Topological insulators in three dimensions from spontaneous symmetry breaking

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I. INTRODUCTION

Three dimensional topological insulators (TI) have recently raised considerable interest in both theory and experiments for their nontrivial topological properties, which separate them from conventional band insulators. The hallmark of a TI is its exotic surface electronic properties. In particular, the strong topological insulator has an odd number of Dirac nodes on the surface of the system, which are stable against moderate perturbations that preserve time reversal symmetry. Such a band structure cannot be realized in any two dimensional system with time reversal invariance. There have been experimental realizations of these predictions in bismuth antimony alloys and in bismuth selenium, which have been verified by angle resolved photoemission spectroscopy.

In two dimensions, an analogous state is the quantum spin hall (QSH) phase, which has counter-propagating one dimensional edge modes. Such a state can occur with spin orbit interactions that preserve spin rotation symmetry about an axis, in which case the oppositely propagating modes carry opposite quantum numbers for this component of spin. It was shown in Ref. that even in the absence of such spin rotation invariance, the counter-propagating modes remain protected by time reversal symmetry. The three dimensional weak topological insulator (WTI) can be obtained by stacking such 2D QSH states. However, in order to realize the strong topological insulator, the spin rotation symmetry must be completely broken.

The TI and QSH phases normally exist in the systems with strong spin-orbit interaction (SOI) that explicitly breaks spin rotation symmetry. However, as pointed out in Ref. an extended Hubbard model on a 2D honeycomb lattice can have spontaneous SRS breaking and result in a QSH phase, with the right kind of repulsive interactions. Spin rotation symmetry is only preserved about an axis \( \hat{n} \), which is spontaneously chosen, leading to gapless Goldstone modes. This was termed a topological ‘Mott’ insulator - the separation of energy scales between the low lying magnetic excitations and the gapped charge excitations being typical of Mott insulators. We will also adopt this nomenclature although it must be noted that local moment physics, often associated with Mott insulators, does not occur here. Subsequently, it was argued in that skyrmions of \( \hat{n} \) carry charge \( 2e \).

Here, we consider the analogous problem of a three dimensional system without bare spin orbit couplings, and full spin rotation symmetry, being driven into a topological insulator state by strong interactions. The key difference from the two dimensional case, is that in order to realize the strong topological insulator, spin rotation symmetry must be completely broken. Hence the order parameter in this case is a rotation matrix \( \mathbf{R} \in O(3) \), similar to superfluid Helium-3 A and B-phases, which leads to a richer set of topological textures. We describe a microscopic model, an extended Hubbard model on the diamond lattice that, within a mean field treatment, leads to this phase. The order parameter supports a number of topological defects. In particular, a vortex like line defect occurs, but with a \( Z_2 \) charge. This line defect in the strong TI is found to be associated with a pair of gapless fermionic excitations that travel along its length. These modes are topologically stable against moderate perturbations such as impurities and interactions as long as time reversal symmetry is intact. This is the main result of the paper - an analytical derivation is provided which relies on the properties of the Dirac equation on a two dimensional curved surface.

We now contrast our results with other recent work. Similar exotic behavior also occurs in TIs, along crystal defects such as dislocations. Gapless fermionic excitations emerge there when a \( Z_2 \) parameter formed by the product of the dislocation Burgers vector and three weak topological insulator (WTI) indices is nonzero - which in principle can occur in both the weak and strong TI. In contrast, in the present paper, the fermionic modes along the line defect are solely determined by the more elusive \( Z_2 \) index. They are absent in the case of the weak TI. Thus far, the characterization of the TI phase has relied on the surface behavior. This result provides a route to identifying the strong topological Mott insulator...
via a bulk property.

Similar modes have been identified propagating along a solenoid of $\pi$ flux, inserted into a strong topological insulator [13]. Here, the $2\pi$ rotation of the electron spin around the line defect leads to a Berry’s phase, providing a physical realization of the $\pi$ flux. Analogous phenomena occur in the context of line defects in superfluid He$_3$-B[10].

The order parameter $\mathbf{R}$ admits a skyrmion like texture, which is a point object in three dimensions (Shankar monopole). We find that in contrast to the skyrmion of the quantum spin Hall effect[13], these are uncharged.

In most solids where electron-electron interactions are important tend to have some degree of spin-orbit interactions - which will confine the defects. Hence, we propose realizations of this physics in optical lattices of ultracold atoms, utilizing molecules with multipole moments to obtain the proposed extended Hubbard models. The two dimensional version [12] is found to be naturally realized with electric dipoles. Realizing the three dimensional case is more challenging, however molecules with electric quadrupole moments confined in optical lattice can realize some of the key ingredients required.

This paper is organized as the following: In the next section, we will present the order parameter manifold and the line modes’ $Z_2$ dependence on the winding number; in section III, we will justify our claim with numerical and analytical results; another texture Shankar monopole will be discussed in section IV; in section V, we will establish our model Hamiltonian on a diamond lattice and show the mean field stability of topological Mott insulating (TMI) phases; we give two possible experimental realizations in cold atom systems in section VI; we conclude the main result of this paper in the last section. Hereafter we use $\sigma$ and $\tau$ for the spin and sublattice degree of freedom, respectively.

