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

Robert-Jan Slager,[1] Louk Rademaker,[2] Jan Zaanen,[1] and Leon Balents[2]

[1]*Institute-Lorentz for Theoretical Physics, Leiden University, PO Box 9506, Leiden, The Netherlands*
[2]*Kavli Institute for Theoretical Physics, University of California Santa Barbara, CA 93106, USA*

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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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Silas Hoffman

Journal club

28.4.15

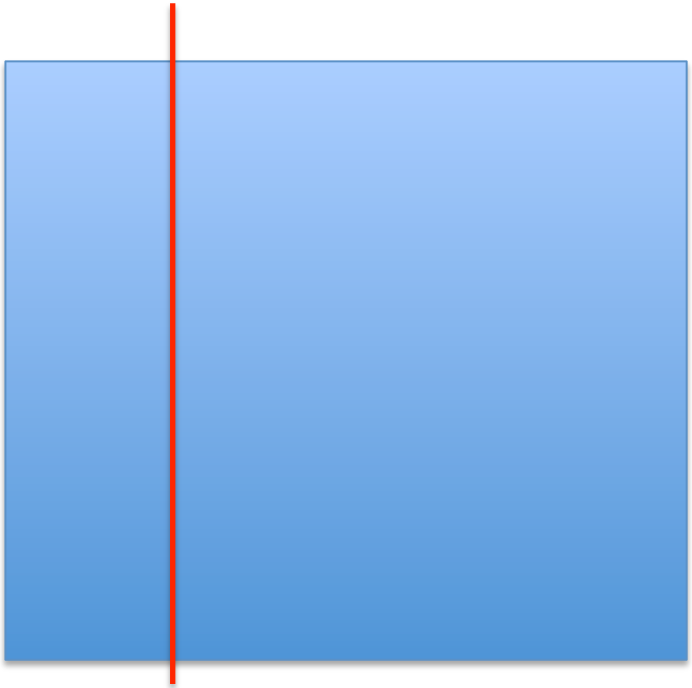
Codimension?

Codimension n-impurity: impurity with **n** fewer dimensions than the **d-**dimensional imbedding material

Codimension?

Codimension **1**-impurity: impurity with **1** fewer dimensions than the **d-**dimensional imbedding material

