Delocalization of edge states in topological phases

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Abstract – The presence of a topologically non-trivial discrete invariant implies the existence of gapless modes in finite samples, but it does not necessarily imply their localization. The disappearance of the indirect energy gap in the bulk generically leads to the absence of localized edge states. We illustrate this behavior in two fundamental lattice models on the single-particle level. By tuning a hopping parameter the indirect gap is closed while maintaining the topological properties. The inverse participation ratio is used to measure the degree of localization.

Topological phases [1–5] constitute one of the most spectacular research fields in quantum matter. Historically, the earliest widely studied example is the quantum Hall effect [6–9]. More recently, topological insulators have attracted much interest [1,10]. The edge states in two dimensions (2D) [9] and the surface states in three dimensions (3D) [11] in topological insulators are commonly seen as a characterizing feature. For notational simplicity, we will henceforth use the term “edge state” for all states localized at a boundary irrespective of dimensionality. Such states have potential applications in spintronics [12], magneto-electronics [13] and opto-electronics [14]. The application of the integer quantum Hall effect in high-precision metrology stands out [15]. Another interesting suggestions are tunable group velocities of edge states to realize delay lines and interference devices [16,17].

The emergence of edge states in non-interacting topological systems is elucidated by the bulk-boundary correspondence [10,18–20] which relates finite discrete topological invariants of the energy bands in the bulk to the existence of edge states at the boundary of finite systems. The underlying idea is as follows. The transition between two bulk systems (one could be the vacuum) with different discrete topological invariants cannot be continuous because of their discrete nature. Thus, there must be in-gap states which link the bands of different topological invariants so that they can no longer be defined for each band separately. Since this argument hinges on the existence of the boundary, it is assumed that these in-gap states are localized at the boundaries, hence represent edge states [10]. For certain Hamiltonians this can be rigorously shown [18–20].

Such topological edge states can be found in topological insulators [10,21], topological semi-metals [22], topological crystalline insulators [23]. Higher-order topological insulators in 3D may not display surface states, but so-called hinge states [24]. In one dimension (1D), there can be localized states at the chain ends [25,26]. Recently, however, we found in 1D that localized end states do not represent the generic scenario if the indirect energy gap between the bands of different topological invariant vanishes [27]. While the direct gap $\Delta_{\text{dir}}$ measures the energetic separation of two bands at a given fixed momentum, the indirect gap $\Delta_{\text{indir}}$ measures this separation if momentum changes are admitted. Clearly, $\Delta_{\text{indir}} \leq \Delta_{\text{dir}}$ and a finite $\Delta_{\text{dir}}$ is sufficient for the bands to be well defined. This surprising finding qualifies the bulk-boundary correspondence in the sense that a finite direct gap does not suffice to guarantee localized edge states.

Since 1D topological systems differ significantly from their higher-dimensional counterparts, the question arises as to which extent the delocalization of edge states occurs in 2D as well if the indirect gap vanishes. The goal of the present letter is to answer this question by a representative proof-of-principle study.

The fermionic tight-binding model proposed by Haldane [28] as a first example of non-trivial topological behavior without magnetic field is a well-established model of a Chern insulator due to its simplicity. Hence, we choose it as our starting point. By adding a spatially
anisotropic hopping it is possible to close the indirect gap while leaving the topological properties of the bands completely untouched. The Hamiltonian reads

\[
\mathcal{H} = \mathcal{H}_{\text{Haldane}} + \mathcal{H}_{\text{diag}},
\]

\[
\mathcal{H}_{\text{Haldane}} = t \sum_{\langle i,j \rangle} c_i \sigma c_j + t_2 \sum_{\langle (i,j) \rangle} e^{\pm i \phi} c_i \sigma c_j,
\]

\[
\mathcal{H}_{\text{diag}} = t'_2 \sum_{\langle (i,j) \rangle} e^{\pm i \varphi} c_i \sigma c_j,
\]

where \(c_i^\dagger\) and \(c_i\) correspond to the creation and annihilation operators at site \(i\), respectively. The hoppings on the honeycomb lattice are shown in fig. 1. A pair of nearest-neighbor (NN) and next-nearest-neighbor (NNN) sites is denoted by \((i,j)\) and by \(\langle (i,j) \rangle\), respectively. The hopping elements \(t, t_2\) and \(t'_2\) are real and \(t\) serves an energy unit. The sign of the complex phase \(\phi\) for the \(t_2\)-hopping is positive for anti-clockwise hopping and negative for clockwise hopping, see blue and red arrows in the plaquettes in fig. 1.

