Correlation Effects in Topological Insulators

Norio Kawakami
Department of Physics, Kyoto University, Kyoto 606-8502

1 Introduction

Recent years have witnessed a surge of interest in topological insulators (TIs), which provide a new research platform in condensed matter physics. TIs have nontrivial band structures due to the spin-orbit coupling. A striking feature in TIs is that they host gapless edge states at boundaries, which are protected topologically. The notion of TI was originally proposed for graphene [1] and also for HgTe/CdTe quantum wells [2]. The latter TI was confirmed experimentally [3]. Also, many examples of TIs in three dimensions have been found in bismuth-based compounds, etc.[4, 5]. Although theory for TIs has been mainly devoted to non-interacting systems so far, correlation effects on them have attracted much attention, since novel aspects of electron correlations would emerge under topologically nontrivial conditions. This issue has further been stimulated by the fact that there are a variety of candidates for correlated TIs [6, 7, 8, 9], such as SmB_6 [10, 11], etc. In spite of extensive studies, understanding of topological phases in correlated systems[12, 13, 14, 15, 16, 17, 18, 19, 20], especially a topological Mott insulator, is still not sufficient. As mentioned above, gapless edge modes which are a source of exotic and rich physics are induced by bulk nontrivial properties in free fermion systems. Even in correlated systems, the nontrivial band structure would lead to novel gapless edge states; for example, edge states composed only of spin excitations in topological Mott insulators.

Here, we report our recent studies on the correlated TIs[21, 22]. We first discuss a topological Mott insulator in one dimension (1D) in Sec.2 to address how the edge Mott states emerge due to the interplay of topology and correlation [21]. We demonstrate, based on DMRG calculations with high accuracy, that the topological Mott insulator accompanied by the edge Mott states is indeed stabilized. In Sec.3, we then address a similar question for a two-dimensional (2D) correlated TIs [22]. In this case, we find a remarkable property caused by the interplay of topology and correlation: the topological properties emerge with increasing temperature in the presence of strong correlations. We demonstrate that the above counterintuitive properties are not specific to the model employed here but rather generic for correlated TIs. In Sec.4, we briefly explain some related topics we have studied in recent years [23, 24, 25, 26]. Brief summary is given in Sec.5.

2 Topological Mott insulator in 1D

We start with a fundamental question: whether a topological Mott insulator really emerges in correlated system, and if so, how the edge states behave in the presence of the interaction. To address this question, we here investigate a prototypical TI with Hubbard interaction in 1D [21]. By examining the bulk topological invariant and the entanglement spectrum of the correlated electron model, we elucidate how gapless edge states in a non-interacting TI evolve into Mott edge states in a topological Mott insulator. Furthermore, we propose a topological Mott transition, which is a new type of topological phase transition. This unconventional transition occurs in spin liquid phases in the Mott insulator and is accompanied by zeros of the single-particle Green's function and a gap closing in the spin excitation spectrum.

We consider a 1D correlated Su-Schrieffer-Heeger (SSH) model, which describes a bond-alternating tight binding model with electron correlation. The Hamiltonian reads,

$$
\begin{aligned}
H_{SSH} &= \sum_{i\sigma}(-tc^{\dagger}_{i+1a\sigma}c_{ib\sigma} + Vc^{\dagger}_{ia\sigma}c_{ib\sigma} + h.c.) \\
&+ U\sum_{i\alpha} n_{i\alpha\uparrow}n_{i\alpha\downarrow} + J\sum_{i} \mathbf{S_{ia}}\cdot\mathbf{S_{ib}} \qquad (1)
\end{aligned}
$$

with $n_{i\alpha\sigma} = c^{\dagger}_{i\alpha\sigma}c_{i\alpha\sigma}$, where $c^{\dagger}_{i\alpha\sigma}(c_{i\alpha\sigma})$ is a creation (annihilation) operator for an electron at site i and in orbital $\alpha = a, b$ and spin $\sigma =\uparrow,\downarrow$ state. We introduce the third term representing the ferromagnetic spin exchange interaction, which is crucial for a topological phase transition induced by electron correlations. We recall that in the non-interacting case, in the region of $-t < V < t$, the system is in a TI phase protected by chiral symmetry, which is characterized by a nonzero winding number. Note that the symmetry is essential for determining the topological properties, and our analysis is valid generically for the 1D chiral-symmetric class. We employ the density-matrix renormalization group (DMRG) method, which provides a powerful tool to compute the ground-state quantities with high precision. In what follows, we choose the hopping integral t as the energy unit.

