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Impurity Bound States and Greens Function Zeroes as Local Signatures of Topology

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We show that the local in-gap Greens function of a band insulator $\mathbf{G}_0(\epsilon, \mathbf{k}_{\parallel}, \mathbf{r}_{\perp} = 0)$, with \mathbf{r}_{\perp} the position perpendicular to a codimension-1 or -2 impurity, reveals the topological nature of the phase. For a topological insulator, the eigenvalues of this Greens function attain zeros in the gap, whereas for a trivial insulator the eigenvalues remain nonzero. This topological classification is related to the existence of in-gap bound states along codimension-1 and -2 impurities. Whereas codimension-1 impurities can be viewed as ‘soft edges’, the result for codimension-2 impurities is nontrivial and allows for a direct experimental measurement of the topological nature of 2d insulators.

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The topological characterization of condensed states of matter has emerged as a prominent research interest over the last few decades. The flourishing of the Quantum Hall effect (QHE) [1] in particular elucidated many connections between physical signatures and topological invariants [2], which supplement the order parameters of the usual symmetry-breaking Landau-Ginzburg paradigm. More recently, however, it became apparent that topological order can also arise by *virtue* of symmetry, and in particular the very common and robust Time Reversal (TR) symmetry is sufficient to establish the existence and stability of topological insulators[3–5]. This is quantified via a \mathbb{Z}_2 invariant, and results in gapless helical edge states or chiral Dirac fermions localized at the perimeter of the sample, in two and three dimensions, respectively. The topological insulator has proven extremely rich both experimentally and theoretically[9, 10]. The concept has been generalized to a ‘‘periodic table’’ describing various discrete symmetries and dimensions [6–8]. Lattice symmetries can similarly lead to further topological distinctions, result in ‘‘crystalline topological insulators’’[11], for which a general classification has been provided [12].

One may ask whether the topology of band insulators has some local signature? In fact, in this Letter, we will show that even the fully *local* in-gap Greens function contains information about the band topology, which is then directly accessible by experiments. The natural way this insight arises is through the study of impurities[13–15], similar to how the space group classification can be probed using lattice defects[16–23]. Consider a codimension-1 impurity line or surface in an insulator. In the limit where the impurity strength diverges, $V \rightarrow \infty$, such an impurity acts like a real edge which, following the bulk-boundary correspondence, should host zero gap metallic bound states in the topological phase. For finite V the codimension-1 impurity surface can thus be viewed as a ‘‘soft edge’’. The codimension-2 impurity lines or points do not host gapless states in the strong V limit, so a priori there is no reason to expect they probe

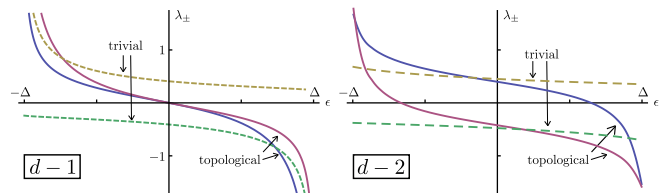


FIG. 1: The eigenvalues of the local Greens function $\mathbf{G}_0(\epsilon, k_{\parallel} = 0, r_{\perp} = 0)$ in the M/B model, relevant for codimension-1 (left) and codimension-2 (right) impurities. In the trivial system (dashed lines, $M/B = -1$) the eigenvalues λ_{\pm} are nonzero. In the topological system (solid line, $M/B = 1$) the eigenvalues are zero for some in-gap energy and hence in-gap bound states always exist.

topology. However, we will see that they in fact inherit the topological structure of the ‘‘soft edges’’. This nontrivial result implies that by probing bound states around a point impurity in a two-dimensional insulator, one can experimentally distinguish between the topological and trivial phase.

Mathematically, the theory for impurity bound states shows that the existence of bound states in the topological phase is directly related to zero eigenvalues of the local in-gap Greens function, see Fig. 1. Consequently, we propose that the presence or absence of zero eigenvalues in the local in-gap Greens function is a signature of the band topology.

The remainder of this Letter is organized as follows. We first introduce the model and the theory of impurity bound states. Then we show that the local in-gap Greens function, relevant for codimension-1 and -2 impurities, has zero eigenvalues if and only if the phase is topological. We then propose an experiment that directly probes the Greens function zeroes for a point impurity in a 2d insulator. Finally, we relate our results to the known \mathbb{Z}_2 classification and the bulk-boundary correspondence.

