Change of an insulator’s topological properties by a Hubbard interaction

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We introduce two dimensional fermionic band models with two orbitals per lattice site, or one spinful orbital, and which have a non-zero topological Chern number that can be changed by varying the ratio of hopping parameters. A topologically non-trivial insulator is then realized if there is one fermion per site. When interactions in the framework of the Hubbard model are introduced, the effective hopping parameters are renormalized and the system’s topological number can change at a certain interaction strength, \( U = \bar{U} \), smaller than that for the Mott transition. Two different situations may then occur: either the anomalous Hall conductivity \( \sigma_{xy} \) changes abruptly at \( \bar{U} \), as the system undergoes a transition from one topologically non-trivial insulator to another, or the transition is through an anomalous Hall metal, and \( \sigma_{xy} \) changes smoothly between two different quantized values as \( U \) grows. Restoring time-reversal symmetry by adding spin to spinless models, the half-filled system becomes a \( \mathbb{Z}_2 \) topological insulator. The topological number \( \nu \) then changes at a critical coupling \( \bar{U} \) and the quantized spin Hall response changes abruptly.

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Recent interest in non-trivial topological properties of insulators \([1,2]\) has spurred intensive search for band models with non-trivial topology. This is because of the possibility that electron interactions in fractionally filled topologically non-trivial bands may lead to the realization of highly correlated fractional quantum Hall states \([3, 6]\). On the other hand, cold atomic gases in optical lattices with tunable interaction strength open the possibility to physically realize topological insulators \([7, 8]\). It is then natural to ask about the effects that electron correlations can have on the topological properties for proposed models.

Indeed, non-interacting topological phases are fairly well understood, so a great deal of attention has recently been given to the effect of interactions \([9–30]\). Studies of the Kane-Mele-Hubbard model \([31, 32]\) have recently been carried out, showing that the topological insulator survives until the Mott insulating phase is attained \([19–23]\). A topological phase can also arise from interactions added to a trivial band model, leading to a topological Mott insulator \([24, 27, 30, 33, 54]\). Also, the instability of quadratic band crossings to arbitrarily weak interactions has been proved \([28, 30]\).

In the present paper we show that yet another possibility exists. Namely, that a purely local interaction, such as that in the Hubbard model, can drive the system from one topologically non-trivial insulating phase into another by changing its topological number, while keeping it finite. This mechanism is particularly relevant for proposed band models with Chern number \( C \) larger than one. We present band models which break time-reversal symmetry explicitly, a situation analogous to the one considered by Haldane for the honeycomb lattice \([31]\). The system is a quantum anomalous Hall insulator when the lowest band is filled. If a Hubbard repulsive interaction is also present, the topological Chern number \( C \), hence the number of chiral edge states, changes at critical values of the Hubbard interaction strength, \( U \), before a Mott insulator phase is attained at higher \( U_c > \bar{U} \). Such transition is signaled by a change in the quantized Hall response. This effect occurs because the interaction effectively renormalizes the Hamiltonian parameters for the fermions, decreasing the longer ranged hopping with respect to the short ranged. Such changes in the effective hopping parameters induce a change of the topological number of bands for the fermions.

The following example models describe electrons in a square lattice with two orbitals per site. The Pauli matrices \( \tau_\mu \) and \( \sigma_\mu \) (\( \mu = 0, 1, 2, 3 \)) act on the orbital (or sub-lattice) space and spin space, respectively, and the subscript “0” refers to the identity matrix. The Hamiltonian has the general form:

\[
\hat{H}(\mathbf{h}) = \mathbf{h}(\mathbf{k}) \cdot \mathbf{\tau} + h_0(\mathbf{k}) \tau_0 ,
\]  

where \( \mathbf{h} = (h_x, h_y, h_z) \) and \( \mathbf{k} = (k_x, k_y) \) denotes the momentum vector. The Chern number for the bands in Hamiltonian Eq. \((1)\) is independent of the choice for \( h_0(\mathbf{k}) \), as computed from the usual expression

\[
C = \frac{1}{4\pi} \int dk_x \, dk_y \, \partial h_x \frac{\partial h_y}{\partial k_x} - \partial h_z \frac{\partial h_y}{\partial k_y} ,
\]  

and we therefore neglect \( h_0(\mathbf{k}) \) for the time being, and comment on it later. Time-reversal symmetry (TRS) requires \( h_{x(z)}(\mathbf{k}) \) to be a even function of \( \mathbf{k} \) and \( h_y \) to be odd. In order to have nonzero \( C \), TRS must be broken. The operation of spatial inversion \([\mathcal{I} : h_x(k) \rightarrow h_x(-k) , \ h_y(z)(k) \rightarrow -h_y(z)(-k)\] does not change \( C \).

