

From edge-state physics to entanglement spectrum: Interactions and impurities in two-dimensional topological insulators

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We present a theoretical approach to incorporate electronic interactions in the study of two-dimensional topological insulators. By exploiting the correspondence between edge-state physics and entanglement spectrum in gapped topological systems, we deconstruct the system into one-dimensional channels. This framework enables a simple and elegant inclusion of fermionic interactions into the discussion of topological insulators. We apply this approach to the Kane-Mele model with interactions and magnetic impurities.

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Introduction. Two-dimensional systems have captivated physicists with their intriguing and often counterintuitive properties [1]. Frequently, they demand the development of new theoretical and numerical tools for investigation [2]. A notable historical example of this behavior is observed in the quantum Hall effect. While the integer quantum Hall effect can be comprehensively explained within the framework of noninteracting particles filling Landau bands, the discovery of noninteger Hall plateaus due to electronic interactions and disorder was a surprising revelation [3]. Recently the better understanding of topological properties in the band structure of two-dimensional systems have yielded new and exciting theoretical and experimental results [4]. However, the interplay of topology and correlations is still a relatively open area of investigation [5].

In the study of strongly correlated two-dimensional systems, one promising approach is to leverage insights gained from one-dimensional models by suitably identifying one-dimensional structures in the higher-dimensional system. Several methods can be employed to achieve this dimensional reduction. One intuitively appealing approach is to first consider quantum wires and subsequently introduce tunneling between them [6–8]. The connection to the two-dimensional system is obtained using renormalization group arguments to the tunneling amplitude. Another approach is to deconstruct the topological system into one-dimensional wires in order to classify the topological phases [9,10]. In a complementary view to this anisotropic starting point, we propose an approach that is particularly well suited for studying impurities in two-dimensional topological systems.

This Letter revolves around a pivotal concept: The spectrum of entanglement [11] in gapped systems provides a valuable insights into the dynamics of local operators [12]. This fresh perspective introduces a fictitious boundary, enabling us to represent the original wave function as a superposition of *bulk states* and *boundary states*. When focusing on the behavior of local operators solely defined on the

boundary, it becomes evident that only the boundary states interact with these operators. However, this introduction of the *boundary* comes at the cost of working within a formalism at a finite fictitious temperature, which is determined by the problem's characteristics, such as the presence of the spectral gap.

By starting with a two-dimensional problem and transitioning to a one-dimensional model at a finite temperature, we gain the ability to incorporate interactions into the problem on much better footing than in a straightforward approach within the original two-dimensional model. This avenue of investigation presents an approach to studying electronic systems, enabling a deeper comprehension of their dynamics and properties. Furthermore, it presents a clear pathway towards two-dimensional bosonization, and possibly new numerical techniques, on these systems.

Though out this Letter we consider natural unit, $\hbar = c = k_B = 1$. The Letter is organized as follows: First, the general formalism is introduced. Subsequently, we delve into the analyses of the prototypical topological band insulators, the *Kane-Mele model*. We add to this model local degrees of freedoms and electronic interactions to investigate the interplay of magnetism, interactions, and topology. We finish with a conclusion and some possible future perspectives.

The physics of a hard-wall boundary. In a two dimensional system, a hard-wall boundary is a one-dimensional surface that prohibits the flow of particles and information. These properties are implemented by specific boundary conditions on the Schrödinger equation that ensures that the current through the boundary is zero. For instance, let us consider *nonrelativistic* fermions in two dimensions with a hard boundary located at $x = 0$. To ensure that the single-particle wave function $\psi(x \geq 0, y) = X(x)Y(y)$ follows the hard wall conditions, we require that

$$\frac{\partial \psi(0, y)}{\partial x} = 0 \quad \text{or} \quad \psi(0, y) = 0. \quad (1)$$

It was shown that for the case of *relativistic* fermions [13–15], the *no-current* condition leads to two very distinct type of $X(x \geq 0)$ functions: *bulk* and *boundary* solutions. Bulk

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solutions correspond to standing waves and must be zero at the boundary,

$$X(x \geq 0) = x_0 \sin[\varepsilon x], \quad (2)$$

with x_0 and ε constants. Conversely, zero-energy boundary solutions can exist. They correspond to exponentially decaying functions

$$X(x \geq 0) = x_0 e^{-\frac{x}{\xi}}, \quad (3)$$

where ξ is the characteristic length of the state. The behavior of $Y(y)$ can depend on the details of the microscopic theory. A well-known example is graphene [16]. In graphene, an *armchair* edge in graphene gives rise to boundary states with energies away from the Fermi level, while a *zigzag* edge introduces states at the Fermi level with no dispersion. The fact that we can classify solutions in the presence of a real hard wall boundary as *bulk* states and *boundary* states is a powerful insight into the spectrum of entanglement.

