B, the $M_2$ order parameter is equivalent to a staggered spin-orbit coupling, $\sim \sum_i (-1)^i s_i z_l_i z$. One can show that when spin-orbit interaction is present, $M_2$ term can be induced as long as $D_3$ sets in, since $D_3$ leads to unequal density between $d_{xz}$ and $d_{yz}$ orbitals. Therefore, we expect that the TDW insulator can be obtained by tuning $V_{2B}$ when $U, U_2 >> t$ at 1/4 filling in the presence of the spin-orbit coupling.

VI. TOPOLOGICAL INSULATORS IN THREE-BAND SYSTEMS

In the preceding sections, we have focused on a two-band tight-binding Hamiltonian, which consists of $d_{xz}$ and $d_{yz}$ orbitals. However, the main idea for realizing topological insulators using two density wave order parameters with opposite symmetries under reflections is valid in general and applicable to more realistic multi-orbital systems. Here we extend our analysis to a three-band model composed of $d_{xz}, d_{yz}$, and $d_{xy}$ orbitals. In particular, we apply our idea to a more realistic model Hamiltonian relevant to the iron pnictide system, which is a representative itinerant multi-band system manifesting a density wave ground state with the ordering wave vector $Q = (π, 0)$. Here we adopt the three-orbital model proposed by Daghofer et al. which captures the main physical properties of the Fe-pnictide systems. In the momentum space, the effective three-band tight-binding Hamiltonian is given by

$$H_{\text{3-band}} = \sum_{\mathbf{k}, \sigma} \sum_{\mu, \nu} d_{\mu, \sigma}^\dagger(\mathbf{k}) T^{\mu \nu}(\mathbf{k}) d_{\nu, \sigma}(\mathbf{k}), \quad (37)$$

where

$$T^{11} = 2t_2 \cos k_x + 2t_1 \cos k_y + 4t_3 \cos k_x \cos k_y - \mu_c,$$

$$T^{22} = 2t_1 \cos k_x + 2t_2 \cos k_y + 4t_3 \cos k_x \cos k_y - \mu_c,$$

$$T^{33} = 2t_5 (\cos k_x + \cos k_y) + 4t_6 \cos k_x \cos k_y - \mu_c + \Delta_{xy},$$

$$T^{12} = T^{21} = 4t_4 \sin k_x \sin k_y,$$

$$T^{13} = (T^{31})^* = 2iT_7 \sin k_x + 4it_8 \sin k_x \cos k_y,$$

$$T^{23} = (T^{32})^* = 2iT_7 \sin k_y + 4it_8 \sin k_y \cos k_x.$$ 

Here we use the unfolded Brillouin zone satisfying $-π < k_x, k_y ≤ π$ as before, which corresponds to one iron atom per unit cell. In real iron pnictide materials, the unit cell contains two Fe atoms due to the buckling of the $\text{As}$ atoms. Therefore the unit translations along the $x$ ($T_x$) and $y$ ($T_y$) directions by the nearest neighbor Fe-Fe distance, are not the symmetries of the system. However, as pointed out in Ref. $^{43}$, the system is invariant under the translations combined with the reflection $P_z$ with respect to the $xy$ plane, i.e. $P_z T_x$ and $P_z T_y$. Then the eigenstates can be labeled by a pseudo-crystal momentum corresponding to the eigenvalues of the combined operations $P_z T_x$ and $P_z T_y$ with one iron atom per unit cell. We use this pseudo-crystal momentum to label states for the momentum space representation of the Hamiltonian in Eq. (37).

In Eq. (37) and (38), $\mu = 1, 2, 3$ indicate $d_{xz}, d_{yz}$, and $d_{xy}$ orbitals, respectively. $\Delta_{xy}$ represents the atomic potential of $d_{xy}$ orbital relative to $d_{xz}$ and $d_{yz}$ orbitals. The chemical potential is given by $\mu_c$. The hopping parameters are displayed in Table IV, which are determined in Ref. $^{39}$. For the 2/3 filling, there are two hole pockets near the $\Gamma$ point and two electron pockets at the $X$ and $Y$ points, which are consistent with the LDA calculations and ARPES measurement for LaOFeAs.

Density wave order parameters with the momentum $Q = (π, 0)$ can be described by the following Hamiltonian,
The order parameter represented by $3 \times 3$ Hermitian matrix $\hat{M}$ (\(\tilde{D}\)) has nine independent components $D_{ij}$ ($M_{ij}$). The transformation properties of these density wave order parameters under the reflections $P_x$, $P_z$, and $P_y$, inversion $I$, and time-reversal $T$ are summarized in Table V and VI. Notice that the reflections $P_x$ and $P_y$ are not the symmetries of the system. The Hamiltonian is invariant only under the combined transformations $P_xP_z$ and $P_yP_z$.

To obtain a nodal spin density wave ground state, we consider the simplest uniform charge density wave order parameter, $D_{\text{uniform}} \equiv \text{diag}(d_0,d_0,d_0)$ with the finite diagonal components of $D_{11} = D_{22} = D_{33} = d_0$. This generates many Dirac points along an axis with a reflection symmetry in the momentum space, whenever a band touching occurs between two bands with opposite reflection parities. Now let us introduce another density wave order parameter to get a gapped phase. To open a full gap between neighboring bands we need a density wave order parameter which is odd under the reflection symmetries $P_xP_z$ and $P_yP_z$. Imposing the time reversal symmetry, the imaginary part of the spin density wave order parameter $M_{12} \equiv \text{Im}(M_{12})$, is the unique choice to obtain a topological insulator.