Theory of impurity bound states- We begin with a translationally invariant system, described by a minimal time-reversal invariant two-band model. The generic

Hamiltonian assumes the form

$$H_0 = \sum_{\mathbf{k}\alpha\beta} c_{\mathbf{k}\alpha}^\dagger d_\mu(\mathbf{k}) \gamma_{\alpha\beta}^\mu c_{\mathbf{k}\beta} \quad (1)$$

where γ^μ are the 4×4 Dirac gamma matrices satisfying a Clifford algebra. We choose $\gamma^0 = \sigma^0 \otimes \tau^3$ and $\gamma^i = \sigma^i \otimes \tau^1$. Here, the σ and τ Pauli matrices act in the spin and orbital space, respectively. Time reversal (TR) symmetry then implies that $d_0(\mathbf{k})$ must be even and $d_i(\mathbf{k})$ must be an odd function. In particular, we focus on the representative cases that $d_0(\mathbf{k}) = M - 2B \sum_i (1 - \cos k_i)$ and $d_i(\mathbf{k}) = \sin k_i$ [24–26]. This is the familiar class of models displaying topological nontrivial regimes for parameter range $0 < M/B < 4d$. This specific choice is not expected to restrict our results, as a topological insulator generically has by adiabatic continuity the form of a lattice regularized massive Dirac Hamiltonian. The following results also apply to other lattice symmetries, as long as there are two orbitals per unit cell, such as the original Kane-Mele model on the honeycomb lattice.[3] Moreover, extra terms that respect TR symmetry will not change the results described below.

The real frequency Greens function in the gap reads

$$\mathbf{G}_0(\omega, \mathbf{k}) = \frac{1}{\omega - d_\mu(\mathbf{k})\gamma^\mu} = \frac{\omega \mathbf{1}_4 + d_\mu(\mathbf{k})\gamma^\mu}{\omega^2 - |d(\mathbf{k})|^2}. \quad (2)$$

Subsequently, we introduce an impurity into the system, which in general can be described by the Hamiltonian

$$H_V = \sum_{\mathbf{r}\alpha\beta} c_{\mathbf{r}\alpha}^\dagger V_{\alpha\beta}(\mathbf{r}) c_{\mathbf{r}\beta}. \quad (3)$$

To find the corresponding spectrum in the presence of the impurity, one needs to solve the (differential) Schrödinger equation

$$(H_0 + H_V)\psi_\epsilon(\mathbf{r}) = \epsilon\psi_\epsilon(\mathbf{r}) \quad (4)$$

where ϵ is the energy of the state. This can be transformed into an integral equation, [27]

$$\psi_\epsilon(\mathbf{r}) = \sum_{\mathbf{r}'} \mathbf{G}_0(\epsilon, \mathbf{r} - \mathbf{r}') V(\mathbf{r}') \psi_\epsilon(\mathbf{r}'). \quad (5)$$

For an insulator, the real-frequency Greens function is well-behaved inside the gap and displays exponential decay as a function of \mathbf{r} . This implies that an in-gap solution of Eqn. (5) will yield a bound state around the impurity.

The existence of an in-gap bound state depends on H_0 and the shape of the impurity potential $V(\mathbf{r})$. However, the qualitative difference between topological and trivial band insulators is found in Greens function features, and is therefore largely independent of the choice of impurity potential. Let us therefore consider the simplest possible choice: a constant $V(\mathbf{r})$ along a n -dimensional plane in

a d -dimensional system (hence codimension $d - n$). The d -dimensional position vector \mathbf{r} can be split into the perpendicular coordinates \mathbf{r}_\perp and the parallel coordinates \mathbf{r}_\parallel , so that the impurity potential is given by

$$V(\mathbf{r}) = \mathbf{V}_0 \delta_{\mathbf{r}_\perp=0}^n \quad (6)$$

where we have used a Kronecker delta to signify our use of lattice models and introduced the 4×4 Hermitian matrix \mathbf{V}_0 . We note that even if the potential $V(r)$ just couples directly to the electron density, \mathbf{V}_0 is not necessarily diagonal when expressed in terms of the second quantized operators.