(a) *Topological Mott phase with spinon edge states*

Let us start with a Topological Mott insulator by setting $J = 0$ in the model Hamiltonian [21]. The obtained results are shown in Fig. 1. It is seen from Fig. 1(a) that even in the presence of U, the winding number takes $N_1 = 1$, implying that the system is always in a topological phase. Although the noninteracting TI continuously changes to the Mott insulator in the bulk with keeping $N_1 = 1$, the edge

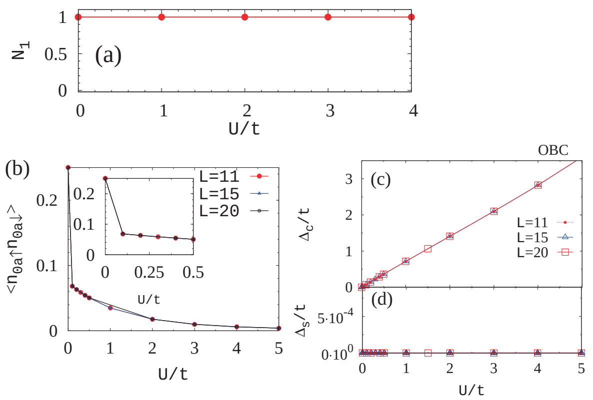

Figure 1: Results obtained for the parameters $(J, V) = (0, -0.4)$ [21]: (a) winding number N_1 for chain length $L = 11$, (b) double occupancy of orbital a at the edge site for several choices of L, (c) ((d)) single particle (spin) excitation gap under open boundary conditions.

site shows a discontinuous change at $U = 0$; namely as seen from Fig. 1(b), the double occupancy abruptly decreases once the interaction U is introduced. This implies the formation of a local spin around the edges. This abrupt change signals the emergence of topological edge-Mott states, where electron correlations play a crucial role. Namely, the emergent local spin is not completely free, but still screened even after the abrupt change, implying that the edge states are strongly correlated. As seen from Fig. 1(c), this abrupt change is accompanied by a gap formation for the single particle excitations at the edges, while the collective spin excitations are still gapless. The latter may be referred to as gapless "spinon edge states". These observations lead us to the conclusion that at $U = 0$ a correlated edge-Mott state with gapful charge (gapless spin) excitations is induced at each edge, while the bulk behaves as a correlated band insulator. Although the single particle excitation spectrum is gapped at edges, degeneracy in the entanglement spectrum is maintained, giving rise to gapless edge modes in the spin excitation spectrum (Fig. 1(d)). Furthermore, the analysis with the entanglement spectrum (not shown here [21]) elucidates the above-mentioned fragility of edge states upon introduction of U.

Summarizing the results obtained for the correlated SSH model with $J = 0$, we have a topological Mott insulating phase where the bulk is always in a correlated TI insulator characterized by the Chern number $N_c = 1$, while the edge state is changed from a gapless electron mode to a topological edge Mott mode having gapful charge (gapless spin) excitations. We believe that this gives the first unambiguous example of topological Mott insulators.

(b) *Topological phase transition*
We now consider a topological Mott transition, which is a new type of topological phase transition characterized by zeros of the single-particle Green's function and a gap closing in the spin excitation spectrum [21]. To address this problem, let us switch on the exchange interaction J in the Hamiltonian (1), which can induce an intriguing phenomenon never observed in free fermion systems. If the interaction is ferromagnetic, a topological transition is induced by correlation effects; for example, for $J = -1.5$, the winding number changes from $N_1 = 0$ to $N_1 = 1$ with increasing the interaction U, as shown in Fig. 2(a). Therefore, the trivial insulator changes into a nontrivial one. In contrast to the non-interacting case, the topological properties are changed without a gap closing; as seen in the right panel of Fig. 3, the single particle excitation gap remains finite even at the transition point. Thus, zeros of Green's function are required at this point. Indeed we can see that a zero appears at the transition point (right panel of Fig. 2); at $U = 0$, a locus of the Green's function $G(i\omega = 0, k)$ does not wind the origin, but as the interaction U is increased, the locus approaches the origin and finally crosses it.