Spectrum of entanglement and edge states. The concept of the entanglement spectrum in topological systems was introduced by Li and Haldane in 2008 [17]. They investigated a Hall system on the surface of a sphere and employed the Schmidt decomposition to recast the problem in terms of wave functions defined on each hemisphere of the sphere. The logarithm of the Schmidt coefficients was then coined the *entanglement spectrum*. It encodes the physical information on how the original wave function is weaved at the fictitious boundary created by the choice of basis. Remarkably, through numerical analysis, they observed that the entanglement spectrum accurately reproduces the low-energy spectrum of a genuine boundary in a Hall bar.

Following their pioneering work, subsequent contributions have further support for these findings [12, 18–25]. These studies consistently demonstrate that in topological systems the entanglement spectrum faithfully reproduces the spectrum of genuine edge states, albeit at finite fictitious *temperature of entanglement*, T_E , and low energies.

In what follows, we assume that the initial wave function that we aim to describe, denoted as $|g\rangle$, is the ground-state wave function of a gapped local Hamiltonian of a topological insulator. We proceed by dividing the system into two partitions, $|A\rangle$ and $|B\rangle$, with an arbitrary cut. The Hamiltonian can be written as the sum of Hamiltonians pertaining to the individual partitions, namely $H_{A/B}$, along with the interpartition Hamiltonian H_{AB} ,

$$H_0 = H_A + H_B + H_{AB}. \quad (4)$$

The state $|g\rangle$ can always be expressed using the Schmidt decomposition $|g\rangle = \sum_i \lambda_i |A_i\rangle |B_i\rangle$, where $|A_i/B_i\rangle$ form a complete basis of each partition. These bases comprise both *bulk* and *boundary* states. The key observation is that *bulk* states must vanish at the boundary. As a consequence, any set of operators, $\{\mathcal{O}_i\}$, that live at the cut defining the partitions will couple only to the *boundary* states of the basis [12]. Only the *boundary* states contribute to the expectation values of $\{\mathcal{O}_i\}$. It is convenient to define two boundary theories, H_A^B and H_B^B , which can be used to label these states. In this context, these boundary theories can be called as *entanglement models*. Notably, it has been demonstrated that if the boundary theory is conformal [12], then the maximally entangled conformal



FIG. 1. Partitioning a system using an arbitrary cut establishes a fictitious boundary. The original ground state is rewritten using the basis of each partitions, $\{|A\rangle, |B\rangle\}$. The expectation value of operators defined at the boundary, $\{\mathcal{O}_i\}$, can be done using only “boundary states” in $\{|A\rangle, |B\rangle\}$. Many partitions are possible and they correspond to different one-dimensional channels that correlations can propagate in the bulk.

state, known as the Ishibashi state $|g_*^B\rangle = \sum_i |B_{A,i}\rangle |B_{B,i}\rangle$, is projected into the desired wave function by the *extrapolation length* β ,

$$|g^B\rangle = e^{-\frac{\beta}{2}(H_A^B + H_B^B)} |g_*^B\rangle, \quad (5)$$

where $|g^B\rangle$ is the ground state at the boundary that can be used to evaluate the expectation values of $\{\mathcal{O}_i\}$. A similar discussion can also be found in Refs. [22, 23] and it was established that $\beta^{-1} = T_E$ is proportional to the bulk gap of the topological insulator.

A direct consequence of Eq. (5) is that any two operators situated on the fictitious boundary will have exponentially decaying correlations. This observation can be understood within the framework of the Lieb-Robinson bound [26–28]. In its more restricted form, the bound says that for a system with a uniform gap and local interactions, the two point correlation function of local operators \mathcal{O}_1 and \mathcal{O}_2 calculated over the ground state should decay exponentially. Thus, the fictitious temperature on Eq. (5) enforces the Lieb-Robinson bound along the direction of the cut.