II. TOPOLOGICAL MOTT INSULATORS AND ORDER PARAMETER TEXTURES IN THREE DIMENSIONS

In order to describe the Topological Mott insulating phase, we consider a concrete example in the following. In a subsequent section, we address the question of how such a phase may be microscopically realized. To contrast the TMI phase with the regular topological insulator, consider the model Hamiltonians of a TI introduced in [1]. We consider nearest neighbor hopping ($t_{ij}$) on the sites of a diamond lattice, and spin orbit induced hopping on next-neighbor sites.

$$H_{TI} = H_{\text{hop}} + H_{SO}$$

$$H_{\text{hop}} = \sum_{\langle ij \rangle} t_{ij} c_{i}^{\dagger} c_{j}$$

$$H_{SO} = i \left(8\lambda_{SO}/a^{2}\right) \sum_{\langle\langle ij\rangle\rangle} c_{i}^{\dagger} \vec{\sigma} \cdot \left(\hat{d}_{ij}^{2} \times \hat{d}_{ij}^{2}\right) c_{j} \quad (1)$$

where $c^{\dagger} = (c_{1}^{\dagger}, c_{1}^{\dagger})$ is the electron creation operator and $\vec{\sigma}$ is the spin pauli matrix. The spin-orbit interaction for a pair of second neighbor sites $ij$, depend on $\hat{d}_{ij}^{p}$ ($p = 1, 2$) the two nearest neighbor bond vectors connecting the second neighbor sites $ij$. The spin orbit interactions are thus determined by the crystal structure. Note, the SU(2) spin rotation symmetry is completely broken, which is required to realize the strong topological insulator in three dimensions.

In contrast, in the TMI phase discussed here, the underlying Hamiltonian possesses full SU(2) spin rotation symmetry that is spontaneously broken. The order parameter $\mathbf{R}$ then is a rotation matrix that describes the relative orientation between the real space coordinate system and the spin axes. The spin orbit term then takes the form:

$$H_{SO}^{\text{TMI}} = i \left(8\lambda_{SO}/a^{2}\right) \sum_{\langle\langle ij\rangle\rangle} c_{i}^{\dagger} \vec{\sigma} \cdot \mathbf{R}_{i}^{j} \cdot \left(\hat{d}_{ij}^{2} \times \hat{d}_{ij}^{2}\right) c_{j} \quad (2)$$

There is one important difference between the TI and TMI: since in the latter $\mathbf{R}$ arises from symmetry breaking it can vary spatially to give rise to a topologically nontrivial texture. To identify the topologically stable defects, we first note that the order parameter manifold is a three dimensional orthogonal matrix $\mathbf{R} \in O(3)$. It can represent by $\mathbf{R} = (\hat{e}_{1}, \hat{e}_{2}, \hat{e}_{3})$, where $\hat{e}_{i}$ are orthogonal unit vectors representing the basis vectors of the spin coordinate system. An example is shown in Fig. [1]

The target manifold of this order parameter is $O(3) = SO(3) \times Z_2$, and $Z_2$ determines the chirality $\det (\mathbf{R}) = \pm1$, or whether the rotation is proper or improper. Hereafter we mainly focus on the continuous $SO(3)$ part of the order parameter, for it has nontrivial homotopy groups in two and three dimensions. Then, each proper rotation can be described by the parameters $(\hat{n}, \theta)$, where $\hat{n}$ is the direction of the rotation axis and $\theta \in [0, \pi]$ is the rotation angle around it. To visualize it we can map all proper rotation matrices to a solid ball with radius $\pi$, where $\hat{n}$ maps to the radial direction and rotation angle maps to the radius of the image point. Note a rotation of $\pi$ about $\hat{n}$ is the same as that of $\pi$ about $-\hat{n}$, so opposite points on the spherical surface are identified. The resulting geometry is a three dimensional projective plane $P^3$[21].
We now discuss the topological defects of this order parameter space. The discrete $Z_2$ symmetry breaking implied by the $Z_2 \times SO(3)$ order parameter leads to domain walls in three dimensions. More interestingly, line defects also exist (we assume three spatial dimensions in the following). These can be captured by considering the order parameter along a closed curve in real space, which encircles the line defect. This defines a closed loop in the order parameter space and distinct classes of such closed loops correspond to the topological line defects. There are two classes of closed loops for the $SO(3)$ space described above. In addition to the trivial closed loop, that can be shrunk continuously to a point, there exists a non-trivial loop that connects the antipodal points $(\hat{n}, \pi)$ and $(-\hat{n}, \pi)$. Since these represent the same rotation, this is in fact a closed loop. Thus there is a nontrivial line defect characterized just by a $Z_2$ topological charge. Technically $\pi_1(SO(3)) = Z_2$ [21]. An example is shown in Fig. 1 with translational invariance along $z$ direction although generically, the line can be of arbitrary shape and direction.

The electronic properties of such a line defect is studied in the following section - protected one dimensional modes that propagate along the defect are found in the case of the strong TMI, but not in the case of the weak TMI. We also note that since $\pi_2(SO(3)) = 0$, no nontrivial point defects exist in three dimensions. However, since $\pi_3(SO(3)) = Z$, ‘skyrmiion’ like textures (called Shankar monopoles [18]) exist in three dimensions. In contrast to topological defects, they are smooth textures without a singular core. We investigate the electronic structure of these objects and find that they are neutral in the large size limit, in contrast to skyrmions in the two dimensional quantum spin hall state which carry charge $2e$ [13].