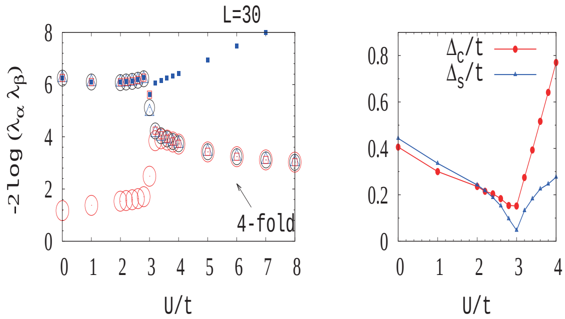

Figure 3: Left panel: Plots of lowest five entanglement spectra as functions of U under periodic boundary conditions for $(J, V) = (-1.5, -1.6)$ [21]. Right panel: Plots of spectral gap for the same parameters; single particle excitation (spin excitation) is denoted as Δ_c (Δ_s). These values are extrapolated to thermodynamic limit with scaling L^{-1}

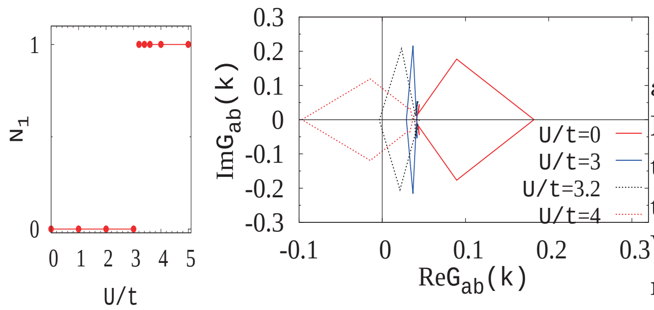

Figure 2: Left panel: Winding number for $(J, V) = (-1.5, -1.6)$ and $L = 11$ as a function of U [21]. Right panel: locus of the Green's function G_{ab}. As the momentum k is increased, $G_{ab}(k)$ draws its locus clockwise. In a trivial phase, at $k = k_{min}$, $G_{ab}(k)$ is positive and real and draws its locus clockwise.

The above-mentioned topological properties are confirmed by the entanglement spectrum. Namely, topological properties described by the winding number are also characterized by the structure of the entanglement spectrum. We can observe in Fig. 3 that the entanglement spectrum becomes degenerate for $3.2 < U$. Note that a change in the degeneracy of the entanglement spectrum requires a gap closing at the transition point, although the single particle gap remains finite at this point. Therefore, the only way to satisfy the condition for this topological Mott transition is to close a gap in a collective excitation spectrum, which corresponds to the spin excitation spectrum in our case. Therefore, we generally expect that a collective excitation spectrum becomes gapless at the topological Mott transition point where the Green's function has zeros.

3 Temperature-induced topological properties in 2D

We now investigate how topologically nontrivial phases evolve at finite temperatures. Specifically, we study a Kane-Mele Kondo lattice shown below at finite temperatures with dynamical mean field theory (DMFT) [22]. We find an intriguing phenomenon: restoration of topological properties at finite temperatures, which is caused by the interplay between topology and correlation. These phenomena are uncovered by analyzing the bulk as well as edge properties: in the bulk, the spin-Hall conductivity which is almost zero around zero temperature increases with increasing temperature, while at the edge, the gapless edge modes emerge with increasing temperature. We thus elucidate that the interplay of the topological nature of the system and the Kondo effect is essential for the restoration of topological properties.

