Topological Hubbard Model and Its High-Temperature Quantum Hall Effect

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The quintessential two-dimensional lattice model that describes the competition between the kinetic energy of electrons and their short-range repulsive interactions is the repulsive Hubbard model. We study a time-reversal symmetric variant of the repulsive Hubbard model defined on a planar lattice: Whereas the interaction is unchanged, any fully occupied band supports a quantized spin Hall effect. We show that at 1/2 filling of this band, the ground state develops spontaneously and simultaneously Ising ferromagnetic long-range order and a quantized charge Hall effect when the interaction is sufficiently strong. We ponder on the possible practical applications, beyond metrology, that the quantized charge Hall effect might have if it could be realized at high temperatures and without external magnetic fields in strongly correlated materials.

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High-temperature superconductivity [1] and the quantum Hall effect (QHE) [2] have been two of the central problems in condensed matter physics of the past three decades. The former is related to electrons hopping on a two-dimensional (2D) lattice close to (but not at) half filling, while the latter focuses on fermions in doped semiconductor heterostructures or graphene in a high magnetic field. High-temperature superconductors are strongly interacting systems, with the potential energy about an order of magnitude larger than the kinetic energy. In the QHE, the kinetic energy is quenched by the external magnetic field. Moreover, interactions are important only in understanding the fractional QHE but not in understanding the integer QHE (IQHE).

The possibility that the IQHE could arise in a lattice Hamiltonian without the Landau levels induced by a uniform magnetic field was suggested by Haldane in 1988 [3]. The essence is that, despite the absence of an uniform magnetic field, the system still lacks time-reversal symmetry. More recently, it was shown that the fractional QHE could also emerge in flat topological bands when they are partially filled [4–9] (see also [10]). These recent developments point to a natural marriage between the QHE and partially filled [4–9] (see also [10]). These recent developments point to a natural marriage between the QHE and partially filled [4–9] (see also [10]).

In this Letter, we study a quintessential strongly correlated lattice 2D system but with a twist. We consider a time-reversal symmetric fermionic Hubbard model in the limit of large on site repulsion $U$ compared to the bandwidth $W$ of the hopping dispersion but with hopping terms yielding topologically nontrivial Bloch bands in that they each support a quantized spin Hall conductivity when fully occupied [11]. The time-reversal symmetric Hubbard model with a single half filled nested Bloch band has a charge insulating ground state that supports antiferromagnetic long-range order [1]. In contrast, the ground state of our time-reversal symmetric Hubbard model with topologically nontrivial Bloch bands simultaneously displays Ising ferromagnetic long-range order and the IQHE at some commensurate filling fraction. The energy scales that can be attained in lattice models are typically rather high, of the order of atomic magnitudes, i.e., electronvolt. If an interacting system with topological bands can be found so as to display the IQHE at high temperatures, it could be of practical use, as we shall explain after we substantiate our claims.

Study of the topological Hubbard model.—We consider spinful electrons hopping on a bipartite square lattice $\Lambda = A \cup B$ with sublattices $A$ and $B$, where each sublattice has $N := L_x \times L_y$ sites. The Hubbard Hamiltonian with repulsive interactions ($U > 0$) can be written

$$H := \sum_{k \in \text{BZ}} c^\dagger_k H_k c_k + U \sum_{\alpha = A, B} \sum_r n_{k,\alpha} n_{k,\alpha} - \sum_{r, \alpha, \beta} \sum_{\alpha = A, B} n_{k,\alpha} n_{k,\beta}.$$  

The component $c_{k,\sigma,\alpha}^\dagger$ of the operator-valued spinor $c_k^\dagger$ creates an electron with momentum $k$ from the Brillouin zone (BZ) of sublattice $A$ and with spin $\sigma = \uparrow, \downarrow$, whose Fourier transform $c_{r,\sigma,\alpha}^\dagger = \sum_k e^{-ik r} c_{k,\sigma,\alpha}^\dagger$ is exclusively supported on sublattice $\alpha = A, B$. The $4 \times 4$ Hermitian matrix $H_k$ obeys the time-reversal symmetry (TRS)

