Interaction-induced topological phase transition in the Bernevig-Hughes-Zhang model

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Abstract – We study interaction-induced topological phase transition in Bernevig-Hughes-Zhang model. The topological nature of the phase transition is revealed by directly calculating the \(Z_2\) index of the interacting system from the single-particle Green’s function. The interacting \(Z_2\) index is also consistently checked through the edge spectra. Combined with \textit{ab initio} methods, the present approach is a useful tool for searching for correlated topological insulating materials from the first-principle point of view.

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Introduction. – \textit{Ab initio} methods got great success in predicting topological insulating materials thus far [1–4]. One reason behind is that the correlation effect is relatively weak in relevant materials. Another reason is that the topological property is more robust than the magnetic or the superconducting properties against systematical errors in the first-principle calculations. Studying the interplay of the correlation effect and the topological order is interesting from both the fundamental and application points of view. The interacting effect on topological phases already received much attention recently. Various analytical or numerical tools have been applied to several models for topological insulators [5–9]. However, most of these studies used the conventional non-topological quantities such as the long-range order parameter [10], the excitation gap [7,11] to indirectly characterize the interacting topological phases. How to extract the interacting topological index from many-body calculations remains a challenge.

Indeed some progress has been made along this line. For Chern TI, the quantum Hall conductance can be calculated using the twisted-boundary-condition [12] or the linear response formula [8]. For \(Z_2\) TI, ref. [13] suggested a definition of the interacting \(Z_2\) index based on the single-particle Green’s function:

\[
Z_2 = \frac{\pi^2}{15} \epsilon_{\mu \nu \rho \tau \rho} \text{Tr}\int \frac{d^4k d\omega}{(2\pi)^5} G \partial_\mu G^{-1} G \partial_\nu G^{-1} G \partial_\rho G^{-1} G \partial_\tau G^{-1},
\]

where \(G(k, i\omega)\) is Matsubara Green’s function\(^1\), \(\epsilon_{\mu \nu \rho \tau \rho}\) is the five-order antisymmetric tensor, the \(\mu, \nu, \ldots, \tau\) indices denote the frequency-momenta \((\omega, k_x, k_y, k_z, k_\lambda)\). For three- (two-) dimensional topological insulator, one (two) of them is the pumping parameter extending the momenta to four dimensions [13]. Note the difference of eq. (1) with the quantum (spin) Hall conductivity coefficient [8]. Since the formula contains the five-dimensional frequency-momenta integration and here the conservation of spin quantum number is not assumed, the Green’s function is in general a matrix in the spin-orbital space. Although being very general, the introduction of the pumping parameter and invoking the derivatives with respect to frequency-momenta hinder a precise numerical implementation of eq. (1).

There are some attempts of integrating eq. (1) numerically for typical forms of interacting Green’s functions [14]. It is highly desirable to have a recipe for extracting topological informations for \(Z_2\) TI directly from

\(^1\)The system should be gapped, otherwise integrating out fermions is invalid and in general there is no quantized topological index.
many-body calculations. It would be even more useful if the method could be easily combined with the first-principle approaches. This will accelerate the search for correlated topological materials.

In this letter, we propose a numerical scheme for calculating the interacting $Z_2$ index. The $Z_2$ index of an interacting system equals the $Z_2$ index of a noninteracting auxiliary system [15]. The auxiliary system is constructed such that its noninteracting bath mimics the effect of local self-energy due to the interaction $H_1$. See text for details.

Fig. 1: (Colour on-line) Illustration of the strategy for calculating the interacting $Z_2$ index. The $Z_2$ index of an interacting system equals the $Z_2$ index of a noninteracting auxiliary system [15]. The auxiliary system is constructed such that its noninteracting bath mimics the effect of local self-energy due to the interaction $H_1$. See text for details.

noninteracting bath mimics the effect of local self-energy due to the interaction $H_1$. Study its effect on the topological properties of the BHZ model:

\[
H_1 = U \sum_i (n_{s\uparrow} n_{s\downarrow} + n_{p\uparrow} n_{p\downarrow}) - \frac{U}{2} \sum_{\sigma} (n_{s\sigma} + n_{p\sigma}).
\]