Model for spinless fermions with \( \mathbb{Z} \) topological
number. — We consider
\begin{align}
h_x &= \sqrt{2}t_1 (\cos k_x + \cos k_y), \\
h_y &= \sqrt{2}t_1 (\cos k_x - \cos k_y), \\
h_z &= 4t_2 \sin k_x \sin k_y + 2t_1' (\sin k_x + \sin k_y) + \delta.
\end{align}

The terms $t'_1$ and $h_y$ break TRS and are responsible for a non-zero Chern number. The terms $t_2$ and $h_y$ break spatial inversion symmetry. If $t_2 > t'_1 - \delta/4$ then Eq. (2) gives $C = 2$, and if $t_2 < t'_1 - \delta/4$ then $C = 1$. The spectrum obtained in the ribbon geometry is shown in Fig. 1(a) for $t_2 > t'_1 - \delta/4$, the $C = 2$ case. Two pairs of counter propagating edge modes, running along the opposite edges of the ribbon, are clearly seen. The case $t_2 < t'_1 - \delta/4$ is shown in Fig. 1(b). Compatible with $C = 1$, now only one edge mode runs along each edge of the ribbon. We take the case where the lowest band is filled with spin polarized (or spinless) electrons, that is, where one electron occupies one of the two orbitals per lattice site. The system is then a band insulator with a number of chiral edge modes equal to the Chern number (see Fig. 1). We now assume that the parameters in Eq. (3) are such that $C = 2$ and introduce electron-electron interactions via the Hubbard term:
\begin{align}
\hat{H}_{\text{int}} &= \frac{U}{2} \sum_j \left( \sum_s \hat{n}_{j,s} - 1 \right)^2
\end{align}

where $s = 1, 2$ denotes the orbital index at lattice site $j$ and $\hat{n}_{j,s}$ is the electron number operator. A suitable approach to the Hubbard model at half-filling is the slave-rotor method. In this approach a rotor $e^{i\theta_j}$ is assigned to every lattice site and the charge at every site is identified with the rotor’s angular momentum, $\hat{L}_j = \sum_s \hat{n}_{j,s} - 1 = -i\partial/\partial\theta_j$. The electron operator is decomposed into a fermion and a rotor as $\hat{c}_j = \hat{f}_j e^{-i\theta_j}$. The interaction can then be simply rewritten as: $\hat{H}_{\text{int}} = \frac{U}{2} \sum_j \hat{L}_j^2$. We shall employ the $X$-boson treatment by equating $e^{i\theta_j} = X_j$ with the constraint $|X_j|^2 = 1$. Such a treatment has the advantage that it allows the calculation of the rotor correlation function between arbitrary sites of the lattice, as the decay of this correlation function with distance in the boson condensed phase is of crucial importance in what follows. Previous studies with this method concentrated on nearest neighbor boson correlation and were focused on the Mott transition. The method is well explained in Ref. and has been applied to the study of Mott transitions in topological insulators a number of times. The Hamiltonian Eq. (1) must be Fourier transformed to real space in order to make the substitution $\hat{c}_j = \hat{f}_j e^{-i\theta_j}$ and becomes a function of $f$-fermions and $X$-bosons, $\hat{H}(\hat{f} X, \hat{f} X^*)$. The partition function is $Z = \int D\lambda D\bar{f} Df DX^* DX \exp[-S]$ where the action $S$ reads
\begin{align}
S &= \int_0^{1/T} dt \left[ \sum_{j,s} \bar{f}_j (\partial_r - \mu) f_j + \sum_j \frac{1}{2U} |\partial_r X_j|^2 \\
&\quad + H(\bar{f} f, X X^*) + i \sum_j \delta/j \left( |X_j|^2 - 1 \right) \right]
\end{align}