$$H_{-k} = \sigma_2 H_k^* \sigma_2,$$  

and, owing to a strong intrinsic spin-orbit coupling, the residual spin-rotation symmetry (RSRS)

$$H_{-k} = \sigma_3 H_{+k} \sigma_3 \equiv \begin{pmatrix} h^{(l)}_k & 0 \\ 0 & h^{(l)}_k \end{pmatrix}. $$
where the Pauli matrices $\sigma_1$, $\sigma_2$, and $\sigma_3$ act on the electronic spin-1/2 degrees of freedom. Hence, the two $2 \times 2$ Hermitian matrices $h^{(\sigma)}_k$ with $\sigma = \uparrow, \downarrow$ obey

$$h^{(\sigma)}_{k, \alpha \beta} = h^{(\sigma)}_{-k, \beta \alpha} \quad \forall \, k \in \text{BZ}, \quad \alpha, \beta = A, B, \tag{1d}$$

because of the condition of TRS (1b). Finally, the operator $n_{r, \sigma, \alpha} = c^\dagger_{r, \sigma, \alpha} c_{r, \sigma, \alpha}$ measures the electron density on site $r$ in sublattice $\alpha$ and with spin $\sigma$.

The Hubbard Hamiltonian defined by Eq. (1a) thus has a global $\mathbb{Z}_2 \times U(1)$ symmetry that arises because of the TRS (1b) and the RSRS (1c). We are going to show that TRS is spontaneously broken while the continuous RSRS is shared by the ground state, when this Hubbard Hamiltonian acquires suitable topological properties.

It is the choice for the matrix elements $h^{(\sigma)}_{k, \alpha \beta}$ entering the kinetic energy (1c) that endows the Hubbard Hamiltonian (1a) with topological attributes. We choose

$$h^{(\sigma)}_{k, AB} = h^{(\sigma)}_{k, BA} := w_k e^{-i\pi/4} (1 + e^{i(k_x - k_y)})$$

$$+ e^{i\pi/4} (e^{-ik_x} + e^{ik_y}), \tag{2a}$$

$$h^{(\sigma)}_{k, AA} = -h^{(\sigma)}_{k, BB} := w_k [2t_2 (\cos k_x - \cos k_y) + 4\mu_x],$$

where

$$w_k^{-1} := \kappa \varepsilon_k (1 - \kappa), \quad \kappa \in [0, 1], \tag{2b}$$

and

$$\varepsilon_k := \sqrt{1 + \cos k_x \cos k_y + [2t_2 (\cos k_x - \cos k_y) + 4\mu_x]^2}. \tag{2c}$$

In the noninteracting limit ($U = 0$), this model features four bands with two distinct twofold degenerate dispersions $\pm w_k \varepsilon_k$ [4]. This twofold degeneracy is a consequence of the Kramers degeneracy implied by the TRS (1b). If we denote the corresponding eigenspinors $\chi_{k, \sigma, \lambda} = (\chi_{k, \sigma, \lambda, A}, \chi_{k, \sigma, \lambda, B})$, where $\lambda = \pm$, and choose the normalization $\chi^\dagger_{k, \sigma, \lambda} \chi_{k, \sigma, \lambda'} = \delta_{\lambda, \lambda'}$, $\forall \, k$, then the kinetic energy is diagonalized by using the fermionic creation operators

$$d^\dagger_{k, \sigma, \lambda} := \sum_{\alpha = A, B} \chi^*_{k, \sigma, \lambda, \alpha} c^\dagger_{k, \sigma, \alpha}, \tag{2d}$$

as

$$H_0 := \sum_{k \in \text{BZ}} \sum_{\sigma = \uparrow, \downarrow} \sum_{\lambda = \pm} \lambda d^\dagger_{k, \sigma, \lambda} w_k \varepsilon_k d_{k, \sigma, \lambda}. \tag{2c}$$

Hence, the Bloch states created by $d^\dagger_{k, \sigma, \lambda}$ are generically spread on both sublattices $A$ and $B$. We shall consider only the case in which these bands are separated by an energy gap, i.e., $|t_2| \neq |\mu_x|$. The parameter $\kappa$ controls the bandwidth of these bands. For $\kappa = 1$, the bands are exactly flat with eigenvalues $\pm 1$. The case $\kappa = 0$ corresponds to a tight-binding model on the square lattice that involves only nearest-neighbor ($|t_1| = 1$) and next-nearest-neighbor hopping ($t_2$) together with a staggered chemical potential $\mu_x$ that breaks the symmetry between sublattices $A$ and $B$ [4]. For $\kappa \in (0, 1]$, longer-range hopping is introduced. However, we stress that the Hamiltonian remains local for all $\kappa \in [0, 1]$ since all correlation functions decay exponentially due to the presence of the band gap [4].