In the following discussion, we focus on $m = -3$ and $\lambda = 0.3$. The chemical potential term ensures that the system has particle-hole symmetry and on average there are two particles per site. For $U = 0$ the system lies in the normal band insulator region. The $s$ and $p$ orbitals are well separated. Occupation of the two orbitals are $(2^-, 0^+)$, small deviation is due to hybridizations. With increasing $U$, some of the electrons residing on the $s$-orbital will be pushed to the $p$-orbital. The occupation number of each orbital will approach $(1^+, 1^-)$ at large $U$. In the following calculations, a spin symmetry is conserved, where we have $\langle n_{s\uparrow} \rangle = \langle n_{s\downarrow} \rangle \equiv \langle n_s \rangle$ and $\langle n_{p\uparrow} \rangle = \langle n_{p\downarrow} \rangle \equiv \langle n_p \rangle$.

We perform the dynamical-mean-field-theory (DMFT) [18] calculations for the interacting BHZ model. By solving the two-orbital Anderson impurity model (AIM) self-consistently, DMFT gives a good approximation of the local Green’s function and self-energy. Here, the AIM is solved with the Lanczos exact diagonalization (ED) impurity solver\(^2\). The ED solver captures essential features of the correlation and has the advantage of allowing direct access to the pole structure of Green’s function. We employ the Lanczos method [19] to solve the ground state and Green’s function. With the ground state $|g\rangle$ of AIM, we run Lanczos algorithm starting from $c_{\beta}^\dagger |g\rangle$ (or $c_{\alpha} |g\rangle$) to get a set of eigenpairs $\{E_n, |n\rangle\} \{\{E_m, |m\rangle\}$ for adding (removing) one particle subspace ($\alpha, \beta$ denote the combined spin-orbital index $\alpha = \{s(p), \sigma\}$). The local Green’s function is calculated as

\[
G_{\alpha\beta}(z) = \sum_n \frac{(g|c_{\alpha}|n)(n|c_{\beta}^\dagger|g)}{z - E_n + E_g} + \sum_m \frac{(g|c_{\alpha}|m)(m|c_{\beta}^\dagger|g)}{z - E_m + E_g}.
\]

The resulting Green’s function is diagonal in the spin-orbital space, i.e. $G_{\alpha\beta} = G_{\alpha\beta} \delta_{\alpha\beta}$. By rewriting eq. (5) to $G_\alpha(z) = \sum_{i=1}^{N_G} W_{\alpha i} Q_{i\alpha}^\dagger$, we have direct access to poles and weights of the local Green’s function $\{Q_{i\alpha}, W_{\alpha i}\}$. The number of poles $N_G$ are limited by the basis size as well as the number of Lanczos vectors. We have checked that the finial $Z_2$ index does not change as more Lanczos vectors are included. We then get the pole-expansion of the local self-energy $\Sigma_\alpha(z) = \Sigma_\alpha(\infty) + \sum_{i=1}^{N_G-1} \Sigma_{\alpha i}^\dagger Q_{i\alpha}^\dagger$.

\(^2\)We include three sites to represents the bath. At each step we determine the energy level and the coupling strength of bath sites to the impurity site from the center of mass of and weight of the hybridization function.
following ref. [20], with
\[
\Sigma_\alpha(\infty) = \sum_{i=1}^{N_G} W^i_\alpha Q^i_\alpha, \tag{6}
\]
and
\[
\sum_{i=1}^{N_G} W^i_\alpha P^i_\alpha - Q^i_\alpha = 0, \tag{7}
\]
and
\[
V^j_\alpha = \left[ \sum_{i=1}^{N_G} W^i_\alpha \right]^{-1} \left( P^j_\alpha - Q^j_\alpha \right)^2. \tag{8}
\]

We explicitly check that the self-energies constructed in this way agree with the self-energies obtained directly from the Dyson equation, see fig. 2 (see footnote 3). With \{\Sigma_\alpha(\infty), P^i_\alpha, V^j_\alpha\} we construct the noninteracting pseudo-Hamiltonian according to [15,21]:
\[
\tilde{H}_k = \begin{pmatrix}
H_k + \text{diag}(\Sigma_\alpha(\infty)) & \text{diag}(\sqrt{V^j_\alpha}) \\
\text{diag}(\sqrt{V^j_\alpha}) & \text{diag}(P^j_\alpha)
\end{pmatrix}.
\tag{9}
\]

The \(Z_2\) index of \(\tilde{H}_k\) is calculated using the algorithm for noninteracting systems [22]. According to [15] it is identical to the interacting \(Z_2\) index of the original model.