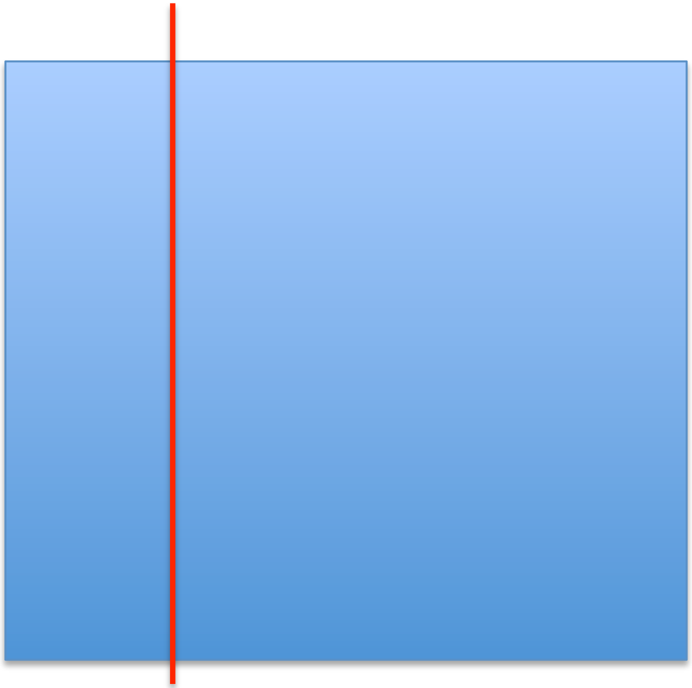
2-dimensional material: (2-1=1)
a line



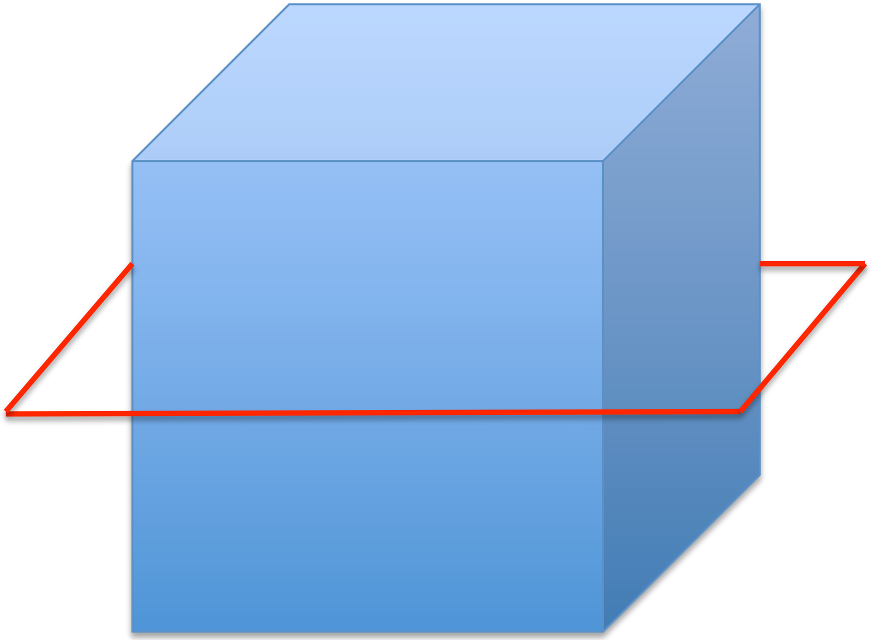
Codimension?

Codimension **1**-impurity: impurity with **1** fewer dimensions than the **d-**dimensional imbedding material

2-dimensional material: (2-1=1) a line



3-dimensional material: (3-1=2) a plane



Codimension?

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a line

3-dimensional material: (3-1=2)
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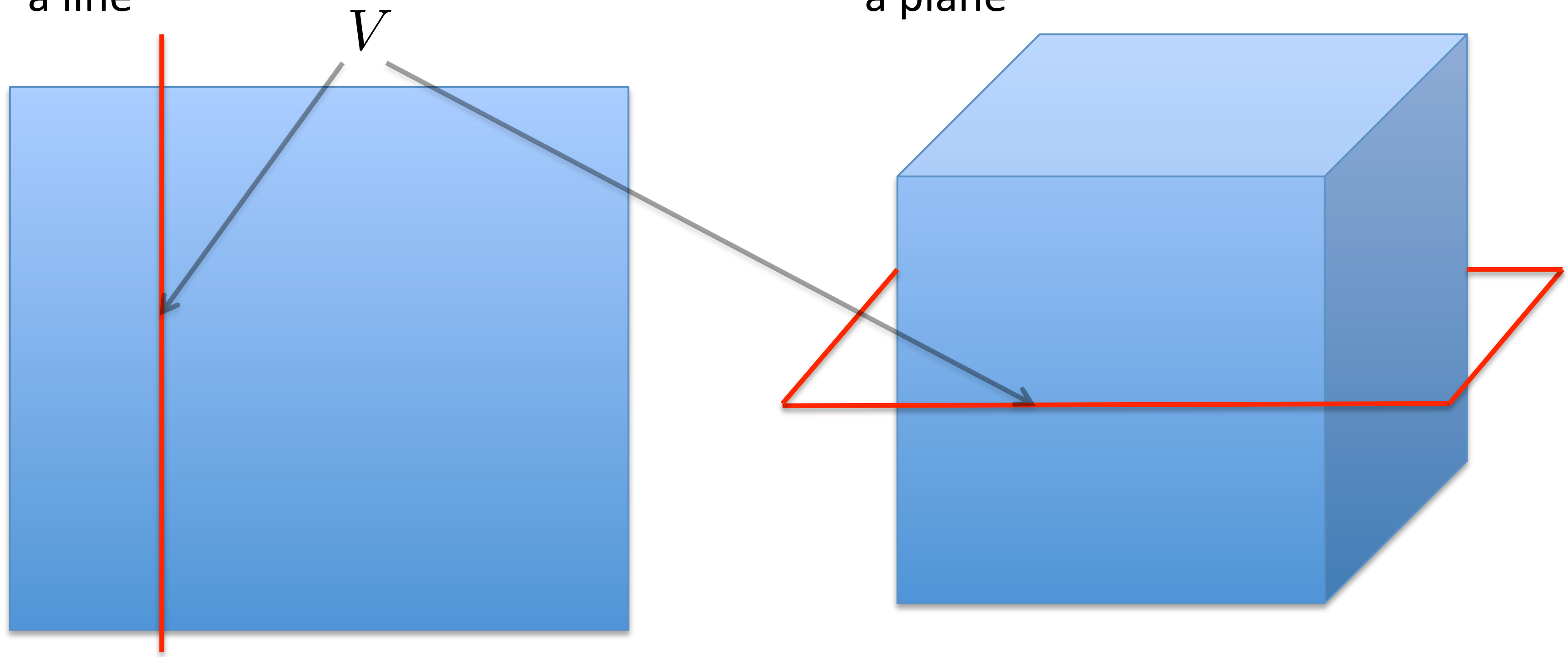

Codimension?