The imaginary time $\tau$ is not to be confused with the Pauli matrices above. The Hamiltonian in the action reads
\begin{align}
H(\bar{f} f, X X^*) &= \sum_{ij} \sum_{ss'} h_{ij} \cdot \tau^s s' \bar{f}_{i,s} f_{j,s'} X_i X_j^*,
\end{align}

with $h_{ij} = \frac{t}{\sqrt{N}} \sum_k h(k) e^{i(kr_i - r_j)}$, where $N_s$ denotes the number of lattice sites. We do the standard mean-field decoupling of the fermions and bosons, whereby the Hamiltonian becomes a sum of a fermionic and a bosonic term, $H(\bar{f} f, X X^*) = H_f(\bar{f}, f) + H_X(X, X^*)$. The $f$-fermion Hamiltonian, $H_f$ back in momentum space is given by expressions in Eq. (1) and Eq. (3), but where the hopping parameter between sites $i$ and $j$ is now multiplied by $\langle X_i X_j^* \rangle$, i.e., $h_{ij} \to h_{ij} \langle X_i X_j^* \rangle$. The boson Hamiltonian has the form:
\begin{align}
H_X &= \sum_{ij} h_{ij} \sum_{ss'} \langle \tau^s s' \bar{f}_{i,s} f_{j,s'} X_i X_j^* \rangle \\
&= J_1 \sum_{ij} X_i X_j^* + J_2 \sum_{ij} X_i X_j^*
\end{align}

where $j'$, $j''$ denote first and second neighbors to the site $i$, respectively, and where $J_{1(2)}$ is obtained by averaging the fermion fields in Eq. (6). $H_X$, enjoys in this case the square lattice symmetry. The action is, accordingly, a sum of two parts, $S = S_f + S_X$, with
\begin{align}
S_X &= \int_0^{1/T} dt \left[ \sum_{ij} \frac{1}{2U} |\partial_r X_j|^2 + \sum_j \delta/j \left( |X_j|^2 - 1 \right) + H_X \right]
\end{align}

where the rescaling $U \to U/2$ has been made in order for the slave-rotor method to reproduce the correct atomic limit. In momentum space and Matsubara frequency, the boson field can be written as
\begin{align}
X_j(\tau) &= \frac{1}{\sqrt{N}} \sum_{i\nu, k} X(i\nu, k) e^{i(kr_j - \nu \tau)} + \sqrt{x_0}
\end{align}
where \(x_0\) is a density of the condensate of the boson field at zero momentum and frequency. The summation in Eq. (8) excludes the point \((\mathbf{i}u, \mathbf{k}) = (0, 0)\). The action for the bosons then reads

\[
S_X = \frac{1}{T} \sum_{\mathbf{i}u, \mathbf{k}} |X(\mathbf{i}u, \mathbf{k})|^2 \left[ \frac{\nu^2}{U} + J_1 \gamma_1(\mathbf{k}) + J_2 \gamma_2(\mathbf{k}) + i\lambda \right].
\]

(9)

with \(\gamma_1(\mathbf{k}) = 2\cos(k_x) + 2\cos(k_y)\) and \(\gamma_2(k) = 4\cos(k_x)\cos(k_y)\). Assuming a spatially constant \(i\lambda_j\), the constraint \(|X|_j^2 = 1\) can be implemented on average in imaginary time and space as

\[
1 = x_0 + \frac{\sqrt{U}}{2} N_s \sum_{\mathbf{k}} \frac{1}{\sqrt{J_1 \gamma_1(\mathbf{k}) + J_2 \gamma_2(\mathbf{k}) + i\lambda}}.
\]

(10)

If the interaction is not strong enough to enter in the Mott regime, the condensate density is finite and this requires the dispersion relation for the bosons \(\sqrt{J_1 \gamma_1(\mathbf{k}) + J_2 \gamma_2(\mathbf{k}) + i\lambda}\) to vanish at \(\mathbf{k} = 0\). The Lagrange multiplier is then fixed to the value \(\lambda = -4(J_1 + J_2)\). The instantaneous boson spatial correlation function reads

\[
\langle X_i X_j \rangle = 1 - \frac{\sqrt{U}}{2} N_s \sum_{\mathbf{k}} \frac{1 - e^{i\mathbf{k} \cdot (r_j - r_i)}}{\sqrt{J_1 \gamma_1(\mathbf{k}) + J_2 \gamma_2(\mathbf{k}) + i\lambda}}.
\]

(11)

The result in Eq. (11) must be inserted back into the f-fermion Hamiltonian \(H_f\), until convergence is attained.