III. ELECTRONIC STRUCTURE OF A LINE DEFECT: NUMERICAL AND ANALYTICAL RESULTS

We study the electronic structure of the $Z_2$ line defect in the diamond lattice model of a topological Mott insulator discussed before. We choose the nearest neighbor hopping in three directions to be equal $t_{ij} = t > 0$ while the fourth is different $t_{ij} = t + \delta t$. A strong (weak) TI phase occurs if $\delta t > 0$ ($\delta t < 0$) [1]. We choose an order parameter texture that incorporates line defects:

$$H = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + i \left(8\lambda_{SO}/a^2\right) \sum_{\langle\langle ij \rangle\rangle} c_i^\dagger s^z R_i \cdot \left(d_{ij}^\dagger \times d_{ij}^\dagger\right) c_j$$

(3)

with

$$R_i(\varphi) = \begin{pmatrix} \cos(\varphi) & \sin(\varphi) & 0 \\ -\sin(\varphi) & \cos(\varphi) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

where $R_i$ depends only on the azimuthal angle of the atom connecting sites $i$ and $j$. Note, only the parity of $l$ is topologically stable. Here we study a system of $24 \times 24$ with a maximally separated vortex ($l = 1$) and anti-vortex ($l = -1$), and with periodic boundary condition in $x - y$ plane and translational invariance in $z$ direction. Note, time reversal symmetry is preserved by this Hamiltonian.

For a $\delta t > 0$ strong TMI system with $l = \pm 1$, two pairs of conducting line modes are found in the bulk gap. These states’ density profiles are strongly localized at the cores or the two defects (Fig. 2 top, shows only one of them for clarity). Therefore a Kramer pair of modes is localized along the thread of core. Given the particle hole symmetry that happens to be present in this model, they cross at zero energy (Fig. 2 bottom). In contrast, these modes are absent in the cases of the weak TMI $\delta t < 0$ or if $l = 0, \pm 2$ in either type of TMI, and the bandstructure remains fully gapped. This is direct evidence that these $Z_2$ dependent line modes within the bulk identify the strong TMI.

An analytical argument for these modes can be developed in several ways. We can derive these modes based on the 3D Dirac continuum limit of the Hamiltonian [3]; however, below we consider deriving these modes using the known properties of surface states of strong topological insulators. Consider a bulk sample with a infinitely long cylindrical hole of radius $R$ drilled through its center. We consider the low energy states on the cylindrical surface, both without and with a line defect inserted in the cylindrical hole Fig. 3. We show that in the limit of $R \rightarrow 0$, a propagating midgap mode survives only when the defect is present; otherwise a fully gapped insulator results. Interestingly, the key ingredient here is the property of the two dimensional surface Dirac state, on a curved manifold. In contrast to the states of a particle on a ring, where the zero angular momentum
main, and the bulk insulator is recovered. However, if a
face, which excludes the zero angular momentum state.

On a curved surface there should be additional terms
due to the curvature. The effective Hamiltonian can be
systematically derived \[22\], as described in the Ap-
pendix. Here we just present the result in the general
case when the radii of curvature along the two tangent
directions \(\hat{n}_1, \hat{n}_2\) are \(R_1, R_2\) respectively (which are
defined via \((\hat{n}_i \cdot \vec{p}) \hat{n}_j = i\hbar \delta_{ij} \hat{n}_1 \times \hat{n}_2 / R_i\) for \(i = 1, 2\)):

\[
H_{\text{curved}} = \sigma_1 \hat{n}_1 \cdot \vec{p} + \sigma_2 \hat{n}_2 \cdot \vec{p} + \frac{\hbar}{2} \frac{1}{R_1} \sin \theta + \frac{1}{R_2} \left[ \sin \theta + i \cos \theta (\hat{n}_1 \times \hat{n}_2) \cdot \vec{σ} \right]
\]

We now apply this result to the problem of surface
states on the cylindrical surface of radius \(R\) with axis
along \(\hat{z}\) and radius \(R\) with strong TMI outside and vac-
uum inside (see Fig. 3). We use cylindrical coordinates
\(z, \phi\), hence \(\hat{n}_z = (0, 0, 1)\) and \(\hat{n}_\phi = (-\sin \phi, \cos \phi, 0)\),
\(\hat{n}_r = -\hat{n}_z \times \hat{n}_\phi\) the two radii of curvature \(R_1 = \infty, R_2 = R\). For simplicity we consider \(\theta = 0\). The effective Hamil-
tonian in the absence of a defect is:

\[
H_0 = (\hat{n}_z \cdot \vec{σ}) p_z + (\hat{n}_\phi \cdot \vec{σ}) p_\phi + \frac{\hbar}{2} i \vec{σ} \cdot \hat{n}_r
\]

where \(p_z = -i\hbar \partial_z\) and \(p_\phi = -i\hbar \partial_\phi\). We can solve for
the energies \(E_0 \psi = E \psi\) by first performing the unitary transformation \(\psi = U_z(\phi) \psi'\) where \(U_z(\phi) = e^{i\phi \sigma_z / 2}\). Note,
since \(U_z(\phi + 2 \pi) = -U_z(\phi)\), the new wavefunc-
tions \(\psi'\) satisfy antiperiodic boundary conditions. The
transformed Hamiltonian \(H'_0 = p_z \sigma_z + p_\phi \sigma_y\) has eigen-
ectors \(\psi' = e^{ikz} e^{i\phi \chi}, \phi\), where \(\chi\) is a fixed spinor. The
energy eigenvalue \(E\) then satisfies:

\[
E^2_0(k) = \hbar^2 (k^2 + n^2 / R^2)
\]

now, due to the antiperiodicity of the \(\psi'\), we require \(n + \frac{1}{2}\)
to be integer. Hence, \(E_n(k)\) in equation\[7\]above, all corre-
spond to massive Dirac dispersions whose mass increases
as \(R \to 0\).