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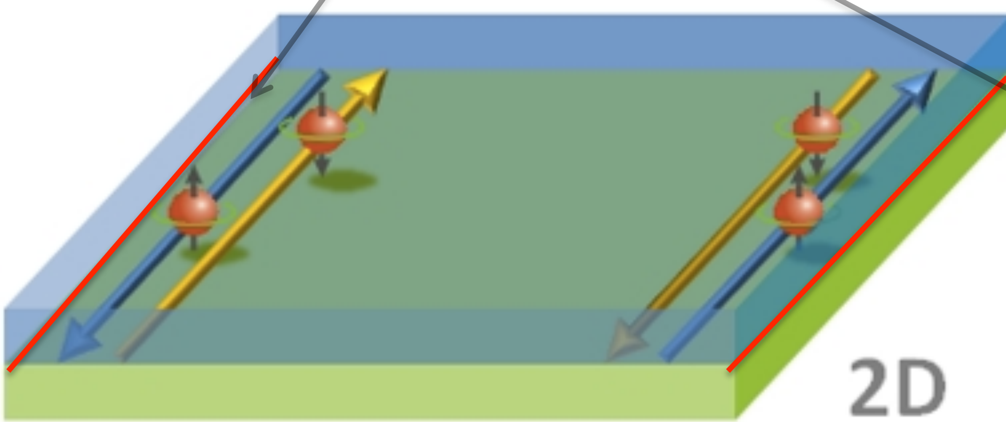
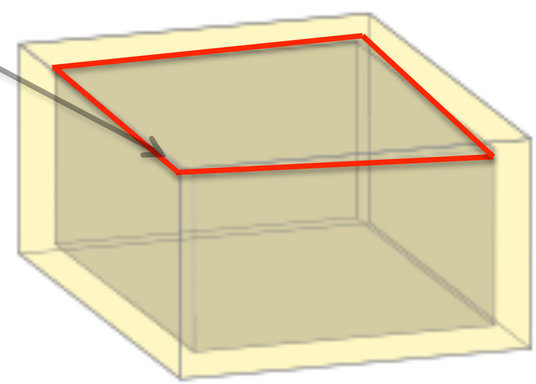
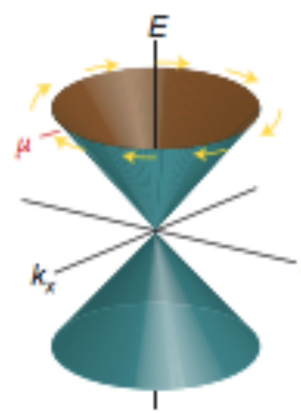
When there is a ('hard') edge, we expect a localized in-gap state

No surprise if we find a localized in-gap state at a 'soft edge'