The topological properties of the lower pair of bands are characterized by their spin Chern number

$$C_\sigma := (C^\uparrow - C^\downarrow)/2, \tag{3a}$$

where $C_\sigma$ is to be computed from the orbitals of spin-$\sigma$ electrons according to

$$C_\sigma := \frac{i}{4 \pi} \int_{k \in \text{BZ}} \frac{d^2 k}{2 \pi} \nabla_k \cdot (\chi^\dagger_{k, \sigma, -} \chi_{k, \sigma, -}). \tag{3b}$$

Time-reversal symmetry implies $C_1 = -C_\downarrow$ and therefore entails a vanishing of the total (charge) Chern number $C := (C^\uparrow + C^\downarrow) / 2$ of the lower bands. The spin Chern number of the lower pair of bands is given by

$$C_\sigma = \frac{1}{2} \left( \text{sgn} h^{(\sigma)}_{(0, 0), AA} - \text{sgn} h^{(\sigma)}_{(\pi, 0), AA} \right). \tag{3c}$$

Hence, the Bloch bands are topologically trivial whenever $|t_2/\mu_x| < 1$, while the model at half filling exhibits the physics of a quantum spin Hall insulator whenever $|t_2/\mu_x| > 1$. In an open geometry, the spin Hall conductivity is quantized to the value $\sigma_{xy}^{\text{SH}} = eC^2/2\pi$, where $e$ denotes the electric charge of the electron.

We now consider the system with a repulsive Hubbard interaction $U > 0$ at 1/2 filling of the lower band (1/4 filling of the lower and upper bands), i.e., with

$$N_e = L_x \times L_y = N \tag{4}$$

electrons. In all that follows, we assume that $U$ is much smaller than the gap $\Delta_0$ induced by a strong intrinsic spin-orbit coupling between the two pairs of bands. If so, we can restrict the $N_e$-body Hilbert space to the Fock space arising from the single-particle Hilbert spaces of the lower pair of bands.

In the limit of flat bands $\kappa = 1$ and at the commensurate filling fraction (4), the kinetic energy (2e) at fixed spin polarization $S := |\langle \sigma \rangle| = 0, 2, \ldots, N$ in units of $\hbar/2$ has a ground state degeneracy

$$N_g = \left( \frac{N}{N - |\langle \sigma \rangle|} \right)^2. \tag{5}$$

The repulsive Hubbard interaction lifts this degeneracy whenever any one of these states allows a site of $\Lambda$ to be doubly occupied with a finite probability. The only two states with full spin polarization $S = N$,

$$|\Psi_\sigma \rangle = \prod_{k \in \text{BZ}} d^\dagger_{k, \sigma, -}|0\rangle, \quad \sigma = \uparrow, \downarrow, \tag{6a}$$

are immune to the presence of the Hubbard repulsion. More formally, observe that Hamiltonian $H - \mu N_e$ is a
positive semidefinite operator for \( \kappa = 1, U > 0 \), and the chemical potential \( \mu = -1 \). Since
\[
\langle \Psi_{\sigma} | (H + N_c) | \Psi_{\sigma} \rangle = 0, \quad \sigma = \uparrow, \downarrow, \quad (6b)
\]
the two states (6a) belong to the ground state manifold of \( H + N_c \) for any \( U > 0, t_2, \) and \( \mu_c \).