Results. – In fig. 3 we plot the interacting \(Z_2\) index (red line) as a function of the interaction strength, it shows a jump from 0 (trivial) to 1 (nontrivial) at \(U = 2.2\), i.e., indicating an interaction induced topological phase transition.

We then validate and explore the nature of this topological transition by considering other physical quantities. First, we note that the static part of the self-energy \(\Sigma_\alpha(\infty) = 2U(N_s^\alpha - N_p^\alpha)\Sigma_2 \otimes \sigma^z\). It renormalizes parameter \(m\) in \(H_0\) to \(m_{\text{eff}} = m + U(\langle n_s \rangle - \langle n_p \rangle)/2\). In fig. 3 we plot the effective mass as a function of \(U\). It can be seen that the topological phase transition occurs whenever \(m_{\text{eff}}\) exceeds \(-2\). The topological transition occurs due to the interaction-induced relative level shift of \(s\) and \(p\) orbitals, which drives the system into an effective inverted band region.

The effective mass shows nonmonotonous behavior for larger \(U\). This is due to the fact that in the large-\(U\) limit fillings of \(s\) and \(p\) orbital tend to be evened out to \((1^+, 1^-)\). Since \(\langle n_s \rangle - \langle n_p \rangle\) decays faster than \(1/U\), \(m_{\text{eff}}\) turns back to the noninteracting value \(m\) (see the following). Interestingly, the interacting \(Z_2\) index calculated in this region disassociates from the effective mass. The system always shows a nontrivial topological property even when \(m_{\text{eff}}\) goes back to its noninteracting value. However, a simple consideration based solely on the effective mass would predict a trivial phase in this region. The above analysis shows that the dynamical part of the self-energy is important in determining the topological properties in a correlated topological insulator.

We further calculate the edge spectrum \(A(k_x, \omega)\) by projecting the interaction Green’s function on to the open edges\(^4\). In fig. 4(a)–(c), the edge states are in accordance with the \(Z_2\) index calculated from pole-expansions

\(^3\)Different from ref. [20] where they employ Hubbard-I solver, here we need to further exclude poles and corresponding weights from hybridization with bath sites. This can be easily done since we have discrete bath sites in the ED solver, whose hybridization function is known.

\(^4\)When calculating the edge spectrum, we assume that the self-energy on the edge is the same with the bulk one, this is of course a crude approximation. It would be interesting to study position-dependent (although local) self-energies in the formalism of the real-space DMFT [23,24].
(TI phase for $U > 2.2$). Inside the TI phase, the bulk gap first increases (due to band inversion) then shrinks (due to the correlation effect) with increasing $U$. Since the bulk gap never closes after the first transition at $U = 2.2$, it is expected that the topological index is unchanged. For $U = 8.0$, the edge state is still visible, but the bulk gap is very small, fig. 4(d). Physically, this tiny gapped TI phase corresponds to a state proximate to Mott transition with a tiny quasi-particle weight. Due to the presence of energy splitting between the $s$ and $p$ orbitals, the system does not reach $\langle n_s \rangle = \langle n_p \rangle = 1$, thus preventing the Mott transition to happen. As long as there is a finite quasi-particle weight, the system is topological nontrivial. Reduction of the bulk gap for a correlated insulator is also observed in [6,25].