The notation \(\langle (i,j) \rangle\) restricts the hopping to next-nearest neighbors in the \(y\)-direction. Therefore, it breaks the point group symmetry \(C_3\) of the bulk system. The sign of its phase \(\varphi\) is positive in the \(y\)-direction and negative in the \(−y\)-direction. This additional term may seem artificial, but it is very suitable for the intended proof-of-principle. Its realization in ultracold atom systems appears feasible [29].

In reciprocal space the bulk Hamiltonian reduces to a \(2 \times 2\) matrix due to the two sites in a unit cell; it can be expressed in terms of Pauli matrices. One finds that \(\mathcal{H}_{\text{diag}}\) is given by \(2t'_2 \cos(k_y + \varphi)\sigma_0\), where \(\sigma_0\) is the identity matrix. Hence the \(t'_2\)-hopping only induces an energy shift without having any effect on the eigenstates at a given momentum. The topological properties derived from the eigenstates such as the Berry curvature and the concomitant Chern number [30] are preserved. The bulk dispersion, however, is altered due to \(t'_2\).

On the left-hand side of fig. 2 we illustrate the dispersion for \(t_2 = 0.2t\), \(\phi = \pi/2\) without \(t'_2\). If \(t'_2\) is switched on at \(\varphi = 0\) the dispersion changes significantly as shown on the right-hand side of fig. 2. The direct energy gap at each given \(k\)-value does not change so that the two bands stay well separated. But the indirect gap is given by the energy difference between the green and the blue dashed line and hence vanishes and becomes even negative as displayed clearly in fig. 2(b) at fixed \(k_x = \pi\).

To take the orientation of the boundary into account we define the indirect gap \(\Delta_{cv}(k_x)\) as the smallest energy difference between the conduction and valence band at a fixed \(k_x\), but for varied momentum \(k_y\). The relevant band edge for the conduction band \(\varepsilon_{\text{bu, } c}(k_x) := \min_{k_y} \omega_{\text{bu, } c}(k_x, k_y)\) is displayed as green dotted line. For the valence band \(\varepsilon_{\text{bu, } v}(k_x) := \max_{k_y} \omega_{\text{bu, } v}(k_x, k_y)\) it is marked by the blue dotted line. Thus, one has

\[
\Delta_{cv,y}(k_x) = \varepsilon_{\text{bu, } c}(k_x) - \varepsilon_{\text{bu, } v}(k_x).
\]

This gap can take formally negative values. Tuning \(t'_2\) from 0t to 0.5t at \(\varphi = 0\) closes the indirect gap at \(k_x = \pi\).

Next, we pass from the bulk to a finite, confined system considering a strip with zigzag edges as shown in fig. 1. We investigate the existence of localized edge states. The boundaries are chosen to run in the \(x\)-direction and, thus, \(k_x\) continues to be preserved, but \(k_y\) does not. Upon turning on the diagonal \(t'_2\)-hopping, the topological properties in the bulk remained completely unaffected, but we find a significant impact on the system with boundaries: the exponentially localized edge states at \(t'_2 = 0\) become less and less localized till they delocalize completely. We want to explore this phenomenon here.

In order to measure the localization of states the inverse participation ratio [31,32] (IPR) is most suitable. We want to quantify the localization to the edges of the strip, so we
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Fig. 3: (a)–(c) The IPR, $\Delta_{cv,y}$, and $\Delta_y$ of the right-moving edge state vs. diagonal hopping $t'_2$ are shown for various momenta $k_x$ as computed for $N = 500$. $\Delta_y$ of both edge states at $k_x = 1.5\pi$ lie on top of each other.

define the IPR of a normalized eigenstate by

$$I_n(k_x) = \sum_i p_{n,i}^2(k_x) = \sum_i |\langle n, i | n, i \rangle|^2(k_x) \in [0, 1],$$

where $p_{n,i}$ is the probability of finding a particle at site $i$ in the unit cell in fig. 1 if the system is in the $n$-th eigenstate at momentum $k_x$. The IPR of localized states is finite, even for $N \to \infty$, while it converges towards zero for delocalized, extended states in this limit. Hence, in numerics an IPR of $O(1/N)$ indicates a delocalized state while larger values indicate localization.