In order to demonstrate the above-mentioned phenomena explicitly, we here employ a topological Kane-Mele Kondo model on a two-dimensional (2D) honeycomb lattice. The Hamiltonian reads

$$\begin{aligned} H_{KMK} &= H_{KM} + J\sum_i \mathbf{s}_i \cdot \mathbf{S}_i, \\ H_{KM} &= -t\sum_{\langle i,j\rangle\sigma} c^\dagger_{i,\sigma}c_{j,\sigma} \\ &+ it_{so}\sum_{\langle\langle i,j\rangle\rangle} \mathrm{sgn}(i,j)\mathrm{sgn}(\sigma)c^\dagger_{i,\sigma}c_{j,\sigma}, \end{aligned} \quad (2)$$

with $\mathbf{s}_i = \frac{1}{2}c^\dagger_{i,s}\sigma_{s,s'}c_{i,s'}$ and $\mathrm{sgn}(\sigma) = 1$ (-1) for $\sigma =\uparrow$ $(\downarrow)$. Here $c^\dagger_{i,s}$ creates an electron with spin $s =\uparrow,\downarrow$ at site i. $\mathbf{S}_i$ denotes a localized moment of spin $S = 1/2$ at site i on the honeycomb lattice. The effect of spin-orbit coupling is incorporated in $\mathrm{sgn}(i,j)$, which takes 1 (-1) when the electron hops clockwise (counter clockwise), respectively.

At $J = 0$, conduction electrons on the Kane-Mele lattice are completely decoupled from localized spins, and therefore the conductivity takes a finite quantized value at zero temperature, which is proportional to the topological invariant. At finite temperatures, it takes a finite but not quantized value. Nevertheless, if the temperature is smaller than the bulk gap, we have a spin-Hall conductivity close to the quantized value. This temperature region is regarded as a "topological insulator region" approximately, although the quantization is not well defined at finite temperatures.

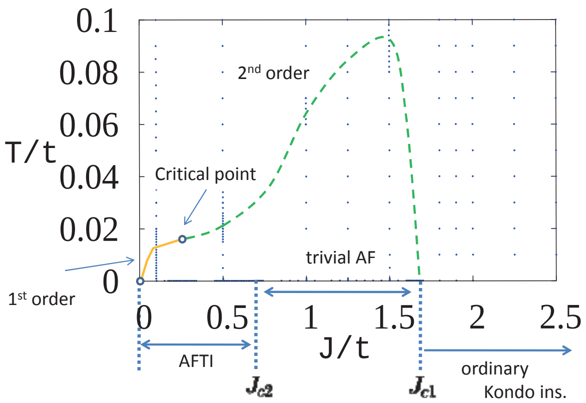

Figure 4: Phase diagram of temperature (T) vs. the antiferromagnetic coupling (J) [22]. A first order transition (solid orange line) is observed in the weak-coupling region while it becomes second order (dashed green line) with increasing J. For $J < 0.683t$ a topological antiferromagnetic phase (AFTI) is stabilized. This phase changes to a trivial antiferromagnetic phase and an ordinary Kondo insulator with increasing J. The topological structure is well-defined only at zero temperature.

Before addressing the topological properties, let us briefly summarize the obtained phase diagram shown in Fig. 4. For weak exchange interaction J, there is an antiferromagnetic topological phase, which is induced by the RKKY interaction. With increasing J, this phase changes to a trivial antiferromagnetic phase. Further increase in J stabilizes an ordinary (trivial) Kondo insulator. When the temperature increases, the antiferromagnetic order disappears via a first (second) order transition for weak (strong) interaction strength J. We find that the system shows the topologically nontrivial properties for $J < 0.683t$, while the increase in J induces a topological transition. At this continuous topological transition point, gap-closing in the density of states is observed.

In the following, we reveal that the interplay between electron correlations and topological properties leads to an intriguing crossover behavior; topological properties are restored at finite temperatures in the region where the topological structure of the ground state is destroyed. We confirm these intriguing properties in the following two steps: we start with the nonmagnetic phase then move to the antiferromagnetic phase.

In order to capture the essence, let us first restrict ourselves to paramagnetic solutions. The calculated conductivity is plotted in Fig. 5(a). At low temperatures, the spin-Hall conductivity is zero for $J = 0.5t$ since the topological invariant is no longer well-defined due to the Kondo effect; the singlet formation between electrons and localized spins leads to zeros of the Green's function (i.e., divergence of the self-energy) [see Fig. 5(b)]. With increasing temperature, the Kondo effect is suppressed, and the conductivity increases. For $T > 0.03t$, the conductivity approaches the values of $J = 0$ which are almost quantized. The increase of the spin-Hall conductivity is also observed for $J = 0.7t$, even though increasing the coupling strength J suppresses the conductivity at finite temperatures due to enhancement of the Kondo effect.

