Interacting surface states of three-dimensional topological insulators

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We numerically investigate the surface states of a strong topological insulator in the presence of strong electron-electron interactions. We choose a spherical topological insulator geometry to make the surface amenable to a finite size analysis. The single-particle problem maps to that of Landau orbitals on the sphere with a magnetic monopole at the center that has unit strength and opposite sign for electrons with opposite spin. Assuming density-density contact interactions, we find superconducting and anomalous (quantum) Hall phases for attractive and repulsive interactions, respectively, as well as chiral fermion and chiral Majorana fermion boundary modes between different phases. Our setup is preeminently adapted to the search for topologically ordered surface terminations that could be microscopically stabilized by tailored surface interaction profiles.

Introduction.—Three-dimensional topological insulators (3DTIs) [1–6], since their prediction in 2007, realize a quantum state of matter which triggered enormous interest in condensed matter physics, and have been subsequently discovered in various material classes [7–11].

When viewed as a symmetry-protected topological phase, 3DTIs exhibit a gapped bulk with two-dimensional gapless edge states protected by U(1) electron number conservation and time reversal symmetry (TRS), forbidding any adiabatic deformation into a trivial insulator. The effective electromagnetic field theory characterizing the 3DTI contains a topological axial term, with quantized coefficient $\theta = \pi$ for fermionic 3DTIs as compared to $\theta = 0$ for TRS trivial insulators [12]. On the surface of a 3DTI, where $\theta$ changes from 0 to $\pi$, the gauge invariance of this topological field theory demands the presence of a half-integer Chern–Simons term at the surface. In the absence of symmetry breaking, this Chern–Simons term is precisely what allows a single Dirac cone state to be gauge invariant and hence consistently defined on the 3DTI surface, whereas a single massless Dirac field in odd space-time dimensions would usually exhibit a parity anomaly [13–15].

When the protecting U(1) particle number symmetry is broken, such as by a superconducting proximity effect, the 3DTI surface yields an unconventional gapped s-wave superconductor with Majorana modes in its vortex cores [16]. Upon breaking TRS, such as by a magnetic coating on the surface, the single surface Dirac cone gaps out, and the Chern-Simons boundary term of the axion bulk action manifests itself as a $\nu = 1/2$ quantum Hall effect [12] without fractionalized excitations. The axion term implies the Witten effect [17] by which a odd-half integer charge binds to magnetic monopoles in the bulk of a 3DTI (see also e.g. Ref. 18).

All aforementioned properties of 3DTIs do not involve interactions in the bulk or at the surface. Assuming that the gapped 3DTI bulk is negligibly renormalized by interactions, it remains to be investigated how interactions could affect the 3DTI surface. To begin with, interactions could contribute to breaking the protecting symmetries explicitly or spontaneously. Transcending the mean-field picture, however, interactions could also give rise to a gapped surface state with intrinsic topological order, allowing a new kind of phase to enter the realm of competing quantum states of matter on a 3DTI surface. Investigations of bosonic 3DTI surface states established that such gapped surface states in the absence of symmetry breaking are indeed possible for certain kinds of topological order [18–22]. Soon thereafter, this idea has been formulated for the physically more relevant fermionic analogue [23–26]. All these conceptually important works rely on consistency arguments on the level of topological field theories and constructions that employ contrived exactly soluble models. What type of physically attainable Hamiltonians would exhibit these exotic ground states remains a challenging question. [27]