We are going to argue that this pair of degenerate Ising ferromagnets spans the ground state manifold for any \( U > 0 \) and \( |t_2/\mu_c| \neq 1 \). This is achieved by arguing that they are separated from excited states by a many-body gap, a departure from the usual ferromagnetism in flat bands when full spin-1/2 \( SU(2) \) symmetry is not explicitly broken [12]. First, particle-hole excitations of \( |\Psi_{\sigma} \rangle \) that keep \( S = N \) fixed cost an energy \( \Delta_0 > 0 \) and are thus gapped. Second, we ask whether excitations of \( |\Psi_{\sigma} \rangle \) that flip one spin \( (S = N - 2) \) are gapped as well. Any such state can be written as
\[
|\Phi_{\sigma, Q} \rangle = \sum_{k \in BZ} A_k^{(Q)} d_{k+Q, \sigma, \varepsilon}^\dagger d_{k\sigma, \varepsilon} |\Psi_{\sigma} \rangle, \quad \sigma = \uparrow, \downarrow, \quad (7a)
\]
where the center of mass momentum \( Q \) is a good quantum number, and thus \( \langle \Phi_{\sigma, Q} | \Phi_{\sigma, Q} \rangle = \delta_{Q, 0} \) if the normalization \( \sum_{k \in BZ} A_k^{(Q)} A_k^{(Q)} = 1 \) is imposed. One verifies that [13]
\[
\langle \Phi_{\sigma, Q} | (H + N_c) | \Phi_{\sigma, Q} \rangle = U - \frac{U}{N} \sum_{k \in BZ} \left( \sum_{Q} A_k^{(Q)} \chi_{k, \sigma, \varepsilon} \chi_{k, -Q, \sigma, \varepsilon, \varepsilon} \right)^2, \quad (7b)
\]
where the lowest energy state with one spin flipped is characterized by the \( A_k^{(Q)} \) that minimizes Eq. (7b) while satisfying the normalization condition. For example, if the single-particle orbitals are fully sublattice polarized, e.g., \( \chi_{k, \sigma, \varepsilon} \propto (1, 0) \) (topologically trivial), the choice \( A_k^{(Q)} = N^{-1/2} \) minimizes Eq. (7b) with the right-hand side equal to zero. Hence, the fully spin-polarized state \( |\Psi_{\sigma} \rangle \) is a gapless ground state in this case. On the other hand, let us assume that
\[
\chi_{k, \sigma, \varepsilon} \neq (1, 0) \quad \text{and} \quad \chi_{k, \sigma, \varepsilon}^\dagger \neq (0, 1) \quad (8)
\]
hold almost everywhere in the BZ, i.e., up to a set of measure zero. In the thermodynamic limit, where the sum over \( k \) becomes an integral, this delivers from Eq. (7b) the strict inequality [13]
\[
\langle \Phi_{\sigma, Q} | (H + N_c) | \Phi_{\sigma, Q} \rangle > 0. \quad (9)
\]
Hence, assumption (8) is sufficient to show that the spin-polarized state \( |\Psi_{\sigma} \rangle \) is a gapped ground state of the Hamiltonian with flat bands in the thermodynamic limit, provided that one also assumes that the lowest energy states with more than one spin flipped are higher in energy than those with one spin flipped.

Ruling out the possibility that states with many spin flips have lower energies than states with few spin flips relative to the Ising ferromagnetic ground state is plausible in the regime when the intrinsic spin-orbit coupling generates the largest energy scale \( (\Delta_0 \gg U) \).

Equation (8) is a reasonable assumption when the Bloch states stem from a band with a nonzero (spin) Chern number, since the spinor \( \chi_{k, \sigma} \) maps out the entire surface of the unit sphere as \( k \) takes values in the BZ. The assumption underlying Eq. (8) can also be understood by constructing the Wannier wave functions, centered at the lattice point \( z \), of the lowest energy band with spin \( \sigma \) and Chern number \( C_\sigma \):
\[
\psi_{z, r, \sigma, \varepsilon} = \frac{1}{N} \sum_{k \in BZ} e^{ik(r-z)} \chi_{k, \sigma, \varepsilon}. \quad (10a)
\]
The gauge-invariant part of their spread functional [14] satisfies
\[
\langle \psi_{0, \sigma, \varepsilon} | r^2 | \psi_{0, \sigma, \varepsilon} \rangle - \sum_z \langle \psi_{0, \sigma, \varepsilon} | r | \psi_{z, \sigma, \varepsilon} \rangle^2 \geq |C_\sigma| A_c/(2\pi), \quad (10b)
\]
where \( A_c \) denotes the area of the unit cell. This inequality relates the Chern number of the band and the “minimum width” of the Wannier states [13]. In particular, in the nontopological phase, one can imagine a limit in which the wave function is entirely localized on a given sublattice, while the nonzero Chern number in the topological phase implies that the Wannier wave function has amplitudes on both sublattices.