$V \to \infty$







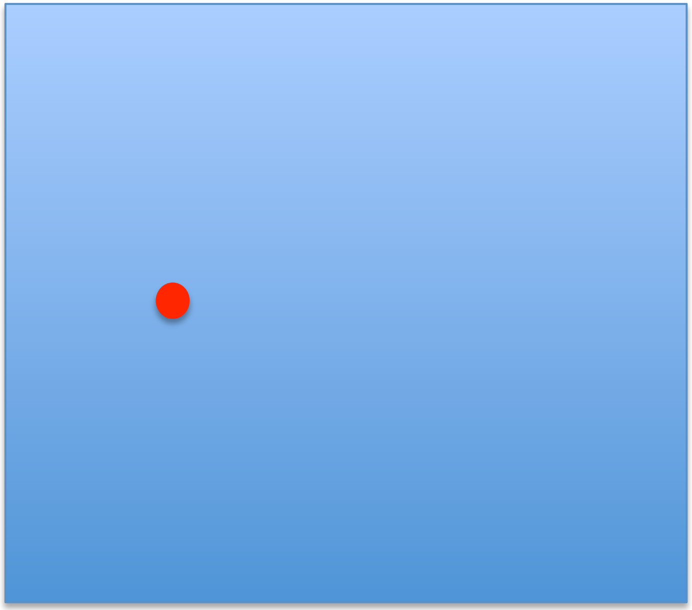
Th. Schapers, Forschungszentrum Julich

Cong and Cui, 2011

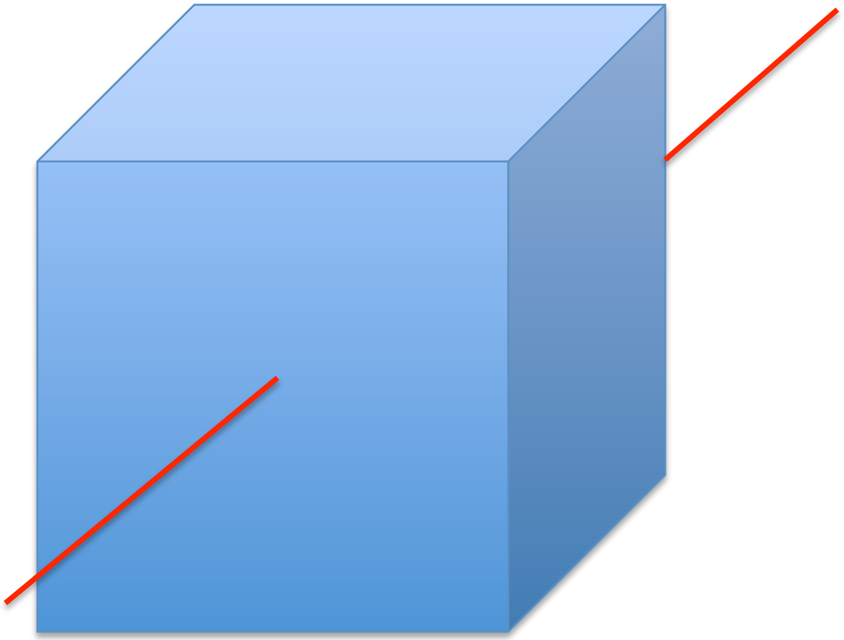
Codimension?

Codimension **2**-impurity: impurity with **2** fewer dimensions than the **d-**dimensional imbedding material

2-dimensional material: (2-2=0)
a point



3-dimensional material: (3-1=2)
a line



Codimension?

Claim: codim. 1 and 2-impurities in TI's always host bound states

Codimension **2**-impurity: impurity with **2** fewer dimensions than the **d-**dimensional imbedding material

2-dimensional material: (2-2=0)
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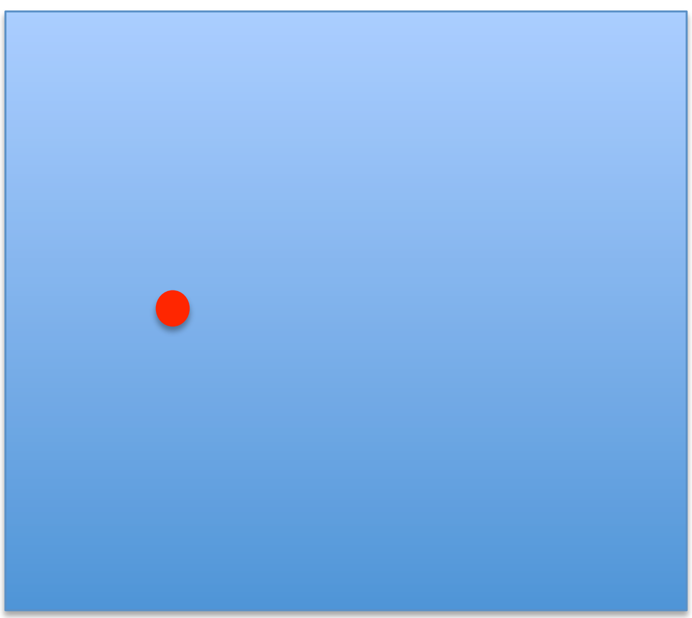
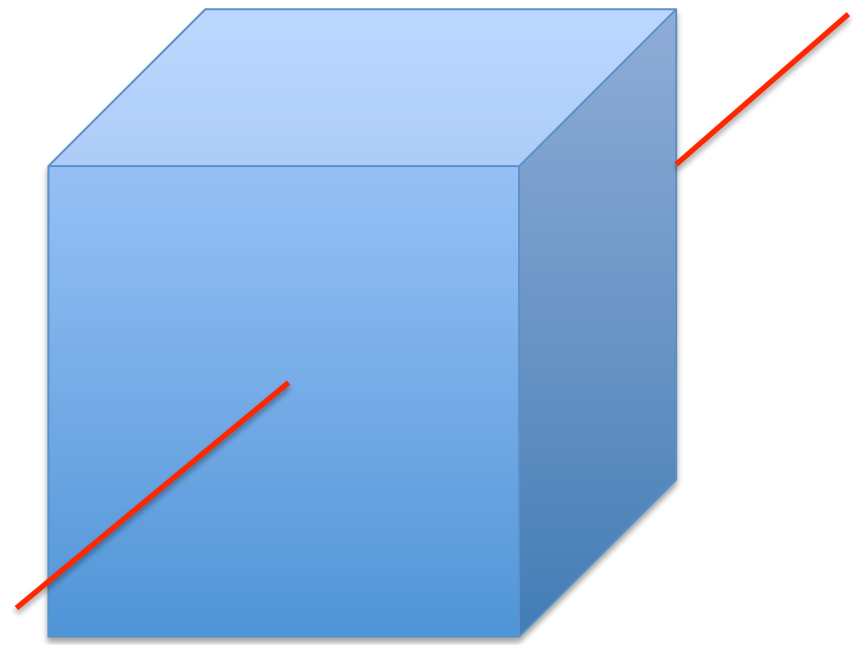