Haldane [28] has recently pointed out that, as the topological surface state only has support in a 2D $k$-space region with an area $A_k$ that may be much smaller that the Brillouin zone, the surface electrons obey an “uncertainty principle” where they cannot be localized within an area smaller than $(2\pi)^2/A_k$, analogous to the “magnetic area” $h/|eB|$ for electrons confined to a 2D Landau level. He noted that this makes the surface dynamics insensitive to the atomic-scale features of the surface, and leads to a continuum “fuzzy quantum geometry” description in which exact diagonalization (ED) studies of strongly-interacting systems becomes practical, as in the fractional quantum Hall effect. Here we will describe an implementation of this idea using the spherical geometry, instead of the periodic (torus) geometry of Ref. [28]. As a consequence of the inherent “fuzziness”, one might expect that, in the presence of interactions, featureless quantum liquid ground states may be favored over translational-symmetry-breaking order such as lattice-scale antiferromagnetism or charge-density waves.
In this Letter, we develop a microscopic framework for numerically studying strong interaction effects on 3DTI surfaces. While a consensus regarding possible states of matter consistent with the constraints given by the 3DTI setup is emerging, little is known which of these states might actually be realized for which kind of interaction profile. For this purpose, we investigate the surface states of a 3DTI on a sphere [29], the geometry where these states have the maximally attainable symmetry but no boundary. The single Dirac cone at the surface is intimately related to the Landau level quantization on the sphere [30], with an individual magnetic monopole of unit (anti-)charge for spin up (down) electrons at the center of the sphere, so as to respect TRS. We study the effect of a density-density contact interaction $U$. We find an $s$-wave superconductor triggered by attractive $U$ as a consequence of spontaneous U(1) symmetry breaking. For repulsive $U$, the gapless Dirac cone persists in an extended regime of parameter space. In the limit of strong interaction, however, we find ferromagnetic phases of broken TRS. These are the $\nu = 1/2$ anomalous quantum Hall effect and the gapless anomalous Hall effect for fillings at and away from the Dirac point, respectively.

3DTI surface states on the sphere.—In the limit of long wavelengths, the surface states of a strong 3DTI are described by a two-dimensional Dirac equation given by

$$H = v\hat{n} \times \sigma$$

(1)

where $v$ denotes the Dirac velocity of the surface states, $\hat{n}$ is the surface normal, and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ twice the physical electron spin vector. For a spherical TI with radius $R$, Imura et al. [29] derived that (1) becomes

$$H_0 = \frac{v}{R} (\sigma_x \Lambda_\theta + \sigma_z \Lambda_\varphi)$$

(2)

where

$$\Lambda = -i \left[ \sigma_x \frac{\partial}{\partial \theta} - \sigma_y \frac{1}{\sin \theta} \left( \frac{\partial}{\partial \varphi} - \frac{i}{2} \sigma_z \cos \theta \right) \right]$$

(3)

is the dynamical angular momentum of an electron in the presence of a magnetic monopole with strength $2\pi \sigma_z$, and $(r, \theta, \varphi)$ are spherical coordinates. The monopole strength or Berry flux through the sphere is hence $2\pi$ for $\uparrow$ spins (i.e., spins pointing in $e_r$ direction) and $-2\pi$ for $\downarrow$ spins (i.e., spins pointing in $-e_r$ direction) [31]. The origin of this Berry phase is easily understood. Since the coordinate system for our spins (to which our Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ refer to) is given by $e_\varphi, -e_\theta, e_r$, it will rotate as the electron is taken around the sphere. For general trajectories, the Berry phase generated by this rotation is given by $\frac{1}{2}$ times the solid angle subtended by the trajectory. Formally, this phase is generated by a monopole with strength $2\pi$ at the origin. Since the model preserves time reversal invariance, the monopole must be of opposite sign for opposite spins.

Substitution of (3) into (2) yields

$$H_0 = \frac{v}{R} \hbar_0, \quad \hbar_0 = \begin{pmatrix} 0 & \hbar^+ \\ \hbar^- & 0 \end{pmatrix},$$

(4)

with

$$\hbar^\pm = \mp \left( \partial_\theta + \frac{1}{2} \cot \theta \right) + i \hbar_\varphi \sin \theta,$$

(5)