A simulation with \(t_1 = 1\), \(t_2 = 0.7\), \(t_1^0 = 0.8t_2\) and \(\delta = 0\), yields a transition from the Chern number \(C = 2\) at \(U < \tilde{U}\) to \(C = 1\) at \(\tilde{U} > \tilde{U}\) where \(\tilde{U} \approx 1.4\). The critical interaction for the Mott transition obtained is \(U_c \approx 2.9\). For \(U > \tilde{U}\) we then expect a discontinuous change in the Hall conductivity. At \(\tilde{U}\) the f-fermions bands touch and close the gap. As long as \(t_2 > t_1^0 - \delta/4\), there is a \(U < U_c\). If \(t_2 < t_1^0 - \delta/4\), then \(C = 1\) for all \(U < U_c\).

On the Mott insulating side, \(U > U_c\), the condensate \(x_0\) vanishes and the boson correlation function is proportional to \(\sqrt{U}\), so that the ratio between first and second neighbors, \(\langle X_i X_j \rangle / \langle X_i X_j \rangle\), is independent of \(U\). Therefore, the above mechanism is not effective inside the Mott phase.

The physical electron’s Green’s function has a coherent part where the boson condensate \(x_0\) is the quasi-particle weight and the excitations are those of the Hamiltonian \(H_f\). We have checked that the Chern number obtained from \(H_f\) and Eq. (2) agrees with that obtained from the physical electron’s full Green’s function for an interacting system (equation (6) in Ref. 39). In the Green’s function point of view, the change in the topological number occurs because a pole of the Green’s function moves across zero energy [39].

Some of the models for flat bands that have been proposed in the literature with the purpose of realizing the fractional anomalous quantum Hall effect, have topological numbers similarly unstable with respect to the Hubbard interaction before the Mott phase is attained. For instance, the three-band model presented in Ref. 3 and which is expected to be realizable in an optical lattice has a transition from \(C = 1\) to \(C = 0\) at \(\tilde{U}/U_c \approx 0.4\), according to the above mechanism.

**A model with spin and Z topological number.**—We consider a system with a spinful orbital at each site described by a Hamiltonian of the form of Eq. (1) with the matrices \(\tau_i\) replaced by the matrices acting on spin space, \(\sigma\), and with

\[
h_x = \alpha \sin k_y, \quad h_y = -\alpha \sin k_x,
\]

\[
h_z = 4t_2 \cos k_x \cos k_y + 2t_1 (\cos k_x + \cos k_y) + \delta
\]

(12)

where \(h_0(\mathbf{k}) = -2t [\cos(k_x) + \cos(k_y)]\). Here \(\alpha\) is a Rashba spin-orbit coupling, the term proportional to \(t_1\) may be seen as an intrinsic spin-orbit coupling and \(\delta\) as a uniform magnetic field. Time reversal implies in this case \(h_1(\mathbf{k}) \rightarrow -h_1(-\mathbf{k})\). The term \(h_z\) in Eq. (12) breaks TRS. In general, due to the presence of the \(h_0(\mathbf{k})\) term there is an indirect band overlap and the system is metallic. Even though the bands are topologically non-trivial they will be in general partially filled. Considering \(h_0(\mathbf{k}) = 0\) and placing the chemical potential at zero energy one naturally gets a half-filled band insulator with non-zero Chern number. The expression in Eq. (2) gives \(C = 2\) if \(|t_1| < |t_2 + \delta/4|\); the Chern number reduces to \(C = 1\) if \(|t_1| > |t_2 + \delta/4|\). Turning on the Hubbard interaction, a transition between the different topological phases may be obtained as in the previous model at a suitable \(\tilde{U} < U_c\). Considering \(h_0\), one possible way to find an insulating phase is by having a large Rashba term. By varying \(t_2\) one finds regimes where the gap becomes
zero and a band overlap occurs, hence a metallic state. Interestingly, increasing further \( t_2 \) takes the system back to an insulating phase with different Chern number. The width of this metallic phase depends on the Rashba coupling. Starting from a \( C = 2 \) phase and turning on the Hubbard interaction we induce a sequence of transitions from the topological insulator through an anomalous Hall metal and back to another insulating phase with different Chern number. This is illustrated in Fig. 2, where we plot the indirect gap between the two bands and the Hall conductance as a function of the Hubbard coupling. There is a smooth crossover between the two quantized values of the Hall conductance in the two insulating phases. The Hall conductance is evaluated using a Kubo formula.