The degree of arbitrariness in choosing the cut that creates the partitions is an important question. When evaluating the expectation value of an operator at the same spatial position, the particular cut is irrelevant. The main advantage to use the spectrum of entanglement in this case is to leverage the knowledge of the boundary theory and its symmetries. This approach enables us to incorporate, for instance, fermionic interactions into the analysis, expanding the scope of the discussion.

However, it is when evaluating observables $\{\mathcal{O}_i\}$ at different positions we truly capture the underlying physics [see Fig. 1]. It is instructive to initially consider a noninteracting theory. Following Ref. [11], it is straightforward that for any tight-binding model the one-particle propagator $C_{ij} = \langle g | c_i^\dagger c_j | g \rangle$ on a lattice \mathcal{L} can be rewritten as $C_{ij} = \text{tr}(\mathcal{K} e^{-\mathcal{H}} c_i^\dagger c_j)$ over a subset of points $\{n, m\} \in \mathcal{M} \subset \mathcal{L}$, with the spectral of entanglement

$$\mathcal{H} = \sum_{\{n, m\} \subset \mathcal{M}} H_{nm} c_n^\dagger c_m \quad (6)$$

and \mathcal{K} a normalization constant. A unitary transformation U , that is \mathcal{M} dependent, diagonalizes the entanglement spectrum and separates the bulk and boundary modes, i.e., $U^\dagger \mathcal{H} U = \mathcal{H}_{\text{boundary}} + \mathcal{H}_{\text{bulk}}$. In particular, if we choose $\{i, j\}$ on the boundary of \mathcal{M} the projection of $c_i^\dagger c_j$ over the boundary modes guarantees that we acquire the same original propagator regardless of \mathcal{M} . Consequently, we possess the liberty

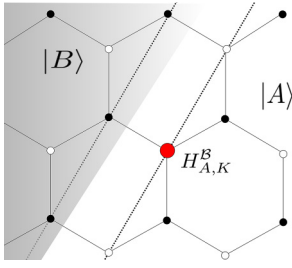


FIG. 2. The Kane-Mele model with Coulomb interactions between the electrons. A magnetic impurity is represented as a red dot. A fictitious cut creates the two partitions, $|A\rangle$ and $|B\rangle$ (white and gray areas), and zigzag edges (dotted lines). The boundary theory on partition $|A\rangle$ is $H_{A,K}^B$, and a Kondo model in an L.L. at finite temperature T_E is defined on the dotted line the cross the impurity.

to opt for the partition that yields the simplest mode expansion. Generally, this corresponds to a partition characterized by reflection symmetry, consequently implying a boundary theory with the shortest distance between points i and j . This argument holds true for an interacting theory as well since the choice of \mathcal{M} does not change the correlation function that is being evaluated. We now use the Kane-Mele model to illustrate the use of the spectrum of entanglement as a calculation tool.

Kane-Mele model with an IRLM. Arguably the simplest topological model that preserves time-reversal symmetry is the Kane-Mele model of free fermions on a honeycomb lattice [29]. Let us consider this model in its standard form [29] and introduce a Hubbard interaction between the fermions

$$H_0 = \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + i\Delta \sum_{\langle\langle i,j \rangle\rangle, \sigma, \sigma'} v_{ij} s_{\sigma\sigma'}^z c_{i\sigma}^\dagger c_{j\sigma'} + u \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (7)$$

where $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, Δ is the next-nearest-neighbor hopping strength, $v_{ij} = \pm 1$ depending on the hopping orientation, s^z is the z Pauli matrix, and u is the Hubbard interaction strength.