Eq. (4) describes a Dirac hamiltonian in the sense that the eigenvalues of $\Lambda_\theta$ are diagonal. Apart from an overall numerical factor, $\Lambda_{s_0} = -\frac{1}{\sin \theta} \sin \theta \partial_\theta - \frac{1}{\sin^2 \theta} (\partial_\varphi - is_0 \cos \theta)^2$ is the hamiltonian of an electron moving on a sphere with a monopole of strength $4s_0$ in the center [30]. The Landau levels on the sphere are spanned by two mutually commuting SU(2) algebras, one for the cyclotron momentum ($\mathbf{S}$) and one for the guiding center momentum ($\mathbf{L}$). The Casimir of both is given by

$$L^2 = S^2 = s(s+1),$$

(8)

where $s = |s_0| + n$ and $n = 0, 1, \ldots$ is the Landau level index. With $A^2 = L^2 - s_0^2 = (n+1)^2 - \frac{1}{4}$ for $|s_0| = \frac{1}{2}$, we see that the eigenvalues of $\hbar_0^2$ are given by $\epsilon^2 = (n+\frac{1}{2})^2$.

In terms of the spinor coordinates $u = \cos \frac{\theta}{2} e^{i\frac{\varphi}{2}}$, $v = \sin \frac{\theta}{2} e^{-i\frac{\varphi}{2}}$ introduced by Haldane [32], and their complex conjugates $\bar{u}, \bar{v}$,

$$S^z + iS^y = S^+ = u\bar{u} - v\bar{v},$$

$$S^- = iS^y = S^- = \bar{v}\bar{u} - \bar{u}\bar{v},$$

$$S^x = \frac{1}{2} (u\partial_u + v\partial_v - v\partial_u - u\partial_v),$$

$$L^z + iL^y = L^+ = u\partial_u + \bar{v}\partial_v,$$

$$L^- = iL^y = L^- = v\partial_v \bar{u} - \bar{u}\partial_v,$$

$$L^x = \frac{1}{2} (u\partial_u - v\partial_v - v\partial_u + u\partial_v),$$

(9)

(10)

The physical Hilbert space is restricted to states with $S^z$ eigenvalue $s_0$. $S^z\phi = s_0\phi$ [30]. With the $\uparrow$ and $\downarrow$ spin components of the eigenstates of $\hbar_0$ thus restricted respectively (i.e., $S^z\phi^\uparrow = \frac{1}{2}\phi^\uparrow$ and $S^z\phi^\downarrow = -\frac{1}{2}\phi^\downarrow$), it is easy to show that $\hbar^-\phi^\uparrow = -S^-\phi^\uparrow$ and $\hbar^+\phi^\downarrow = -S^+\phi^\downarrow$, and hence that

$$\hbar_0 = \begin{pmatrix} 0 & -S^+ \\ -S^- & 0 \end{pmatrix}.$$

(11)

The Dirac property of $\hbar_0$ and the eigenvalues of $\hbar_0^2$ imply that the eigenstates take the form

$$\hbar_0\psi_{nm}^\lambda = \lambda(n+1)\psi_{nm}^\lambda, \quad \psi_{nm}^\lambda = \begin{pmatrix} \phi_{nm}^\lambda \\ \lambda\phi_{nm}^\lambda \end{pmatrix},$$

(12)
where $\lambda = \pm 1$ distinguishes positive and negative energy solutions, and $m$ is the eigenvalue of $L^z$. With $h^+ h^- = S^- S^+ + 1$, we find [30]

$$\phi^{\dagger}_{nm} = (L^-)^{s-m}(S^-)^n u^{2s} = (L^-)^{s-m}\bar{v}^n \bar{u}^{n+1}, \quad (13)$$

where $s = n + \frac{1}{2}$ and $m = -s, -s + 1, \ldots, s$. With (12),

$$\phi^{\dagger}_{nm} = -\frac{S^-}{n+1} \phi^{\dagger}_{nm} = -(L^-)^{s-m} u^n \bar{v}^{n+1}. \quad (14)$$

The number of degenerate states in the $(n+1)$-th Landau level with energy $\epsilon = \lambda(n+1)$ is hence $2(n+1)$, and grows linearly with $|\epsilon|$, as required for a Dirac cone (see Fig. 1).