\( \text{Model with } \mathbb{Z}_2 \text{ topological number.} \) — We extend the model in Eq. (3) so as to describe a bilayer square lattice, with one orbital per site and where the superscripts in \( \tau^{ss'} \) denote layer indices. We introduce spin by coupling the spin operator \( \sigma \) to the terms that break TRS. The model reads

\[
\begin{align*}
\mathcal{H}_x &= \sqrt{2}t_1 (\cos k_x + \cos k_y) + t_\perp, \\
\mathcal{H}_y &= \sqrt{2}t_1 (\cos k_x - \cos k_y) \sigma_z, \\
\mathcal{H}_z &= 4t_2 \sin k_x \sin k_y + 2t_1' (\sin k_x + \sin k_y) \sigma_z + \delta.
\end{align*}
\]

where \( t_\perp \) is real and couples the atom in lattice site \( j \) of one layer (denoted by an index \( s \)) to the one that sits directly above it in the other layer \( s' \neq s \). Although TRS has been restored by the spin-orbit coupling, the model still lacks particle-hole symmetry, however. This puts the model in the AII class \([40]\). Studies of the Mott insulating phase for systems with spin-orbit coupling and TRS, using other techniques, exist in the literature \([19]\). The half filled system is a \( \mathbb{Z}_2 \) topological insulator characterized by a topological number \( \nu \) which is given by the parity of the Chern number: \( \nu = 0 \) if \( C = 2 \) and \( \nu = 1 \) if \( C = 1 \). Equation (6) for this case reads

\[
H(fX, fX^*) = \sum_{ij} \sum_{ss'} h_{ij} \cdot \tau^{ss'} \sigma_{f_{i,s,s'}f_{j,s',s}} X_{is} X^*_{js'},
\]

where \( \sigma = \uparrow, \downarrow \) denotes the spin projections. We make a similar decoupling of the X-bosons and fermions as above, with the difference that the bosons now have an extra layer index, \( X_{is} \). A calculation with model parameters: \( t_1 = 1, \ t_2 = 0.7, \ t_1' = 0.56, \ t_\perp = -1 \) yields a transition from \( \nu = 0 \) to \( \nu = 1 \) for \( \bar{U} = 0.44U_c \) with \( U_c = 4.3 \). If \( t_1' = 0.42 \) then one obtains \( \bar{U} = 0.84U_c \) with \( U_c = 4.2 \). In Fig. 3 we show the phase diagram so obtained. Because of TRS, no Hall conductivity exists, but the quantized spin Hall conductance, which is given by \( \sigma_{xy} = eC/(2\pi) \), displays an abrupt change at the transition, since the number of edge modes changes discontinuously (see Fig. 1). Since \( \nu = 0 \) is not protected by additional terms with TRS then, if disorder is present, the system may actually go from zero spin-Hall conductivity to finite (quantized) spin-Hall conductivity.

It is interesting to see that in the Kane-Mele-Hubbard model, when either a trivial Dirac mass (staggered potential) \([41]\) or a nearest-neighbor Rashba spin orbit coupling \([42]\) are present, the present mechanism would destroy the topological insulating phase for a certain \( \bar{U} < U_c \). This is so because, similarly to the model in Eq. (13), the topological insulator in the Kane-Mele model is induced by a second nearest neighbor hopping, which is thus susceptible to be renormalized by the interaction.

**Conclusions.** — We have shown that a short ranged repulsive interaction can induce a change from a system’s non-trivial topological phase to another, and presented several examples. The effect occurs because the renormalization of parameters in the Hamiltonian is such that the longer ranged hopping is decreased with respect to the short ranged. It is an interesting direction for future investigations to explore how the renormalization group technique for interacting fermions will renormalize interaction and kinetic energy parameters so as to induce changes in the topological class of a fermionic system.

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