First, we focus on the case $k_x = \pi$ being the crossing point of the dispersion of the right- and left-moving in-gap state. Its energy lies precisely in the middle between the conduction and valence band rendering the spectrum at this value of $k_x$ similar to the spectrum of the 1D case studied previously [27]. Figure 3(a) depicts the IPR as a function of $t'_2$. For comparison, the indirect gap $\Delta_{cv,y}$ is shown in fig. 3(b). As in 1D, the IPR at $k_x = \pi$ decreases monotonically to its minimum value $O(1/N)$ upon increasing $t'_2$. The IPR reaches this value at the same value $t'_2$ where the indirect gap $\Delta_{cv,y}$ vanishes. This delocalized in-gap state remains extended for $\Delta_{cv,y} < 0$.

If $k_x$ takes other values the situation is more complex because the energy of the in-gap states is closer to one of the two bands, conduction or valence, respectively. We observe that the delocalization $I \approx 0$ occurs for smaller values of $t'_2$ than the zero of the indirect gap $\Delta_{cv,y}$, see fig. 3(a) and (b). So we conclude that the existence of an indirect gap and delocalization are linked, but not in a straightforward manner, see discussion below.

In order to achieve a better understanding we define a specific indirect gap $\Delta_y$ referring to the energy of the in-gap state. This piece of information is available once the strip geometry is analyzed quantitatively. Let the in-gap energies be denoted by $\omega_{in,\alpha}$ where $\alpha$ denotes the different in-gap branches. Then $\Delta_y$ is the smallest energy difference of $\omega_{in,\alpha}$ to one of the bands at fixed $k_x$

$$\Delta_y(k_x, \alpha) := \min \{\omega_{in,\alpha} - \epsilon_{bu,v} - \epsilon_{bu,c} - \omega_{in,\alpha}\}.$$  \hspace{1cm} (4)

If the in-gap states enter the continua of either conduction or valence band we set $\Delta_y(k_x, \alpha) = 0$. Thus, $\Delta_y(k_x, \alpha) = 0$ measures the energy distance of in-gap states to the extended bulk modes. It is to be expected that it is closely related to delocalization.

The indirect gap $\Delta_y$ as a function of $t'_2$ is shown in fig. 3(c). For $k_x = \pi$, $\Delta_y$ behaves like $\Delta_{cv,y}$ since in this particular symmetric case both quantities are proportional to each other. For other momenta, however, differences appear. In contrast to $\Delta_{cv,y}$, $\Delta_y$ at $k_x \neq \pi$ vanishes exactly at the value of $t'_2$ where the IPR essentially vanishes. This shows that localization can be attributed to a finite $\Delta_y$. Note also the possible non-monotonic behavior of IPR and $\Delta_y$ as a function of $t'_2$, e.g., at $k_x = 0.3\pi$.

For the sake of comprehensibility we visualize the evolution of the band structure as a function of the hopping amplitude $t'_2$. In fig. 4 we depict four representative cases $t'_2 = \{0, 0.25t, 0.5t, 0.75t\}$. On increasing $t'_2$ the conduction and valence bulk bands are approaching each other and the edge states are becoming covered by them more and more, see fig. 4(a) and (b). At the marginal value $t'_2 = 0.5t$ shown in fig. 4(c), all in-gap states are covered by bulk states and therefore are delocalized. This coincides with the closing of the indirect gap $\Delta_{cv,y} = 0$ at $k_x = \pi$. Increasing $t'_2$ further, see fig. 4(d), the range of $k_x$-values increases where $\Delta_{cv,y}$ is zero or negative.

There is a large number of further aspects worth investigating: i) In the Supplementary Material (SM) we study the case $\varphi = \pi/2$ which confirms our conclusion that the vanishing of the indirect gap $\Delta_y$ goes along with delocalized in-gap states. But better localized states may have a smaller $\Delta_y$ which shows that both quantities are not linked by a simple monotonic relation. ii) We find that if the additional hopping runs along $\pi$ and not along $y$ the additional term reads $2t'_2 \cos(k_x + \varphi)\rho_0$ and does neither change the bulk topology nor the localization in the strip in fig. 1. iii) Samples which are finite in both directions are also studied (see SM). We find that their chiral edge states become extended precisely if along one of the edges the in-gap states delocalize. Finally, we point out that different boundaries imply different edge states dispersions. For instance, a bearded boundary [16] in the Haldane model has its crossing point at $k_x = 0$ implying a different $\Delta_y(k_x)$ so that the localization persists up to larger values of $t'_2$. 