We now consider introducing a texture in the order
parameter. A strength ‘\(l\’\) is readily introduced by the
spin rotation \(U_z(l\phi)\). The Hamiltonian then is:

\[
H_l = U_z(l\phi) H_0 U_z(-l\phi)
\]

The eigenstates \(\psi\) of \(H_l\) can be obtained by the unitary transformation \(\psi = U_z([-l \phi] \psi')\), and the transformed

\[\text{Dirac Theory on a Curved Surface:}\]

On a flat surface, the eigenstate remains at low energy even when the ring ra-

radius is shrunk to zero, here, the Dirac particle acquires a

Berry’s phase of \(\pi\) on rotating around the cylinder sur-

face, which excludes the zero angular momentum state. Hence on shrinking the radius, no low energy states re-

main, and the bulk insulator is recovered. However, if a
topological defect of the spin-orbit coupling matrix is in-

tered through the cylinder, an additional Berry’s phase of

\(\pi\) is now acquired by the electrons. This ultimately
results from the rotation of the electron’s spin by \(2\pi\), on

following the texture. With this additional phase, the zero angular momentum mode is allowed, and a low en-
ergy propagating mode results when the cylinder radius is

shrunk to zero. These are the topologically protected

one dimensional modes in the core of the defect. Note,
since we are establishing the presence of a topologically

protected excitations, it is sufficient to use a simple Dirac
dispersion for the surface states of the strong topologi-

cal insulator, since a general surface state can always be

adiabatically mapped to it. We first describe the surface

Dirac hamiltonian in the presence of curvature, and ap-

ply this to the case of a cylinder with a defect inserted

through it.

\[\text{FIG. 2: Up: The density distribution of a midgap mode}\]

\((k = 1.05, E = 0.25)\) in the \(\hat{a}_1, \hat{a}_2\) plane, the mode is

well localized at the \(l = 1\) vortex, the other state \((k = 1.05, E = -0.25)\)

is well localized at the \(l = -1\) antivortex; Down: Electronic

spectrum of diamond lattice strong TMI along

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IV. SHANKAR MONOPOLE IN THREE DIMENSIONS

The line vortex is not the only nontrivial texture in 3D. The other texture we study is the Shankar monopole, a mapping \( S_3 \rightarrow SO(3) \) characterized by the homotopy classification \( \pi_3(SO(3)) = \mathbb{Z} \) \[18\]. Imagine an identical phase farway from the monopole, where matrix \( \overrightarrow{R}(\hat{n}, \varphi) \) is independent of \( \hat{r} \), we can identify the infinity of real space \( R_\infty \) thus obtain \( S_3 \). As an specific example here the \( \overrightarrow{R} \) matrix connecting \( \vec{p} \) and \( \vec{\sigma} \) is \( \overrightarrow{R}(\hat{r}, r) = \exp \left( i \theta (r) \hat{r} \cdot \vec{J} \right) \), where \( \hat{r} \) and \( r \) are the directional vector and distance from the origin to the site linking \( i \) and \( j \), and \( \vec{J} \) are classical rotation generators in three dimensions. The rotation axis \( \hat{n} = \hat{r} \), and the rotation angle is \( \theta(r) \), a function 0 at the origin and smoothly increases to \( 2\pi (l \in \mathbb{Z}) \) at infinity. The homotopy class \( \pi_3(SO(3)) \) is described by integer \( l \), suggesting the base manifold wraps the target manifold \( l \) times. It is protected against any continuous deformation. This is a zero dimensional defect so the localized states should be localized charge at the monopole, if any.

However, numerical results show this topological defect does not carry localized states even in the strong TMI phase. We studied a single monopole at the center of a \( 32^3 \) unit cell system. To treat the large system size we found a way to sidestep a complete diagonalization of the spectrum. Instead, we estimate the boundaries of the energy eigenstates using ARPACK (Arnoldi Package), and shift the spectrum so that all states below (above) the band gap are at negative (positive) energies. Then, we only need to look at the difference in the number of negative and positive energy eigenvalues, to determine the monopole charge. This can be done via an efficient \( LDL^T \) factorization, where the Hamiltonian is factorized into a lower triangular matrix \( L \) and a diagonal matrix \( D \). The entries of the diagonal matrix preserves the sign of the eigenvalues, but not their magnitude. Counting the number of positive and negative eigenvalues is then readily accomplished. While smaller system sizes sometimes show charged monopoles, at the largest sizes, they are found to be neutral. We conclude that the Shankar monopole texture does not carry charge in the TMI phase.

V. TOPOLOGICAL MOTT INSULATOR IN A MICROSCOPIC MODEL - EXTENDED HUBBARD MODEL ON THE DIAMOND LATTICE

We now discuss the question of realizing the 3D TMI phase beginning with a microscopic model with full spin rotation symmetry. We consider an extended Hubbard model on the diamond lattice within mean field theory.
As always, the results of such a mean field treatment should be treated with caution especially since strong interactions are involved. Nevertheless, we use this analytically tractable approach to obtain a range of parameters where the TMI phase is stabilized over the other obvious candidate phases - the disordered semi-metal, antiferromagnetic insulator (or spin density wave: SDW) and the charge density wave (CDW). Realizing the 3D TMI which completely breaks spin rotation symmetry spontaneously, requires, in mean field theory, further neighbor repulsion (between second than third nearest neighbors) as well as a small antiferromagnetic coupling between second neighbors, as shown in Fig. 5.