The shape of \mathbf{V}_0 can be restricted, though, using symmetry principles. For example, when we consider non-magnetic impurities, TR invariance applies to the impurity potential as well [34]. As a result, the matrix \mathbf{V}_0 has only six degrees of freedom,

$$\mathbf{V}_0 = V\mathbf{1} + V_0\sigma^0 \otimes \tau^3 + V_i\sigma^i \otimes \tau^2 + V_4\sigma^0 \otimes \tau^1. \quad (7)$$

Recall that in this notation, time reversal is $T = i\sigma^2 K$ where K is complex conjugation. Parity, on the other hand, is given by $\gamma^0 = \sigma^0 \otimes \tau^3$. If we require both parity and TR the form of \mathbf{V}_0 is even further constrained to

$$\mathbf{V}_0 = V\mathbf{1} + V_0\gamma^0. \quad (8)$$

Since the translational symmetry is not broken along directions parallel to the impurity, the impurity bound states have a well-defined parallel momenta \mathbf{k}_\parallel . Thus $\psi_\epsilon(\mathbf{r}) \propto e^{i\mathbf{k}_\parallel \cdot \mathbf{r}_\parallel}$ and the integral equation Eqn. (5) reduces to an eigenvalue equation for each \mathbf{k}_\parallel ,

$$\det [\mathbf{G}_0(\epsilon, \mathbf{k}_\parallel, \mathbf{r}_\perp = 0)\mathbf{V}_0 - \mathbf{1}] = 0. \quad (9)$$

We immediately notice that for the case $\mathbf{V}_0 = V\mathbf{1}$, the existence of bound states is directly related to the eigenvalues of the local ($\mathbf{r}_\perp = 0$) in-gap Greens function $\mathbf{G}_0(\epsilon, \mathbf{k}_\parallel, \mathbf{r}_\perp = 0)$.

Codimension-1 impurities- Let us now consider codimension-1 impurities, that is a surface in $d = 3$ and a line in $d = 2$, having only one perpendicular direction $r_\perp = 0$, see Eqn. (9). The corresponding Greens function in the gap, integrated over the perpendicular momentum, can be decomposed in terms of

$$g_\mu(\epsilon, \mathbf{k}_\parallel) = \int \frac{dk_\perp}{2\pi} \frac{d_\mu(\mathbf{k}_\parallel, k_\perp)}{\epsilon^2 - |d(\mathbf{k}_\parallel, k_\perp)|^2}, \quad (10)$$

$$g(\epsilon, \mathbf{k}_\parallel) = \int \frac{dk_\perp}{2\pi} \frac{\epsilon}{\epsilon^2 - |d(\mathbf{k}_\parallel, k_\perp)|^2}, \quad (11)$$

so that $\mathbf{G}_0(\epsilon, \mathbf{k}_\parallel, r_\perp = 0) = g(\epsilon, \mathbf{k}_\parallel)\mathbf{1} + g_\mu(\epsilon, \mathbf{k}_\parallel)\gamma^\mu$.

At any TR-symmetric point for the parallel momentum, for example $\mathbf{k}_\parallel = 0$ or π , the g_\parallel are vanishing. Additionally, g_\perp vanishes since the integrand is an odd function of \mathbf{k}_\perp . At TR-symmetric points we thus only

need to consider g_0 and g . We note that this still holds if we add e.g. Rashba spin orbit coupling terms, that are odd functions of the momentum, to the bare Hamiltonian. As a Rashba term removes the particle hole symmetry of the original Hamiltonian and similar terms can be introduced to eliminate the inversion symmetry, the following results can thus also be verified in the absence of any other symmetry but TR symmetry

We will now show that the eigenvalues of the local in-gap Greens function $\mathbf{G}_0(\epsilon, \mathbf{k}_\parallel^S, \mathbf{r}_\perp = 0)$,

$$\lambda_\pm(\epsilon) = g(\epsilon) \pm g_0(\epsilon), \quad (12)$$

have the shape displayed in the left panel of Fig. 1. The difference between a topological insulator and a trivial insulator, is whether the in-gap Greens function has a zero eigenvalue or not.