In Fig. 10 (a) we plot the band structure of the uniform charge density wave state with $D_{\text{uniform}} \neq 0$ along the $k_y$ axis. Since $D_{\text{uniform}}$ preserves the $P_xP_z$ reflection symmetry, the imaginary part of the spin density wave order parameter $M_{12}$ is still conserved, the spin Chern number is a well-defined quantity. In Table VII, we show the distribution of the spin Chern numbers for several cases.
values of $M_{12}$ supporting fully gapped phases. Here $C_{S,n}$ indicates the spin Chern number of the $n$th band defined as $C_{S,n} = N_{C,n,↑} - N_{C,n,↓}$ where $N_{C,n,σ}$ denotes the Chern number of the $n$th spin-up band. We label that the band 1 has the highest energy and the band index $n$ increases as the energy eigenvalue decreases. In the case of the gapped phase that is obtained by adding a small $M_{12}$ on the nodal charge density wave state with $D_{\text{uniform}} \neq 0$, only the 4th and 5th band support nonzero spin Chern numbers shown in the 2nd column of Table VII. Interestingly, however, as the magnitude of $M_{12}$ increases, band gap closing and reopening occur successively. For instance, for the uniform density wave state with $D_{\text{uniform}} = 0.5$, the first gap closing happens between the band 1 and 2 for $M_{12} \approx 0.15$. As $M_{12}$ increases further, another fully gapped phase is obtained with the spin Chern numbers displayed in the 3rd column of Table VII. It is interesting to notice that after the gap closing and reopening process, the number of the bands supporting finite spin Chern numbers has increased. Similar gap closing happens again for $M_{12} \approx 0.22$ to the redistribution of the spin Chern numbers shown in the last column of Table VII. Note that all cases with 1/3 filling give TDW insulators, while TDW phase with 5/6 filling occurs only for the $M_{12} = 0.2$ and 0.3.

VII. SUMMARY AND DISCUSSION

In this paper, we investigate theoretically if topological insulators can be achieved from a nodal density wave state with broken translational symmetry. While a nonzero density wave order parameter in general opens a gap between the degenerate states connected by the ordering wave vector, nodal density wave phases occur in multi-orbital systems via translational symmetry breaking due to the distinct symmetry properties of orbitals. Such a nodal density wave state supports a large number of Dirac nodes between neighboring bands. We have explicitly proved that a pair of inversion symmetric Dirac points share the same topological winding numbers in nodal density wave states contrary to the Dirac points in the honeycomb lattice. If we introduce an additional order parameter whose transformation property under reflection symmetries is opposite to that of the underlying order parameter, the system can be a gapped insulator at certain filling factors. Among those insulators, time-reversal invariant TDW insulators with helical edge states are identified.

The existence of a nodal density wave ground state is experimentally verified in a recent ARPES measurement on BaFe$_2$As$_2$ and quantum oscillation experiments on BaFe$_2$As$_2$ and SrFe$_2$As$_2$. It is interesting to notice that, according to these experimental studies, the velocity of Dirac fermions is estimated to be 14 - 20 times slower than that in graphene. This implies that the Dirac fermions in nodal density wave states are more susceptible to interaction effects. However, according to our mean field calculation, it seems to be difficult to realize quantum spin Hall insulators in Fe pnictides system, as it favors a conventional spin density wave state ($M_0$).

Our results in general imply that transition metal materials with two-dimensional square lattice structure possessing partially filled $t_{2g}$ orbitals are good candidates for TDW insulators. In particular, in the case of the effective two-orbital (three-orbital) model, the 1/4 filled (1/3 filled) system is the most promising for the realization of TDW insulators. However, to make a prediction on real materials with layered perovskite structure, it is important to generalize our study to three dimensional systems taking into account interlayer couplings. Stacking of two dimensional TDW insulators simply leads to a weak topological insulator. Therefore identifying three dimensional TDW phases with a nontrivial strong topological invariant in the layered perovskite structure is an interesting but challenging future work.

Finally, it is worthwhile to comment the consequences of relaxing the constraint of time-reversal invariance. When an imaginary charge density wave state ($D_{2g}$) breaking time-reversal symmetry occurs in the presence of a nodal density wave state, a gapped topological phase with topologically protected edge modes can be developed. In contrast to the case of the quantum spin Hall insulator, here the spin-up and down bands have the same Chern number, which gives rise to an insulator with finite Hall conductance. Interestingly, the imaginary charge density wave state is one of the competing ground states in iron pnictide systems which is expected to be achieved in real materials. Thus searching for gapped phases proximate to nodal density wave states is a new avenue to topological phases.

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We choose $Q = (\pi, 0)$ for simplicity but the general criteria for obtaining TDW phase do not depend on the choice of $Q$. In Ref. 39, $t_8$ and $t_7$ was fixed by $t_8 = -t_7/2$ to make the electron pockets have pure $xy$ character along $\Gamma - X$ and $\Gamma - Y$ directions. Since this additional constraint generates accidental band crossing points, we introduce 10 percent modulation in the magnitude of $t_8$, which does not affect the overall band structure and the shape of the Fermi surfaces.