In Fig. 2, we introduce a cut that separates the two sublattices of the Kane-Mele model, resulting in two zigzag edges that can be described in terms of Luttinger liquids [29]. These edges exhibit fermionic currents, namely $J_{A/B}^{R\uparrow}$ and $J_{A/B}^{L\downarrow}$. The fact that the model preserves time-reversal symmetry implies that, at low energies, only marginal forward-scattering interactions need to be considered. These interactions can be described by the boundary Hamiltonians,

$$H_{A/B,I}^B = \frac{v_f}{4\pi} \int dx \sum_{a \neq b \in \{R\uparrow, L\downarrow\}} [g_2 J_{A/B}^a J_{A/B}^b + g_4 (J_{A/B}^a)^2], \quad (8)$$

where v_f represents the Fermi velocity. By employing Abelian bosonization [30–32], the low-energy theory of *each* boundary shown in Fig. 2 can be expressed as

$$H_{A/B,0}^B + H_I^B = \frac{\tilde{v}}{8\pi} \int_{-\infty}^{\infty} dx \frac{1}{g} \partial_x \phi_{A/B}^2 + g \partial_x \theta_{A/B}^2, \quad (9)$$

where $[\phi_{A/B}(a), \partial_x \theta_{A/B}(b)] = -4\pi i \delta(a-b)$, $g = \sqrt{(1+g_4-g_2)/(1+g_4+g_2)}$ is the Luttinger parameter and $\tilde{v} = v_f \sqrt{(1+g_4-g_2)(1+g_4+g_2)}$ is the bosonic

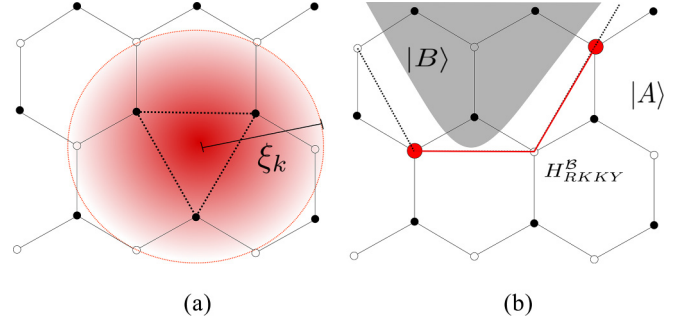


FIG. 3. (a) If $T_E \ll T_k$, then a Kondo singlet is formed (red region of length ξ_k). We expect that edge states exist at the end of the Kondo cloud (depicted as dotted lines in the figure). (b) In the perturbative regime, $T_k \lesssim T_E$, an effective RKKY interaction controls the dynamics of the magnetic impurities.

velocity. The energy gap and the interactions in the bulk system determine the Fermi velocity and the band width, which can be approximated as $\Lambda \sim T_E$.

At a site on the edge of partition A we introduce a single-impurity Anderson model with on-site repulsive interactions $H_{A,1}^B = H_{A,0}^B + V \sum_{\sigma} c_{0,\sigma}^\dagger d_{\sigma} + \text{H.c.} + U N_{\uparrow} N_{\downarrow}$, with $N_{\sigma} = d_{\sigma}^\dagger d_{\sigma}$. Using the Schrieffer-Wolff transformation [33] and taking the large- U limit, we obtain the Kondo model in a Luttinger Liquid (L.L.) as *one* of the boundary theories [32,34,35],

$$H_{A,K}^B = H_{A,0}^B + H_{A,I}^B + J_z \partial_x \theta_A(0) \cdot S^z + (J_{\perp} \Lambda) e^{-i\phi_A(0)} S^- + \text{H.c.}, \quad (10)$$

where $J_{k=z,\perp} \sim V^2/U$ and \vec{S} is the spin projection of the fermion at the the d level. A single impurity couple to the boundary theory is similar to the introduction of a Unruh-DeWitt detector [36] in the Unruh effect. Therefore, it completes the analogy introduced by Swingle and Senthil [22] between the spectrum of entanglement and the Unruh effect. The scaling equations for this Kondo problem flow to strong coupling for repulsive interactions, $g < 1$, and/or antiferromagnetic Kondo coupling, $J_{z,\perp} > 0$. The Kondo temperature can be estimated using the usual argument as

$$\frac{T_K}{T_E} = J_{\perp} \frac{-1}{1-g+\frac{4J_z}{v}}. \quad (11)$$

The physics of the ground wave function will depend on a comparison between the Kondo temperature, T_k , and the temperature of entanglement, T_E , which acts as an infrared cutoff to the renormalization process.