This increase of the conductivity is interpreted as a restoration of gapless edge modes. Our real-space dynamical mean-field theory (R-DMFT) calculations using the ribbon geometry reveal how finite temperatures affect

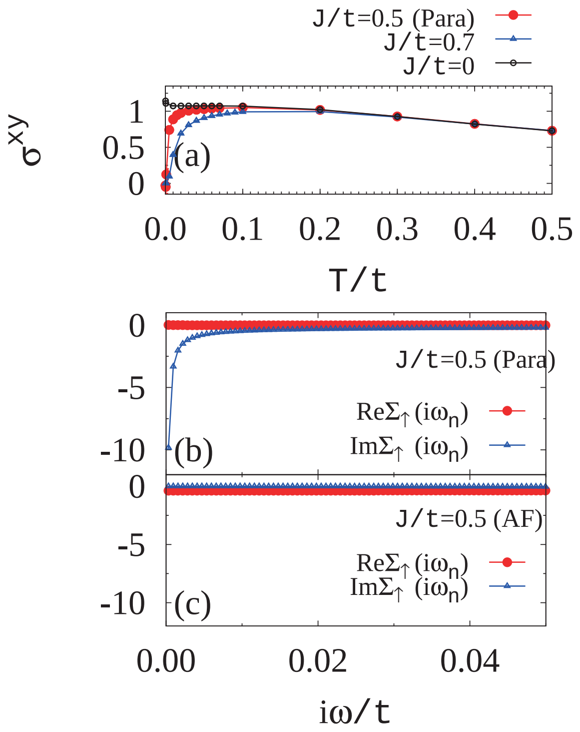

Figure 5: (a): Spin-Hall conductivity at finite temperatures. (b) ((c)): Self-energy of up-spin state in the paramagnetic (antiferromagnetic) phase [22]. For $t_{so} = 0$, the spin-Hall conductivity is zero even in the high temperature region.

the edge modes. From the results (not shown here [22]), we can see that edge modes are destroyed due to the Kondo effect at low temperatures, but are restored with increasing temperature, leading to an increase of the spin-Hall conductivity.

Therefore, we conclude that the origin of this crossover is the competition of the Kondo effect and the topological properties. In the low temperature region, the Kondo effect governs the low energy properties and destroys the topological structure. On the other hand, topological properties (i.e., the conductivity and edge states) are restored if the temperature is higher than the Kondo temperature but smaller than the energy scale of the band gap of the noninteracting topological insulator.

It should be noted that the restoration of topological properties occurs even in the anti-

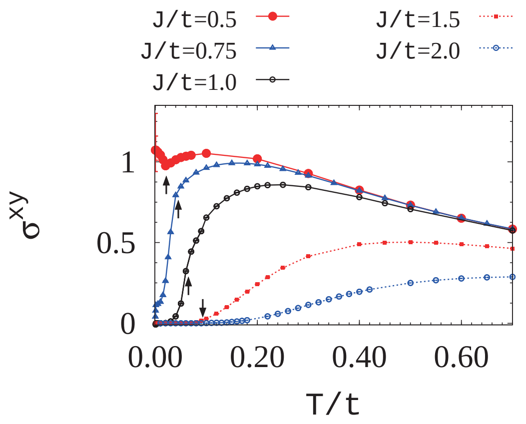

Figure 6: Spin-Hall conductivity for several values of J [22]. The error bars at low temperatures are due to extrapolation to the $\omega \to 0$ limit. At high temperatures these error bars are smaller than symbols. Arrows denote antiferromagnetic transition points.

ferromagnetic phase; the increase of the spin-Hall conductivity is observed in the antiferromagnetic phase. The conductivity in the antiferromagnetic phase is shown as a function of T in Fig. 6. At $J = 0.75t$, where the ground state is topologically trivial, the spin-Hall conductivity vanishes at zero temperature, but increases with increasing temperature. Note that the ground state is an antiferromagnetic topological phase for $J < 0.683$. As seen in Fig. 5(c), the magnetic order removes the pole of the self-energy, and the ground state possesses nontrivial properties. This leads to a dip structure in the temperature dependence of the conductivity for $J = 0.5t$; with decreasing temperature the Kondo effect firstly decreases the conductivity for $0.021t < T < 0.03t$, but with entering the antiferromagnetic phase ($T < 0.021t$), the conductivity increases again because the ground state is the antiferromagnetic topological insulator.