3-dimensional material: (3-1=2)
a line



Model

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

$$H_0 = \sum_{\mathbf{k}\alpha\beta} c^\dagger_{\mathbf{k}\alpha} d_\mu(\mathbf{k}) \gamma^\mu_{\alpha\beta} c_{\mathbf{k}\beta} \quad (1)$$

$\gamma^0 = \sigma_0 \otimes \tau_3$ and $\gamma^i = \sigma_i \otimes \tau_1$

$$d_0(\mathbf{k}) = M - 2B \sum_i (1 - \cos k_i)$$

$$d_i(\mathbf{k}) = \sin k_i$$

BHZ model: topologically nontrivial when $0 < M/B < 4d$.

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

$$H_V = \sum_{\mathbf{r}\alpha\beta} c^\dagger_{\mathbf{r}\alpha} V_{\alpha\beta}(\mathbf{r}) c_{\mathbf{r}\beta} \quad (H_0 + H_V)\psi_\epsilon(\mathbf{r}) = \epsilon \psi_\epsilon(\mathbf{r})$$

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

Model

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 $\mathbf{r}_{||}$

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

$$V(\mathbf{r}) = \mathbf{V}_0 \delta^n_{\mathbf{r}_\perp = 0}$$

$$\mathbf{V}_0 = V\mathbf{1} + V_0\gamma^0$$

According to parity and time reversal (TR) invariance

$$\det\left[\mathbf{G}_0(\epsilon, \mathbf{k}_{||}, \mathbf{r}_\perp = 0)\mathbf{V}_0 - \mathbf{1}\right] = 0$$

At least one in-gap state, for any potential, if there is a zero EV

Existence of in-gap states related to eigenvalue

Codimension-1

One can show:

- Normal insulator has **no** zero eigenenergies
- TI **must** have a zero eigenenergies and therefore supports at least a single bound state
- TI eigenvalues go to +/- infinity at the valence/cond. band