We now discuss the details of this mean field treatment. The model Hamiltonian we study is an extended Hubbard model on a 3D diamond lattice at half filling (Fig. 4)

\[
H = - \sum_{\langle ij \rangle, \sigma} \langle c_{i \sigma}^\dagger c_{j \sigma} + h.c. \rangle + U \sum_i n_{i \uparrow} n_{i \downarrow} + \sum V_{ij} \rho_i \rho_j + J \sum \langle i j \rangle \vec{S}_i \cdot \vec{S}_j
\]

where \( t \) is the nearest neighbor hopping strength, \( J \) is the second nearest-neighbor antiferromagnetic coupling strength between spins \( \vec{S}_i = \vec{c}_i^\dagger \vec{c}_i \), and \( V_{ij} = V_2 \) for second nearest-neighbor repulsion, \( V_{ij} = V_3 \) for third nearest-neighbor repulsion while \( U \) is the onsite repulsion strength. All of these operate within the same sublattice as can be seen from figure Fig. 4. For simplicity, we assume no nearest neighbor interaction: \( V_1 = 0 \); however, as long as \( V_1 \) (or fourth-nearest neighbor repulsion \( V_4 \)) is not so large that a nearest-neighbor charge density wave becomes energetically favored, they can be included but will be irrelevant to our mean field results. We neglect further neighbor interactions. \( n_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma} \) is the number operator on site \( i \) for spin \( \sigma \), and \( \rho_i = n_{i \uparrow} + n_{i \downarrow} - 1 \). Note the Hamiltonian has full \( SU(2) \) spin rotation symmetry.

Without repulsive interaction the system is in a semimetal phase with gapless excitations along lines in the Brillouin zone (‘Dirac lines’) and a vanishing DOS at the Fermi level. We turn on interactions and investigate possible phases including the Topological Mott Insulator, second and third nearest neighbor charge density wave (CDW) insulators, and nearest-neighbor spin density wave (SDW) insulator. Note, the diamond lattice is composed of a FCC Bravais lattice, plus a two site basis that forms the two sublattices. The natural SDW phase has alternating spin densities on two sublattices, resulting from the effective antiferromagnetic coupling from nearest neighbor hopping and \( U \). Note, this is a \( q = 0 \) order, i.e. preserves lattice translations. In contrast, the likely CDW orders resulting from second and third neighbor repulsion break translation symmetry within each sublattice. The phases can be mapped to a 3D Ising model on an FCC lattice[10], and both the second and the third nearest neighbor CDWs has the same charge density distribution for two sublattices but nonuniform distribution from unit cell to unit cell. Finally, in the TMI phase one develops second nearest-neighbor correlations \( \langle c_{ij \sigma}^\dagger c_{j \sigma'} \rangle \sim i\vec{\sigma}_{\sigma'} \cdot \vec{R} \cdot (\vec{d}_i \times \vec{d}_j) \) that mimic the spin orbit interaction and breaks the \( SU(2) \) symmetry completely. Within the mean field approximation we solve the ground state energy for each phases in the following, and the resulting phase diagram with fixed \( J = 0.3t \) is shown in Fig. 5. Note there is a TMI phase in the center.

We now discuss the mean field energetics of these phases in more detail.

(i) Semimetal: For relatively weak interactions, the semimetal phase arising from the nearest neighbor hopping model on the diamond lattice remains stable due to the vanishing density of states at the Fermi energy. This phase retains all symmetries of the Hamiltonian.

(ii) Spin Density Wave In the limit of large onsite repulsion \( U \) the SDW phase with opposite spin on the two sublattices is stabilized. More precisely, if \( U - 24J \gg V_2 \), the SDW phase becomes energetically favorable. Define the order parameter \( \theta \)

\[
\langle c_{j1}^\dagger c_{i1} \rangle = \langle c_{j1}^\dagger c_{j1} \rangle = \cos^2 \theta, \langle c_{i1}^\dagger c_{i1} \rangle = \langle c_{j1}^\dagger c_{j1} \rangle = \sin^2 \theta
\]

The ground state energy per unit cell is calculated using mean field approximation:

\[
E_{SDW} = \frac{U}{2} + \left( \frac{U}{2} - 12J \right) \chi - \frac{1}{L^3} \sum_k \sqrt{(U - 24J)^2 \chi + 4 |t(k)|^2}
\]

Here \( \chi = \cos^2 \theta \). \( \chi = 0 \) denotes the semimetal phase. \( t(k) = \sum c_{n \vec{k}}^\dagger \tau_n \), \( \tau_n = 1, 2, 3, 4 \) are the vector from one atom to its nearest neighbor. \( L \) is the number of points along each direction within the first Brillouin Zone.