As a comparison, we solve the interacting BHZ model with the Hartree-Fock (HF) mean-field theory. In the HF treatment, the interacting term is decoupled as $H_I = U \sum_{1a} (n_{s\sigma} \langle n_{s\sigma} \rangle + n_{p\sigma} \langle n_{p\sigma} \rangle)$. This also effectively modifies the mass term to $m_{\text{eff}} = m + U (\langle n_s \rangle - \langle n_p \rangle)/2$. By solving the mean-field Hamiltonian self-consistently we find that $m_{\text{eff}}$ increases monotonously with $U$. In fig. 3, we see that the effective mass from the DMFT and HF calculations are in accordance with each other for small interacting strength $U < 2$. The interaction-driven band inversion is captured by a Hartree-Fock level shift. However, the HF result deviates from the DMFT one at large $U$. This is because the HF theory does not correctly capture the asymptotic behavior of $\langle n_s \rangle - \langle n_p \rangle$ at large $U$ (see footnote 5). Due to this, we anticipate that HF will favor the existence of topological phase transitions in some strongly correlated materials.

In the HF treatment, the topological properties are simply determined by the mean-field Hamiltonian, i.e., the mean-field $Z_2$ index is determined by $m_{\text{eff}}$. The topological transition occurs whenever $m_{\text{eff}}$ exceeds $-2$. The topological transition point in the HF theory shifts towards a slightly smaller value of $U$ compared to the DMFT result. At the phase boundary, the single-particle excitation gap closes and the effective mass shows a kink in the transition point [9,26].

To summarize our physical results, the mean-field effect first drives the band inversion and turns the system into a correlated TI. Further increasing $U$ will first stabilize the TI phase by a larger band inversion, but soon correlation effect takes over to suppress the quasi-particle weight and hence the bulk gap. The system is academically always in the TI phase with a tiny gap since there is no Mott transition.

**Discussion.** – We have used several ways to determine the topological properties of an interacting model, namely getting the interacting $Z_2$ index from the pole-expansion, looking at the edge spectrum and using the mean-field theory. The mean-field theory is not reliable for strongly correlated systems. Practically, the real-frequency edge spectrum is not directly accessible to many numerical techniques due to the complication of analytical continuation. And it is hard to distinguish odd and even pairs of edge states from the spectrum. The interacting $Z_2$ index, eq. (1), is defined using the Matsubara Green’s function. However, as discussed in [14,15] due to extremely inhomogeneous distribution of the integrand, it is difficult to directly accomplish the integration to get the quantized topological index. The pole-expansion technique, combined with DMFT calculations, thus provides a practical way of determining the topological properties of correlated topological insulators. Since the pole-expansion technique is already widely used in LDA+DMFT calculations (for avoiding the time-consuming numerical matrix inverse for each frequency) [20,21], with the proof-of-principle demonstration here, we anticipate that the combination of the present approach with the \textit{ab initio} tools will be useful for future theoretical searching of correlated TI materials.

**Summary.** – For the parameter region studied in the present paper, the topological phase transition is essentially driven by the mean-field effect (shift of HF levels). However, deep inside the interacting TI phase, the correlation effect plays an important role in modifying the properties of the system. The mean-field theory fails in predicting the topological nature base on the orbital occupations. On the other hand, the interacting $Z_2$ index from the pole-expansion correctly predicts a topological

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A simple estimation based on the two-level model shows that $\langle n_s \rangle - \langle n_p \rangle \sim 1/U^2$; however, HF predicts $\langle n_s \rangle - \langle n_p \rangle \sim 1/U$. 

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57001-p4
nature of the correlated TI phase for the whole range of the interacting strength. This is quite remarkable, because we do not need to calculate dynamical quantities (like the edge spectrum or the real-frequency Green’s function) to determine the topological nature of an interacting system.

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**Additional remark:** After completion of this manuscript, there appeared interesting papers by Wang [27, 28]. We have validated their formula with our numerical Green’s functions. It gives identical topological transition point as the pole-expansion method used in this paper. Independent studies are also reported in [29] and [30].

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\^**6** We diagonalize \( G(k_i, 0) = [−H_k − \Sigma(k_i, 0)]^{-1} \) for \( k_i \) ∈ TRIM points. Denote eigenvectors with positive eigenvalues as \( |\alpha_i\rangle \). They are also eigenvectors of the parity operator \( P = \text{diag}(1, 1, −1, −1) \), i.e. \( P|\alpha_i\rangle = \eta_\alpha |\alpha_i\rangle \). Then \( \frac{1}{2πi} \sum_{\alpha} \ln \eta_\alpha \mod 2 \) gives the \( Z_2 \) index. (0 for trivial insulator, 1 for topological insulator.)