For repulsive interactions and when $T_k \gg T_E$ the Kondo singlet forms. In the limiting case of $J_{z,\perp} \rightarrow \infty$, a c fermion at the the resonant level site is bound to form the Kondo singlet. This effectively removes the site from the lattice and introduces a zigzag edge in the middle of the bulk, see Fig. 3(a). However, for a finite $J_{z,\perp}$ the many-body state is more complex. The fermion at the local level d is entangled with many electrons on the c band, forming what is known as the Kondo cloud [37]. The Kondo cloud is not a well-defined entity in real space, but it is usually assumed to have a characteristic length scale of $\xi_k = \tilde{v}/T_k$. This region of the

material, characterized by the Kondo cloud, is an intriguing state of matter that should be surrounded by gapless real edge states. If a diluted set of these Kondo impurities is separated by distances of the order of ξ_k , then it could allow current to pass through the bulk of the material. This implies that for a linear dimension L , a critical density of magnetic impurities of $n_c = \xi_k/L$ would melt the topological phase. The tunneling of electrons in internal edge states created by impurities have been proposed before as a mechanism to destabilize the topological phase [38]. The difference here is that the region is not related to size of the impurities but rather to the length of the Kondo cloud.

In the limit where $T_k \lesssim T_E$, we enter a perturbative regime where the renormalized $J_{z,\perp}$ remains small due to an irrelevant flow or an infrared cutoff. In this regime, multiple magnetic impurities can interact through the c band. To study this interaction, we need to evaluate the Green's functions of the c electrons that mediate the interaction. For simplicity, let us consider a pair of magnetic impurities, $\{\vec{S}_1, \vec{S}_2\}$, located on the same sublattice of the honeycomb lattice, see Fig. 3(b). We introduce a partition that connects the two impurities through a minimum path of distance Δx along the edge. Since we are in the perturbative regime, it is straightforward to write a Ruderman-Kittel-Kasuya-Yosida– (RKKY) like interaction between the two impurities using the finite-temperature Green's function of the L.L. [31],

$$H_{\text{RKKY}}^B \propto \frac{J_k^2}{\left[\frac{\beta_E}{\pi} \sinh\left(\frac{\pi}{\beta_E} \Delta x\right)\right]^{2g}} \vec{S}_1 \cdot \vec{S}_2 + \text{l.r.t.} \quad (12)$$

The ground state of several pairs of these magnetic impurities are singlets. Therefore, by measuring the distribution of binding energies of these singlets, and independently measuring the bulk gap, it is possible to directly determine the Luttinger parameter.

The physics of a dense array of magnetic impurities will ultimately depend on the interplay of the three energy scales in the problem: T_E , T_K , $T_{\text{RKKY}} \sim J_k^2 \bar{v}$. This interplay opens up a wide range of possibilities for exploring the rich

phenomenology of heavy fermions. For instance, for $T_{\text{RKKY}} > T_K > T_E$ it is possible to order the impurities magnetically, in sharp contrast to the the Kondo phase ($T_K > T_{\text{RKKY}} > T_E$). Arguably, the most interesting situation would be $T_K \sim T_{\text{RKKY}} > T_E$, where a conducting-insulating transition could occur as a function of temperature and/or pressure.

Conclusions. In this Letter we propose a theoretical approach for incorporating electronic interactions in the study of two-dimensional topological insulators. Building on the established correspondence between edge-state physics and the entanglement spectrum in gapped topological systems, we leverage this connection to deconstruct the two-dimensional system as one-dimensional channels that connect any two points within in the system. The effective theory of these channels is precisely the edge-state theory at the fictitious temperature of entanglement. The effective theory carries the same topological protection that real edge states have. Consequently, we can elegantly incorporate fermionic interactions into the framework. To analyze these systems we can employ well-known techniques such as Abelian bosonization or the density matrix renormalization group. While considering one-dimensional channels in topological insulators is not a new idea [6–10], our approach naturally emerges from the ground-state wave function.

We follow the general discussion by considering the Kane-Mele model with interactions and in the presence of magnetic impurities. It is well established that impurities can give rise to localized regions, or islands, within a topological system, which harbor edge states [38]. Our findings reveal two intriguing scenarios. First, in the Kondo regime we identify a possible mechanism to destabilize the topological phase. Second, in the perturbative regime we observe that the impurities can order magnetically through an RKKY-like interaction. Interestingly, this magnetic ordering in a dilute impurity system presents a unique opportunity to experimentally measure the strength of fermionic interactions in the topological system.

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