(iii) Charge Density Wave In the limit of strong further neighbor repulsion \( V_2, V_3 \), a CDW is expected. The
problem with just the density repulsion can be mapped to the FCC lattice Ising model. In that context it is known that \( V_2 \) will favor a model is called a Type III CDW phase, while \( V_3 \) will favor a type II CDW phase, described below. The type III CDW phase has Neel state in the (100) plane and frustrated arrangement between neighboring planes which leads to a \( Z_2 \) degeneracy per plane; the type II CDW phase can be described as a combination of four independent simple cubic CDWs. The CDW phase is important despite the frustration. As a matter of fact, in Ref. [12] the second nearest neighbor CDW phase, which the authors neglected, will dominate the large \( V_2 \) region and the Quantum Anomalous Hall phase can be realized only with inclusion of \( U \). To suppress the CDW phases, we choose the ratio of \( V_3/V_2 \) to be 1/2 so the system is close to the transition between type II and type III CDW phases. Hereafter we fix \( V_3 = V_2/2 \), and point out that the phase diagram is similar without \( V_3 \) but the TMI phase will generally occur at a larger \( U \) region.

Assuming inversion symmetry and SRS are intact, we define order parameter \( \rho \) for type III CDW phase
\[
\langle c_{\sigma}^\dagger c_{\sigma} \rangle = \langle c_{\sigma}^\dagger c_{\sigma} \rangle = \frac{1 + \rho}{2}, \langle c_{\sigma}^\dagger c_{\gamma} \rangle = \langle c_{\gamma}^\dagger c_{\gamma} \rangle = \frac{1 - \rho}{2}.
\]
where footnote 1 and 3 are on the first sublattice of two neighboring unit cells and footnote 2 and 4 are on the second sublattice and \( \sigma \) is the spin index. The energy per original unit cell is
\[
E_{\text{CDW}} = 3V_2\rho^2 + U(1 - \rho^2)/2
\]
- \[
\frac{2}{L^3} \sum_k \sqrt{g_1^2 + g_2^2 + g_3^2} \pm \sqrt{4g_1^2(g_2^2 + (g_2g_3^2 + g_2^2g_3^2)^2)}
\]
where \( g_1 = (3V_2 - U/2) \rho \), \( g_2 = t \left(1 + e^{i\vec{d}_1} \right), g_3 = t \left(e^{i\vec{d}_2} + e^{i\vec{d}_3} \right), \) and \( \vec{a}_i \) are the lattice vectors for the FCC lattice. The momentum summation is over \( L^2/2 \) points of the unit cell doubles. The CDW instability is signalled by a non-zero \( \rho \).

(iv) Topological Mott Insulator More importantly, similar to the QSH phase in 2D [12], at intermediate couplings the TMI phase is favored, with order parameters:
\[
\langle c_{\sigma}^\dagger c_{\gamma} \rangle = i \langle \bar{\chi}_{ij} \cdot \hat{\sigma} \rangle_{ss} = i|\chi| \left( \begin{array}{cc} \cos\theta_{ij} & \sin\theta_{ij}e^{-i\varphi_{ij}} \\ \sin\theta_{ij}e^{i\varphi_{ij}} & -\cos\theta_{ij} \end{array} \right)
\]
where \( i, j \) are second nearest neighbors. Our mean field ansatz assumes for simplicity that all \( \bar{\chi}_{ij} \) have the same magnitude but their directions are arbitrary and described by the angles \( \theta_{ij} \) and \( \varphi_{ij} \). Note \( \bar{\chi}_{ij} = -\bar{\chi}_{ji} \) for Hermiticity. Lattice translation, rotation and inversion symmetries are also considered to be intact. This implies that the order parameters on the other sublattice are the negative of these. We decouple the Hamiltonian
\[
H = \frac{UL^3}{2} + 24L^3(V_2 - J)|\chi|^2 - \sum_k \left(t(k)c_k^\dagger I_\sigma \otimes \tau^- c_k \right) + h.c. - \sum_k \left(V_2 - J)|\chi| \sin \left( \vec{k} \cdot \vec{d}_{ij} \right) \right]
\]
where the summation is over the two occupied bands, \( \vec{d}_{ij} \) are the vector from on site to its six second nearest neighbors(one for each opposite pair). We then obtain the ground state energy per unit cell:
\[
E_{\text{TMI}} = \frac{U}{2} + 24(V_2 - J)|\chi|^2
\]
- \[
\frac{2}{L^3} \sum_k \left|\sum_{\langle i<j \rangle} |t(k)|^2 + 4(V_2 - J)^2|\chi|^2 \right| \sum_{\langle i<j \rangle} \sin \left( \vec{k} \cdot \vec{d}_{ij} \right) \tilde{\chi}_{ij}
\]
where \( \tilde{\chi}_{ij} = (\sin\theta_{ij}\cos\varphi_{ij}, \sin\theta_{ij}\sin\varphi_{ij}, \cos\theta_{ij}) \).

It is straightforward to see that the energy only depends on \( |\chi| \) and the relative angles between \( \tilde{\chi}_{ij} \). Under global rotation to all \( \tilde{\chi}_{ij} \) the energy remains invariant and directly leads to an \( SU(2) \) degeneracy.

This is not a TMI phase in the strict sense, since there are dirac nodes at the Fermi level. However, an arbitrarily small distortion of the lattice will introduce anisotropy of nearest neighbor hopping strengths \( t_{\text{dist}}(k) = \sum_{n=1}^4 t_n e^{ik \cdot \vec{d}_n} \) and an effective mass that leads to a gap of size \( \delta \) [1]. In the simplest case that one nearest neighbor hopping strength is different from the other three \( t_{\text{dist}}(k) = t(k) + \delta t \), a stronger bond \( \delta t > 0 \) will lead to a strong TMI phase while a weaker bond \( \delta t < 0 \) will lead to a weak TMI phase.