$H_0$ is invariant under both time reversal $T \equiv -i\sigma_y K$ (where $K$ denotes complex conjugation) and parity $P \equiv \sigma_z P_0$ (where $P_0$ takes $\theta \rightarrow \pi - \theta$). The basis states (12) transform according to

$$T \psi^\lambda_{nm} = \lambda (-1)^m - \frac{1}{2} \psi^\lambda_{n-m,m}, \quad (15)$$

$$P \psi^\lambda_{nm} = \lambda (-1)^{n+m+1} \psi^\lambda_{nm}. \quad (16)$$

**Momentum space cutoff.**—The Dirac Hamiltonian $H_0$ (or $h_0$) governs the behavior of the surface states of a topological insulator for energies close to the Dirac nodal point. At higher and lower energies, the surface states merge with the bulk conduction and valence bands, respectively, and their weight on the surface diminishes. Consequently, even strong electron-electron interactions of the order of the bulk gap will only induce small matrix elements between bulk and surface states. It is hence sensible to study the effects of strong interactions on the surface states alone, when working in the Fock space constructed from the single-particle eigenstates of $H_0$ with $n \leq n_0$ for some Landau level cutoff $n_0$. Importantly, it is impossible to build orbitals in position space that are localized on length scales smaller than $2\pi R/n_0$ in this restricted Hilbert space. Thus even if the interactions are much larger than the kinetic energy scale $v/R$, the problem does not reduce to a classical limit [28]. This is somewhat reminiscent of the Landau level problem, with the important difference that single-particle states are exponentially localizable on long enough distances on the topological insulator surface while they are power-law decaying in a Landau level on a compact manifold.

**Interactions.**—On this restricted single particle Hilbert space, we consider a contact interaction

$$H_{\text{int}} = U \int d^2 \mathbf{r} \rho_\uparrow(\mathbf{r}) \rho_\downarrow(\mathbf{r}), \quad (17)$$

where $\rho_\sigma(\mathbf{r})$ is the density operator of electrons with spin $\sigma$ at position $\mathbf{r}$. This interaction preserves $T$, $P$, the number of particles $N_p$, and the total angular momentum $M = \sum_{i=1}^{N_p} m_i$. We have studied the phase diagram of this model as a function of $UR/v$ and electron filling via exact diagonalization up to $n_0 = 2$ (24 single particle states) (see Fig. 2).

**Magnetic phases.**—At half filling and for $UR/v > 10$, the ground state is a ferromagnet. In the finite system, we find two quasi-degenerate ground states $|FM_\pm\rangle$ with $P = \pm 1$ in the $M = 0$ sector. The magnetization operator in $e_z$ direction, $\Sigma_3 \equiv \int_{S_2} d^2 \mathbf{r} [\rho_\uparrow(\mathbf{r}) - \rho_\downarrow(\mathbf{r})]$, anticommutes with the parity operator $P$, since $\Sigma_3 \psi^\lambda_{nm} = \psi^{-\lambda}_{nm}$. 

**FIG. 1.** (Color online) Single-particle spectrum of (11) that describes the surface states of a spherical topological insulator, including the 24 states closest to the Dirac point. The single-particle quantum numbers are the “Landau level” index $n = 0, 1, 2, \ldots$, the angular momentum $m = -(n + 1/2), \ldots, (n + 1/2)$, and the particle-hole index $\lambda = \pm 1$.

**FIG. 2.** (Color online) Phases of the topological insulator surface states subject to the contact interaction (17) for a Hilbert space restriction $n_0 \leq 3$ as a function of interaction strength $UR/v$ and filling $\nu = N_p/\left[2(n_0 + 1)(n_0 + 2)\right]$. Gapped phases are found as an $s$-wave superconductor (SC) and an anomalous quantum Hall effect (AQHE) coinciding with ferromagnetism. Gapless phases include the semimetal (SM) at half filling, a Fermi liquid (FL), and anomalous Hall effect (AHE) coinciding with ferromagnetism. Left panel: Lower end of the energy spectrum in the limit $UR/v \rightarrow -\infty$ as a function of the particle number $N_p$. The superconducting ground state is evidenced by the degeneracy of the ground states in all sectors of even $N_p$. Right panel: Magnetization $M$ of the 2-fold (4-fold) quasi-degenerate ground state manifold in the limit $UR/v \rightarrow \infty$ as a function of the even (odd) $N_p$. It evidences spontaneously broken TRS in the thermodynamic limit.
finite size energy spectra for a system restricted to the boundary between two ferromagnetic domains and a ferromagnet-superfluid domain wall, respectively. Shown are finite size energy spectra for a system restricted to the $n_0 \leq 2$. Magnetic domains on the northern/southern hemisphere are enforced by Hamiltonian (2) with a mean-field magnetization $m_0 \langle \theta \rangle \sigma_z$ with $|m_0| = 3.5v/R$, while the superfluid domain is interaction-induced with $U = -15v/R$. In (a), the level counting is the one expected for a U(1) mode that consists of six states with $m = -5/2, -3/2, -1/2$ assuming that the levels with $m > 0$ are occupied in the half-filled ground state. In (b), the level counting in the fermion parity sectors are as expected if one assumes that the chiral Majorana mode at the boundary consists of three operators with $m = -5/2, -3/2, -1/2$ which do not annihilate the ground state.