Summarizing this section, we have observed an intriguing crossover behavior due to the interplay between electron correlations and topological properties. At low temperatures, the Kondo effect destroys the topological structure. However, the topological properties are restored if the temperature is higher than the Kondo temperature but smaller than the band gap of the topological insulator. The restoration of topological properties can be observed in the bulk and the edge. The spin-Hall conductivity rapidly increases even if it is almost zero at low temperatures. Edge modes, destroyed by the Kondo effect in the low temperature region, appear with increasing temperatures. The crossover behavior is observed in both of the paramagnetic and the antiferromagnetic phases.

4 Related issues

We have also studied some interesting issues related to topological phases, which we briefly summarize below.

(a) *Topological phase transitions in periodically driven systems* [23, 24]: Recently, concepts of topological phases of matter have been extended to nonequilibrium systems. In particular, periodically driven systems described by Floquet theory have been a topic of intensive studies. We propose a model which shows non-equilibrium topological phase transitions in cold-atomic systems. Namely, we demonstrate that the Rabi oscillation plays an important role to tune the band structure in fermionic optical lattices, driving a non-equilibrium topological phase transitions from the trivial insulator to a time-reversal symmetric (Z_2) TI.

(b) *Hidden topological properties of quantum walks*[25]: Quantum walks provide a unique platform to realize Floquet TIs in a nonequilibrium systems driven by a time-periodic field. So-called discrete quantum walks consists of two operators, i.e. shift and coin operators, which respectively play a similar role of particle hopping and spin-rotation due to spin-orbit coupling. We can thus realize various topological phases in quantum walks for cold atomic systems, photonic systems, etc. We here obtain the phase diagrams of the topological numbers for the 1D discrete quantum walks. This accounts for a hidden topological phase of the 1D photonic quantum walk studied in recent experiments, in which edge states were observed, even though the parameter space was considered to be topologically trivial.

(c) *Topological properties of quasiperiodic correlated systems* [26]: We analyze a quasiperiodic Bose lattice system in 1D, which we call Harper-like Bose-Hubbard model. We compute the Chern number and observe a gap closing behavior as the Hubbard interaction U is changed. Also, we discuss the bulk-edge correspondence in the system. Furthermore, we explore the phase diagram as a function of U and a continuous deformation parameter between the Harper-like model and another important quasiperiodic lattice, the Fibonacci model. We numerically confirm that the incommensurate charge density wave (ICDW) phase is topologically non-trivial and it is topologically equivalent in the whole ICDW region

5 Summary

We have reported our recent studies on correlated TIs and some related topics. We have established the emergence of 1D topological Mott insulator, which is accompanied by edge Mott states carrying only spin currents. This was done by applying the DMRG method to the calculation of the winding number as well as the entanglement spectrum. We have also shown an intriguing topological phase transition from a trivial to nontrivial phase, which is characterized by zeros of Green's function.

We have addressed a similar question for two-dimensional TIs by using a DMFT approach. As a typical example of correlated topological phase in two dimensions, we have considered a Kane-Mele Kondo lattice model, where the Kondo effect becomes dominant, leading to a topologically trivial singlet ground state. However, a remarkable phenomenon is induced by temperature effects, reflecting strong competition between topology and correlation, i.e. topological properties are restored by raising the temperature. We have confirmed that this kind of temperature induced topological properties are not specific to the present model, but applicable more generically to correlated TIs [27].

We have also summarized some other topics related to topological phases, which we studied recently. This includes laser-induced TIs in nonequilibrium conditions, hidden topological properties in quantum walks, and topological properties of correlated quasi-periodic systems.

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