Note that the denominator in the integrand, $\epsilon^2 - |d|^2$, is always negative. In the trivial phase $d_0(\mathbf{k})$ does not change sign throughout the Brillouin zone. This implies that $g_0(\epsilon)$ does not change sign. Additionally, because $\epsilon < |d_0(\mathbf{k})|$, we have $g(\epsilon) + |g_0(\epsilon)| > 0$ and $g(\epsilon) - |g_0(\epsilon)| < 0$. Therefore, in the trivial phase, the Greens function $\mathbf{G}_0(\epsilon, \mathbf{k}_\parallel, \mathbf{r}_\perp = 0)$ *never* has an eigenvalue equal to zero for *all* momenta \mathbf{k}_\parallel and energies ϵ .

On the other hand, in the topological phase, when \mathbf{k}_\parallel is chosen as a TR-symmetric point \mathbf{k}_S associated with the projection describing the topological phase [12], the Greens function for $\epsilon = 0$ satisfies $\mathbf{G}_0(\epsilon = 0, \mathbf{k}_\parallel = \mathbf{k}_S, \mathbf{r}_\perp = 0) = 0$. To prove this, we evaluate

$$\begin{aligned} g_0(0, \mathbf{k}_S) &= - \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{d_0(k, \mathbf{k}_S)}{|d^2(k, \mathbf{k}_S)|} \\ &= - \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\hat{M}(\mathbf{k}_S) - 2B(1 - \cos k)}{\sin^2 k + (\hat{M}(\mathbf{k}_S) - 2B(1 - \cos k))^2}, \end{aligned}$$

where $\hat{M}(\mathbf{k}_S) = M - 2B \sum_{i=1}^{d-1} (1 - \cos(k_i))$ in terms of the coordinates \mathbf{k}_S . Substituting $x = e^{ik}$, the integral becomes a contour integral over the unit circle for which the solution depends on the poles inside the unit circle. We find that *only* in the topological regime $0 < \hat{M} < 4B$, two poles with *opposite* residue reside in the unit circle rendering zero eigenvalues of the Greens function $g_0(\epsilon = 0)$. Together with the universal robust divergence of both $g(\epsilon)$ and $g_0(\epsilon)$ at the band edges, which is of relevance in absence of particle hole symmetry, we arrive at the generic description as shown in Fig. 1.

Consequently, for any impurity strength a topological insulator will always have in-gap states along a codimension-1 impurity, whereas for a trivial insulator it depends on specific details of the impurity and the insulator. The codimension-1 impurity can thus be understood as a 'soft edge'.

Codimension-2 impurities- The above results on the structure of the eigenvalues of $\mathbf{G}_0(\epsilon, \mathbf{k}_\parallel, \mathbf{r}_\perp = 0)$ in the

codimension-1 case can be extended to codimension-2 impurities. In this case, there are two perpendicular directions $\mathbf{k}_\perp = (k_\perp^x, k_\perp^y)$,

$$\mathcal{G}_\mu(\epsilon, \mathbf{k}_\parallel) = \int \frac{dk_\perp^x dk_\perp^y}{(2\pi)^2} \frac{d_\mu(\mathbf{k}_\parallel, \mathbf{k}_\perp)}{\epsilon^2 - |d(\mathbf{k}_\parallel, \mathbf{k}_\perp)|^2}, \quad (13)$$

$$\mathcal{G}(\epsilon, \mathbf{k}_\parallel) = \int \frac{dk_\perp^x dk_\perp^y}{(2\pi)^2} \frac{\epsilon}{\epsilon^2 - |d(\mathbf{k}_\parallel, \mathbf{k}_\perp)|^2}, \quad (14)$$

for $\mu = 0, 1, 2, 3$. It is clear that for any of the perpendicular directions $\mathcal{G}_\perp = 0$, as the integrand is odd.

For the trivial phase, we can show that the eigenvalues of $\mathbf{G}_0(\epsilon, \mathbf{k}_\parallel, \mathbf{r}_\perp = 0)$ are nonzero throughout the gap, since the two-dimensional integral can be done by first integrating in one direction, which yields the results from the codimension-2 impurities, and then integrating along the second direction. Therefore, $\mathbf{G}_0(\epsilon, \mathbf{k}_\parallel, \mathbf{r}_\perp = 0)$ is never zero in the gap.