This implies that $\langle \text{FM}_+ | \Sigma_3 | \text{FM}_+ \rangle = \langle \text{FM}_- | \Sigma_3 | \text{FM}_- \rangle = 0$. The magnetization of the ferromagnetic ground states with spontaneously broken TRS, which emerge in the thermodynamic limit, is hence given by $\mathcal{M} \equiv \langle \text{FM}_+ | \Sigma_3 | \text{FM}_- \rangle$. A ferromagnetically ordered gapped surface termination of a 3D topological insulator features a half-integer Hall effect—a phase that would not be possible in a pure 2D system without intrinsic topological order. Thus, the ferromagnetic phase also constitutes an anomalous quantum Hall phase. Between two domains of opposite magnetization, there exists a chiral boundary state (see Fig. 3a). Upon hole- or electron doping the anomalous quantum Hall phase, the system enters a anomalous Hall phase without a quantized Hall conductance. At high doping, the ground state is a Fermi liquid which does not violate any symmetry. We distinguish these two phases by the different quasi-degeneracies of the ground state and by computing the magnetization $\mathcal{M}$ in this quasi-degenerate subspace (see Fig. 4). [33]

Superfluid phase.—At negative $UR/v$, the system enters a superfluid phase. For $UR/v \to -\infty$, we find a set of degenerate states at $M = 0$, one in each sector of even particle number $N_p$. Physically, these degeneracies manifest themselves in the Goldstone mode of the superfluid. The low energy excitations above the ground state in each sector of even $N_p$ show the same structure as the spectrum of two electrons subject to an infinite repulsive interaction, which consists of three quasi-degenerate states with $M = -1, 0, 1$. This suggests that the low-energy excitations in the superfluid phase are obtained by breaking up an individual Cooper pair into two electrons which do not interact with the condensate. An s-wave superconducting termination of a 3D topological insulator is a topological superconductor in the sense that it supports Majorana zero energy states in vortex cores and a chiral Majorana mode at the boundary with e.g. a ferromagnetic region of the surface (see Fig. 3b). That we obtain a gapped superconducting state in the limit $UR/v \to -\infty$ is a direct manifestation of the localization properties of the single-particle states. If the single particle states were fully localizable in real space, pairs of electrons could bind into point-like particles and the ground state would be exponentially degenerate.

Conclusions.—We have developed a formalism to study interaction effects on fermionic 3D TI surface states numerically. From the analysis of a two-body contact interaction, we found both ferromagnetic and topologically non-trivial superconducting phases, as well as chiral fermion and chiral Majorana fermion boundary modes between different phases. Several branches of future investigation can be anticipated, such as the application to bosons and studies of more sophisticated interaction profiles. The formalism establishes an ideal testing ground for topologically ordered TI surface states scenarios.

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[33] Phases that become gapless in the thermodynamic limit are hard to detect and discriminate using numerically exact diagonalization. Thus, we expect that the location of all the phase transition points that we determine as a function of $U$ are subject to strong finite-size errors. Since we understand the limits at $U = +\infty$, $U = 0$ and $U = -\infty$, however, the structure of the phase diagram is fixed.