While Eq. (9) is strongly suggestive of the existence of a many-body gap \( \Delta \), it does not provide information about its size. To quantify \( \Delta \), we diagonalized the model (1) exactly numerically in the limit of flat bands \( \kappa = 1 \) at the commensurate filling fraction (4). We varied the ratio \( |t_2/\mu_c| \), keeping \( t_2^2 + \mu_c^2 = 1/2 \) constant to drive the system from the topological to the trivial phase. The results are shown in Fig. 1. First, they support the assumption that all states with more than one spin flipped are higher in energy than the many-body one-spin-flipped gap provided \( |t_2/\mu_c| > 1 \). Second, we find \( \Delta \approx 0.3U \) as an extrapolation to the thermodynamic limit for \( \mu_c = 0 \) deep in the topological phase, while \( \Delta \) monotonically decreases toward a much smaller nonvanishing value for \( t_2 = 0 \) in the topologically trivial phase set by the unit of energy \( |t_1| = 1 \). Finally, it should be noted that neglecting the states from the upper band of the noninteracting Hamiltonian delivers the correct excitation many-body gap \( \Delta \) not only in the aforementioned limit \( U \ll \Delta_0 \) but also under the weaker condition \( \Delta < \Delta_0 \), if the limit of flat bands is taken.

Deep in the topologically nontrivial regime \( |t_2/\mu_c| > 1 \), the states \( |\Psi_{\sigma} \rangle \) and \( |\Psi_{\overline{\sigma}} \rangle \) are degenerate ground states related by TRS for any finite \( N \). They are separated from their excitations by a gap that survives the thermodynamic limit \( N \to \infty \). Spontaneous breaking of TRS takes place in the thermodynamic limit \( N \to \infty \) by selecting the ground state to be \( |\Psi_\uparrow \rangle \), say. It is then meaningful to discuss the quantized electromagnetic response of \( |\Psi_\uparrow \rangle \), since TRS is
FIG. 1 (color online). Numerical exact diagonalization results for flat bands \( \kappa = 1 \) at the commensurate filling fraction (4). Markers show the energy of the lowest state in different sectors of total spin \( S \) (in units of \( \hbar/2 \)) measured with respect to the ground state energy for \( L_x = 3 \), \( L_y = 4 \). Here, \( g := (2/\pi) \arctan(\mu_0/\epsilon) \), so that \( g > 0.5 \) and \( g < 0.5 \) correspond to the trivial and topological single-particle bands, respectively. Since there is only one state in the fully polarized sector \( |S| = 12 \), the difference between the asterisks and the squares is the many-body excitation gap \( \Delta(g) \). The thick blue line shows the extrapolation of \( \Delta(g) \) to the thermodynamic limit. In the inset, exact diagonalization in the sector with one spin flipped away from the fully polarized sector is presented for \( \mu_0 = 0 \), \( t_2 = 1/\sqrt{2} \), and \( L_x = L_y \) ranging from 6 to 30. The straight lines are a guide to the eye and make evident an even-odd effect in \( L_x \). Deep in the topologically nontrivial regime \( g \ll 0.5 \), we observe a sizable \( \Delta(g \ll 0.5) \). The topologically trivial regime \( g > 0.5 \) is also characterized by a gap \( \Delta(g > 0.5) \) in the sector with one spin flipped away from the fully polarized sector; however, this gap is much smaller than \( \Delta(g \ll 0.5) \). We refer the reader to the Supplemental Material for a discussion of the regime \( \Delta(g > 0.5) \).