Of more interest is the question of existence of zero energy eigenvalues in the topological regime. Let us focus on the 2-dimensional case, so that there are no parallel directions: we are directly probing the *local, on-site Greens function*. We expect that the terms $\mathcal{G}(\epsilon)$ and $\mathcal{G}_0(\epsilon)$ will diverge close to the band-edge. In fact, these divergences are captured by expanding around the point where the gap is minimal, \mathbf{k}_G ,

$$|d(k^x, k^y)|^2 = \Delta^2 + a(k^x - k_G^x)^2 + b(k^y - k_G^y)^2 + \dots \quad (15)$$

The diverging part of the integral is then captured by the integral

$$\begin{aligned} &\int - \frac{dk^x dk^y}{(2\pi)^2} \frac{1}{2\Delta\delta\epsilon + a(k^x)^2 + b(k^y)^2} \\ &\sim - \int_0^{0^+} \frac{dq}{2\pi\sqrt{ab}} \frac{q}{2\Delta\delta\epsilon + q^2} \sim \frac{\log \delta\epsilon}{4\pi\sqrt{ab}}. \end{aligned} \quad (16)$$

Hence, $\mathcal{G}(\epsilon) \sim \frac{-|\Delta| \log \delta\epsilon}{4\pi\sqrt{ab}}$ and $\mathcal{G}_0(\epsilon) \sim \frac{d_0(\mathbf{k}_G) \log \delta\epsilon}{4\pi\sqrt{ab}}$ in proximity of the valence band. The dependence of the gap Δ on $d_0(\mathbf{k})$ proves that both eigenvalues in the topological phase diverge to positive infinity at the valence band edge, and to minus infinity at the conduction band edge. Consequently, as this functional dependence is robust against small perturbations, in the topological phase the Greens function eigenvalues must be zero somewhere in the gap. Details are provided in the Online Supplementary Information. This proves that in $d = 2$, the completely local in-gap Greens function $\mathbf{G}_0(\epsilon, r = 0)$ has zero eigenvalues if and only if the system is in the topological phase, see Fig. 1, right.

This result carries over to the case of line impurities in $d = 3$ topological insulators, if the remaining parallel momentum is chosen at one of the TR-symmetric points.

Experiment- The existence of these zero eigenvalues can be probed directly in experiments, using impurity

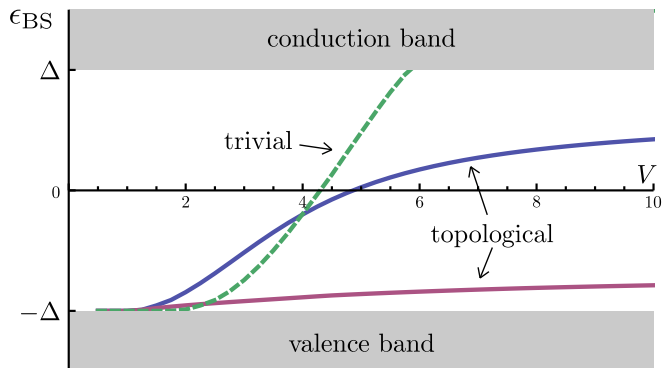


FIG. 2: Typical energy of impurity bound states in a two-dimensional insulator as a function of impurity strength V . Here, we discern between the topological regime (solid lines, $M/B = 1$) and the trivial regime (dashed line, $M/B = -1$). For strong V , bound state in the trivial phase has disappeared in the conduction band, whereas the bound states in the topological phase remain.

bound states as solutions to Eqn. (9). Imagine a two-dimensional insulator, where at one isolated point a tunable gate voltage is applied, serving as the impurity potential V . Then using tunneling spectroscopy, the possible bound states around this impurity can be found. Upon *increasing* the impurity potential V , the energies of the bound states shift: for a trivial insulator, one can make a bound state disappear into one of the bands by a sufficiently strong potential. However, our results show that for a topological insulator, for all strong V there will always be two bound states. Explicitly, the energy of the bound state as a function of V is shown in Fig. 2.