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Fig. 4: (a)–(d) Continua of the two bulk bands and dispersions of the two in-gap states (right-mover in blue, left-mover in green) for $t_2 = 0.2t$, $\phi = \pi/2$, $\varphi = 0$, and $t'_2 = \{0t, 0.25t, 0.5t, 0.75t\}$. Due to the absence of an indirect gap the continua overlap in panels (c) and (d) and no in-gap states can be identified. The magenta and cyan lines indicate the band edges $\varepsilon_{bu,c}$ and $\varepsilon_{bu,v}$, respectively.

The standard lattice studied above has provided a proof-of-principle result allowing us to establish the importance of indirect gaps for the localization of in-gap states so that they represent true edge states. In order to corroborate that this scenario is generic and experimentally relevant we next address the topological checkerboard lattice, see fig. 5, which has been realized by optical lattices [33–35]. This lattice is described by a two-band model [36] with NN ($t$) and NNN ($t'_1$, $t'_2$) hopping,

$$H = -t \sum_{\langle i,j \rangle} e^{\pm i\phi} c_i^\dagger c_j - \sum_{\langle\langle i,j \rangle\rangle} t'_1 c_i^\dagger c_j. \quad (5)$$

For the bulk, Fourier transformation yields a representation in terms of Pauli matrices,

$$H = -s(\cos(k_x) + \cos(k_y))\sigma_0 - d(\cos(k_x) - \cos(k_y))\sigma_z - 4t\cos(\phi)\cos(k_x/2)\cos(k_y/2)\sigma_x - 4t\sin(\phi)\sin(k_x/2)\sin(k_y/2)\sigma_y, \quad (6)$$

where we use $s := t'_1 + t'_2$ and $d := t'_1 - t'_2$ for brevity and $t$ as energy unit. A topological phase occurs for $\phi \neq n\pi$ and $d \neq 0$ [37]. Investigating the strip sketched in fig. 5 one clearly sees the left- and right-moving in-gap states shown in panel (a) of fig. 6. Tuning $s$ while keeping $d$ constant (see SM), the bulk topology is not changed, but the dispersion changes, just as for the Hamiltonian (1). Indeed, we find the same scenario as in fig. 3, see panels (b) to (d) in fig. 6. This strongly corroborates our findings and paves the way to their experimental verification.

Summarizing, non-trivial topological properties of the bulk imply the existence of in-gap states. Often, they are supposed to be localized at the boundaries of the sample. But in generic one-particle models we showed that these edge states can delocalize if they are not protected...
by finite indirect gaps. Mostly clearly, this can be demonstrated by adding terms to the Hamiltonians proportional to the identity matrix. They change the dispersions, but leave the eigenstates unchanged and hence the topological properties. We stress that this holds true independent of the number of bands. This message also implies that the omission of terms proportional to the identity matrix is acceptable for the bulk, but not for confined geometries.

For in-gap states of which the energy is protected by additional symmetries it is sufficient to consider the bulk indirect gap \( \Delta_{\text{CV,g}} \). Generally, this gap is not sufficient to decide on localization and one has to consider the indirect gap \( \Delta_\nu \) which measures the energetic distance of the in-gap states to the closest bulk band. Generically, if \( \Delta_\nu \) is finite the states are localized and thus true edge states. If \( \Delta_\nu \) vanishes delocalization is to be expected.

While the described scenario is the generic one it can vary in special cases. Baum and co-workers [37] pointed out that further symmetries such as momentum and energy conservation can prevent delocalization in topological states of matter in spite of coupling edge states to a gapless bulk. Similarly, Verresen and co-workers [38] discovered edge states at the ends of critical chains. Independent of topological properties, it has been noted that localization can persist notwithstanding hybridization with continua in especially designed systems [39]. The localization may be weak in the sense that it is not exponential, but algebraic [40].

Yet, the results presented in this letter for standard one-particle topological models illustrate that delocalization of edge states is the generic phenomenon if indirect gaps vanish and hybridization with bulk continua occurs. To the best of our knowledge, this fact has not yet been appreciated in the literature even though it has important consequences for realizations of topological phases and their experimental detection. The take-home message is that the lack of localized edge modes does not preclude the existence of non-trivial topology characterized by discrete topological invariants. Then, however, direct techniques to detect topological invariants are required [41–43].

To pave the way towards experimental verifications by ultracold atoms in optical lattices we considered the topological checkerboard model explicitly. Further preliminary results show that the advocated scenario also occurs in the Kane-Mele model including Rashba couplings as a prototypical model with \( \mathbb{Z}_2 \)-topological invariant.

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