spontaneously broken. The transverse charge response \( \sigma_{xy}^H \) of \( |\Psi_f \rangle \) is proportional to the many-body Chern number \( C_{|\Psi_f \rangle} \). The latter takes into account the occupation of the Bloch states [4]. Since all Bloch states of the lower band with spin \( \sigma \) are occupied in \( |\Psi_f \rangle \), while all Bloch states with spin \( \downarrow \) are empty, \( C_{|\Psi_f \rangle} = C_f \). Hence, the ground state has the quantized Hall response

\[
|\sigma_{xy}^H| = |C_f|e^2/h = e^2/h.
\]

(11)

Remarkably, the selection by the repulsive Hubbard interaction of a ground state supporting simultaneously Ising ferromagnetism and the IQHE is robust to a sizable bandwidth as is suggested by numerical exact diagonalization. As shown in Fig. 2, the fully spin-polarized state \( |\Psi_\sigma \rangle \) remains the gapped ground state of the system up to a bandwidth \( W/U \approx 0.7 \).

**Practical applications.**—So what is it good for, a material with a QHE at room temperature without applied external magnetic fields, besides metrology [15,16]? First, we recall that the quantization of the Hall resistance and the accompanying vanishing of the longitudinal resistance is exact only at zero temperature. The longitudinal resistance increases exponentially fast with increasing temperature [16]. However, if a QHE with gaps of the order of hundreds of meV or even eV scales could arise in a strongly correlated lattice material, exceptionally low resistivities could be attained. The resistance of a Hall bar depends on its aspect ratio and the Hall angle \( \delta = \arctan(\rho_{yy}/\rho_{xx}) \) [17], but, for long systems ("wires") near the quantized regime, the longitudinal resistance scales as \( R_x = L/W\rho_{xx} \), and the 2D resistivity \( \rho_{xx} \sim R_x e^{-\Delta/T} \), where \( \Delta \) is the excitation gap. For gaps of the order of 100 meV to 1 eV, one would obtain room temperature 2D resistivities from \( \rho_{xx} \sim 10^3 \Omega \) to \( \rho_{xx} \sim 10^{-13} \Omega \), respectively. Obviously, the exponential behavior is responsible for this gigantic range. Small as they are, these are not perfect conductors. For a benchmark, we consider the conductivity of copper at room temperature per atomic layer. Using the value for the 3D resistivity of copper at \( 20^\circ \)C of \( \rho_{Cu}^{3D} = 1.68 \times 10^{-8} \Omega \)m [18] and that the lattice parameter for FCC lattice is 3.61 Å, we obtain \( \rho_{Cu}^{2D} = 93.3 \Omega \). Therefore, for gaps above \( \Delta \approx .2 \) eV, the Hall system starts to be better conducting than copper at room temperature, and for \( \Delta \approx .3 \) eV it is already almost 3 orders of magnitude better conducting than copper.

The RSRS (1c) is not exact in practice. For example, a Rashba spin-orbit coupling violates this RSRS. However, our analysis of transport at room temperature still applies provided the characteristic energy scale associated to the breaking of the RSRS (1c) is much smaller than the largest energy scale \( \Delta_0 \) induced by the intrinsic spin-orbit coupling. Materials that realize a 2D \( \mathbb{Z}_2 \) topological band insulator [19,20] with a band gap \( \Delta_0 \) are thus candidates to realize a QHE at room temperature if (i) the band gap is larger than the correlation energy and (ii) the chemical
potential can be tuned to half filling of (iii) a reasonably flat valence band. HgTe quantum wells with an inverted band structure realize a 2D $\mathbb{Z}_2$ topological band insulator with a small Rashba coupling [21,22]. The design of a material with the functionalities (i)–(iii) has been proposed in Ref. [8]. Cold atoms trapped in an optical honeycomb lattice [23,24] might offer an alternative to realizing the topological Hubbard model discussed in this Letter.

We would like to close by mentioning that examples such as the topological Hubbard model discussed in this Letter, as well as lattice models displaying the fractional quantum Hall effect studied in Refs. [4–7], could serve as benchmarks for numerical methods of fermionic models in 2D such as dynamical mean-field theory and methods based on tensor product states [25]. In contrast to the single-band repulsive Hubbard model, for which little is known exactly at fractional filling, the topological Hubbard model (1), because of the nonvanishing Chern numbers of its bands, leads to much better understood (topological) ground states. It can thus serve as a yardstick for the performance of these methods.

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