Classification and the bulk-boundary correspondence- The odd number of crossings per spin branch of $\mathbf{G}_0(\epsilon, \mathbf{k}_{\parallel}, \mathbf{r}_{\perp} = 0)$ with the zero eigenvalue axis is a topological property, similar to invariants based on the momentum space Greens function[28–31]. It reflects that in the nontrivial regime the system has an odd number of Kramers degenerate edge states on either side of the surface and hence may be regarded as a consequence of the bulk-boundary correspondence [9, 10]. In particular, the bulk TR Z_2 invariant is in this case simply the product $\prod_{\Gamma_i} \xi_i$ of the parity γ^0 eigenvalues ξ_i over the TR points in the Brillouin zone [32]. Moreover, the two relevant poles have the same residues but multiplied by sign of the mass, i.e. the parity γ^0 eigenvalues. Hence, only if the choice \mathbf{k}_S in the projected plane is associated with two masses of opposite sign, meaning that this cut features a band inversion, the poles cancel in the above integral rendering a zero eigenvalue. This is in accordance with the space group classification [12].

For example, for $d = 2$ the model Eqn. (1) exhibits a Γ ($T - p4mm$) phase for $0 < M/B < 4$ and a M ($T - p4$) phase for $4 < M/B < 8$. From the above considerations we find that \hat{M} has to satisfy $0 < \hat{M} < 4$

for $\mathbf{G}_0(\epsilon, \mathbf{k}_{\parallel}, \mathbf{r}_{\perp} = 0)$ to develop zero eigenvalues. Taking subsequently projections onto k_x and k_y and using that $\hat{M}(\mathbf{k}_s) = M - 2B \sum_i (1 - \cos(k_i))$, we thus conclude that in the Γ phase these k_S choices correspond to an inversion at $\mathbf{k} = (0, 0)$, whereas in the M phase the inversion is at $\mathbf{k} = (\pi, \pi)$. We stress that this analysis still holds if we add Rashba terms, that are odd functions of momentum. Similarly, we may add a next nearest neighbor term $\tilde{d}_0(\mathbf{k}) = -\tilde{B}[1 - \cos(k_x) \cos(k_y)]$, $d_x(\mathbf{k}) = \cos(k_x) \sin(k_y)$, $d_y(\mathbf{k}) = -\sin(k_x) \cos(k_y)$ to the Hamiltonian [12], allowing for an additional $X - Y$ ($p4$) topological crystalline phase [11]. This phase is associated with the inversion momenta $\mathbf{k} = (\pi, 0)$ and $\mathbf{k} = (0, \pi)$. An identical calculation then shows that indeed projections along k_x and k_y yield zero eigenvalues of $\mathbf{G}_0(\epsilon, \mathbf{k}_{\parallel}, \mathbf{r}_{\perp} = 0)$ for *both* $k_S = 0$ and π . These ideas carry over directly to three dimensions. Consider for example a Γ ($T - pm\bar{3}m$) phase with an inversion at $\mathbf{k} = (0, 0, 0)$ for $0 < M/B < 4$, in the projected plane one should now choose $\mathbf{k}_S = (0, 0)$ or on a line $k_S = 0$.

Our method allows to distinguish between a $d = 3$ weak and strong topological insulators (TIs).[5] Since a weak TI can be viewed as a stacking of $d = 2$ TI, it follows that the codimension-1 local Greens function with r_{\parallel} parallel to the $2d$ layers will not have zero eigenvalues.

Conclusions and Outlook- We have shown that topological band insulators can be characterized by the existence of zero eigenvalues in the local in-gap Greens function $\mathbf{G}_0(\epsilon, \mathbf{k}_{\parallel}, \mathbf{r}_{\perp} = 0)$, where \mathbf{r}_{\perp} is the position vector perpendicular to a codimension-1 or -2 impurity. Whereas the codimension-1 impurities can be viewed as soft edges, the nontrivial result for codimension-2 impurities suggests one can experimentally probe the difference between a topological insulator and a trivial insulator using a tunable localized impurity.

We made some simplifying assumptions in the proof presented above, but the results are robust. For example, adding more bands to the system, further away from the Fermi level, might introduce extra impurity bound states whose energies depend strongly on the impurity strength, but one can show that these do not generally remove the states arising from the low energy bands. Furthermore, we showed (e.g. Fig. 2) the persistence of bound states for strong potential V but neglected V_0 ; however, while the shape of bound state energy versus potential strength changes if V_0 is included, the conclusion that they persist is independent of the ratio V_0/V . Additionally, as long as weak electron-electron interactions do not close the gap or spontaneously break a symmetry, the principle of adiabatic continuation suggests our proposed classification applies equally well to gapped weakly interacting systems with a quasiparticle description[33] or topological superconductors[10].

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