Phase Diagram: For each phase, we search for the global minimum with respect to its order parameters and compare different phases. Numerical evaluation of energies was done on a Brillouin zone with \( 40 \times 40 \times 40 \) k space points. For simplicity we present the phase diagram with a fixed next nearest antiferromagnetic coupling strength \( J = 0.3t \), and \( V_3 = 0.5V_2 \) (Fig. 5). The semimetal phase exists at small \( U \) and \( V_2 \) region; the CDW phase occurs at large \( V_2 \); the SDW phase occurs at large \( U \). Most importantly, there is a TMI phase in the center of the phase diagram.

This TMI phase has second nearest neighbor correlation similar to that arising from spin orbit interactions in the Fu-Kane-Mele model on the same lattice, except, of course for an arbitrary SU(2) spin rotation [1], \( \tilde{\chi}_{ij} \sim \vec{R} \cdot (\vec{d}_i \times \vec{d}_j) \) for each second nearest neighbor pair \( i \) and \( j \), where \( \vec{d}_i \) and \( \vec{d}_j \) are nearest neighbor bond vectors connecting this pair of sites, and \( \vec{R} \) is an arbitrary constant three dimensional rotation matrix.
SDW, CDW and TMI are all second order transitions. Other parameters are \( V_3 = V_2/2 \) and \( J = 0.3t \). The system size is \( L = 40 \) for calculation.

If we further increase \( J \) the stability of the TMI phase is enhanced and it now a wider parameter range. However, at still larger values, a different TMI phase, that breaks lattice symmetries is realized via a continuous transition. However, since this occurs in the very large \( U \) regime, where mean field theory may not be accurate, we do not present further details of this phase.

VI. TOWARDS EXPERIMENTAL REALIZATIONS

An experimental realization of the TMI phase must contend with two challenges. First, the system should have weak intrinsic spin-orbit coupling, but strong interactions. Next, the further neighbour repulsion should be substantial compared to the nearest neighbour interactions. We believe these difficulties can be overcome in cold atom system, where intrinsic spin orbit couplings are irrelevant, if particles with electric multipole moments are confined to optical lattice sites. We first discuss a two dimensional example involving electric dipoles, for which a fairly definite experimental setup can be constructed. Although the phase realized here is two dimensional and does not break spin rotation symmetry completely (a \( U(1) \) spin rotation remains unbroken), it illustrates how the necessary ingredients can be assembled. Subsequently we discuss ideas for realizing the three dimensional TMI, the main subject of this paper, using electric quadrupole moments.

2D Case: Electric Dipoles on a diamond lattice layer

Dipole-dipole interactions between hetero-nuclear polar molecules, such as \( \text{Rb}_87 \) and \( \text{K}_{40} \) have already been shown to be strong [24]. Consider a fermionic spin 1/2 molecule, with an electric dipole moment (which is independent of the spin) confined to the sites of an optical lattice. We note here that the diamond lattice has a special property that if the dipole-moment is along the [100] directions, then the nearest neighbor interaction \( V_1 \) vanishes. Thus, the second nearest neighbor interaction \( V_2 \) becomes dominant. However, the difficulty is that within the twelve second nearest neighbors, only interactions between neighbors within a plane perpendicular to the dipole moment are repulsive. This problem can be solved if we restrict the molecules within a two dimensional (111) layer of the diamond lattice (still contain both sublattices and essentially two layers of triangular lattices), as the sites circled in Fig. 1. Then if the dipole moment is perpendicular to the plane all possible nearest neighbor interactions are repulsive.

We solve for the mean field phase diagram of this model, as was done previously for the 3D case. Note, since the lattice is essentially the honeycomb lattice, this is essentially the model studied in Ref. [12]. There exists a 2D-TMI phase at the center of the \( U - V_2 \) phase diagram (Fig. 6). Note this phase diagram differs from the same model in Ref. [12] which has an extended 2D-TMI phase. This is because we also allow for the second nearest neighbor CDW that the authors neglected. Though frustrated, this order will dominate at large \( V_2 \).

The resulting TMI phase in our case has a second nearest neighbor correlation resembling that of a quantum spin Hall state and SU(2) spin rotation symmetry is only broken down to \( U(1) \). The resulting order parameter will be \( SU(2)/U(1) = S_2 \) instead of \( SU(2) \). Since \( \pi_1(S_2) = 0 \) there are no point topological defects - however skyrmions acquire a charge \( 2e \) in this phase. Note, the parameters in the phase diagram seem rather accessible for dipolar molecular systems in this setup, assuming that the onsite \( U \), which results from a combination of dipolar and microscopic interactions, is not too large.

3D TMI: Electric quadrupoles on a distorted diamond lattice

We now discuss some ideas for realizing the 3D TMI. While these are not as straightforward as the ones discussed earlier, we nevertheless offer them as one avenue that presents itself at the current time. Another possible origin of repulsive interaction is the quadrupole-quadrupole interaction. One can show that for two parallel uniaxial quadrupoles (quadrupole tensors are identical and diagonal), the interaction is

\[
E = \frac{3Q^2}{r^5} (3 - 30\cos^2\theta + 35\cos^4\theta)
\]

where \( Q \) is the electric quadrupole moment, \( r \) is the distance between two quadrupoles and \( \theta \) is the angle between the quadrupole symmetry axis and the direction between the quadrupoles.

From this expression if \( \cos^2\theta \approx 0.742 \) the quadrupole-quadrupole interaction will vanish. Therefore, assume the quadrupole moment is along the crystal unit cell \( \hat{z} \)
axis to retain as many symmetries as possible, if we elongate the lattice along one direction to make the nearest neighbor satisfy this condition, we will obtain a system where second nearest neighbor interaction dominates. This gives $c/a \approx 2.40$. Note the distortion brings no change to the Hamiltonian we started with. Within this lattice, the ratio between the repulsive interaction from the second nearest neighbor out of the quadrupole perpendicular plane and that from those in plane is $E_\perp/E_\parallel = 0.945$. The $V_2$ anisotropy is reasonably small, thus we believe the physics we discussed with an isotropic $V_2$ is unchanged. However, in this arrangement, $V_3$ is rather small.

To give an reasonable estimate of the quadrupole strength necessary to drive the system into a TMI phase, we notice the typical nearest neighbor hopping strength in an cold atom system is of order $10^{-8} \sim 10^{-6}$ K limited by the cooling temperature and the typical lattice dimension is about the laser wavelength $0.5 \times 10^{-6}$ m. This leads to a quadrupole of $10^{-18} \sim 10^{-17} e \cdot m^2$, where $e$ is unit charge. This is rather large but maybe realizable in multi-electron molecules. Also, the critical quadrupole moment can be further reduced by lowering the temperature or using lasers with shorter wavelength. Finally, a moderate second nearest neighbor antiferromagnetic coupling may result from second nearest neighbor hopping super-exchange effect. We leave for future work construction of a more realistic setting that can realize the 3D TMI phase.

VI. CONCLUSION

We have argued that appropriate repulsive interactions can induce a spontaneous spin rotation symmetry breaking state, the topological Mott insulator, where spin orbit couplings are induced by interactions.

In addition to exotic surface states, line defects of the order parameter are found to carry protected one dimensional modes along their length in the strong TMI, which provides a bulk signature of this phase. Also, potential experimental directions towards creating these phases in cold atom system are discussed. An interesting open question is whether the form of the spin-orbit interactions near a line defect, and hence these protected line modes, can be realized by suitably modifying the atomic structure in a strong topological band insulator.

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APPENDIX: EFFECTIVE HAMILTONIAN ON A CURVED TI SURFACE

It is known that the effective Hamiltonian for a TI surface has the form of a Dirac equation: $H = \vec{p} \cdot \vec{\sigma}$ when the spin and momentum are parallel and $H = \hat{n} \cdot (\vec{p} \times \vec{\sigma})$ when they are perpendicular, where $\hat{n}$ is the normal direction of the surface. Both the momentum and spin are confined to the surface. More generally, when the angle between spin and momentum is $\theta$ the effective Hamiltonian is:

$$H = (\hat{n}_1 \cdot \vec{\sigma} \cos \theta + \hat{n}_2 \cdot \vec{\sigma} \sin \theta) (\hat{n}_1 \cdot \vec{p})$$

$$+ (\hat{n}_2 \cdot \vec{\sigma} \cos \theta - \hat{n}_1 \cdot \vec{\sigma} \sin \theta) (\hat{n}_2 \cdot \vec{p})$$

where $\hat{n}_1$ and $\hat{n}_2$ are orthogonal directions in plane.

One would tends to apply the same Hamiltonian to a curved surface. However, here we claim the effective Hamiltonian on an arbitrary shaped TI surface is:

$$H = (\hat{n}_1 \cdot \vec{\sigma} \cos \theta + \hat{n}_2 \cdot \vec{\sigma} \sin \theta) (\hat{n}_1 \cdot \vec{p})$$

$$+ (\hat{n}_2 \cdot \vec{\sigma} \cos \theta - \hat{n}_1 \cdot \vec{\sigma} \sin \theta) (\hat{n}_2 \cdot \vec{p})$$

$$+ \frac{\hbar}{2} \left( \frac{1}{R_1} + \frac{1}{R_2} \right) \sin \theta + i \hbar \left( \vec{\sigma} \cdot \hat{n}_3 \right) \left( \frac{1}{R_1} + \frac{1}{R_2} \right) \cos \theta$$

where $\hat{n}_1$ and $\hat{n}_2$ are tangent vectors of the surface with radius of curvature $R_1$ and $R_2$, respectively, and $\hat{n}_3$ is the normal vectors. $\theta$ is the constant angle between spin and momentum in the corresponding flat surface effective theory. Note when the surface is flat, the last two terms vanish and the Hamiltonian goes back to the one describing the flat surface mode.
This Hamiltonian can be systematically derived from the inclusion of the connection form for a curved space\[21, 22\], but an alternative method we used is to ensure hermiticity and anticommutation relation \(\{H, \hat{\sigma} \cdot \hat{n}_3\} = 0\) since the spin is in the surface plane\[23\], with the help of the relations: \((\hat{n}_i \cdot \vec{p}) \hat{n}_j = i \hbar \delta_{ij} \hat{n}_3/R_i\), \((\hat{n}_i \cdot \vec{p}) \hat{n}_3 = -i \hbar \hat{n}_i/R_i\) for \(i = 1, 2, 3\), and 
\[\left(\hat{\sigma} \cdot \hat{A}\right) \left(\hat{\sigma} \cdot \hat{B}\right) = \hat{A} \cdot \hat{B} + i \hat{\sigma} \cdot \left(\hat{A} \times \hat{B}\right).\]

The additional terms arising from the space curvature are canceled by the inclusion of the connection form. Thus, the above effective Hamiltonian well describes a curved TI surface.

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