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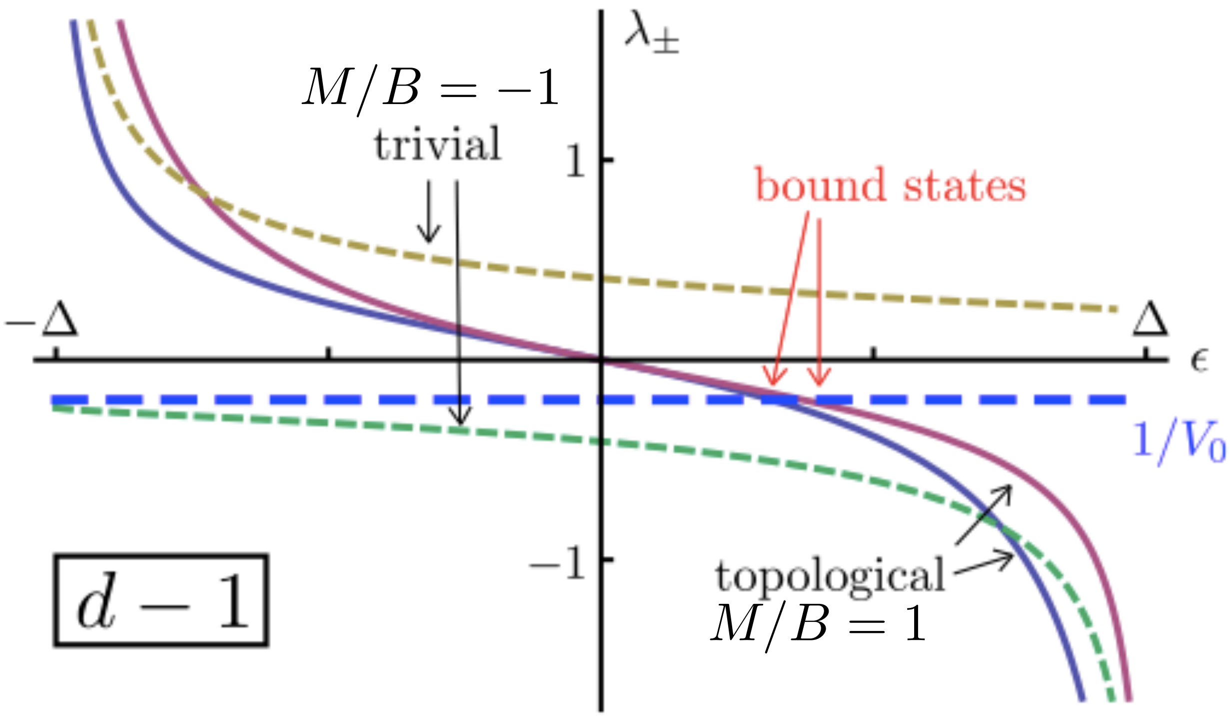
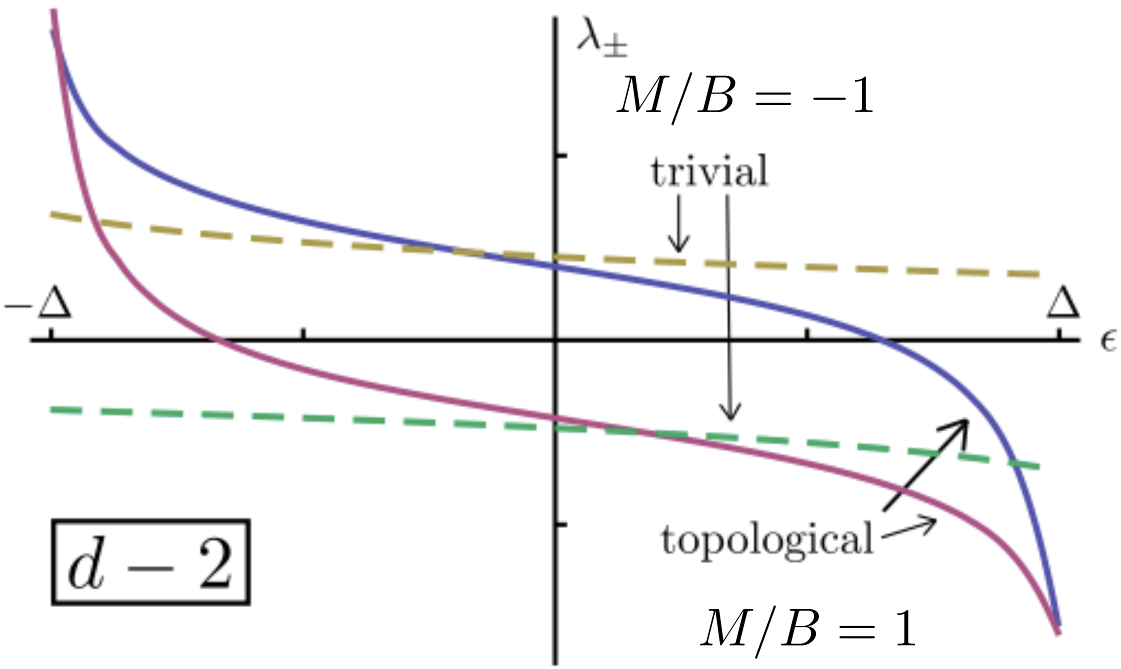


Codimension-2

One can show:

- Normal insulator has **no** zero eigenenergies
- TI **must** have a zero eigenenergies and therefore supports at least a single bound state
- TI eigenvalues go to +/- infinity at the valence/cond. band



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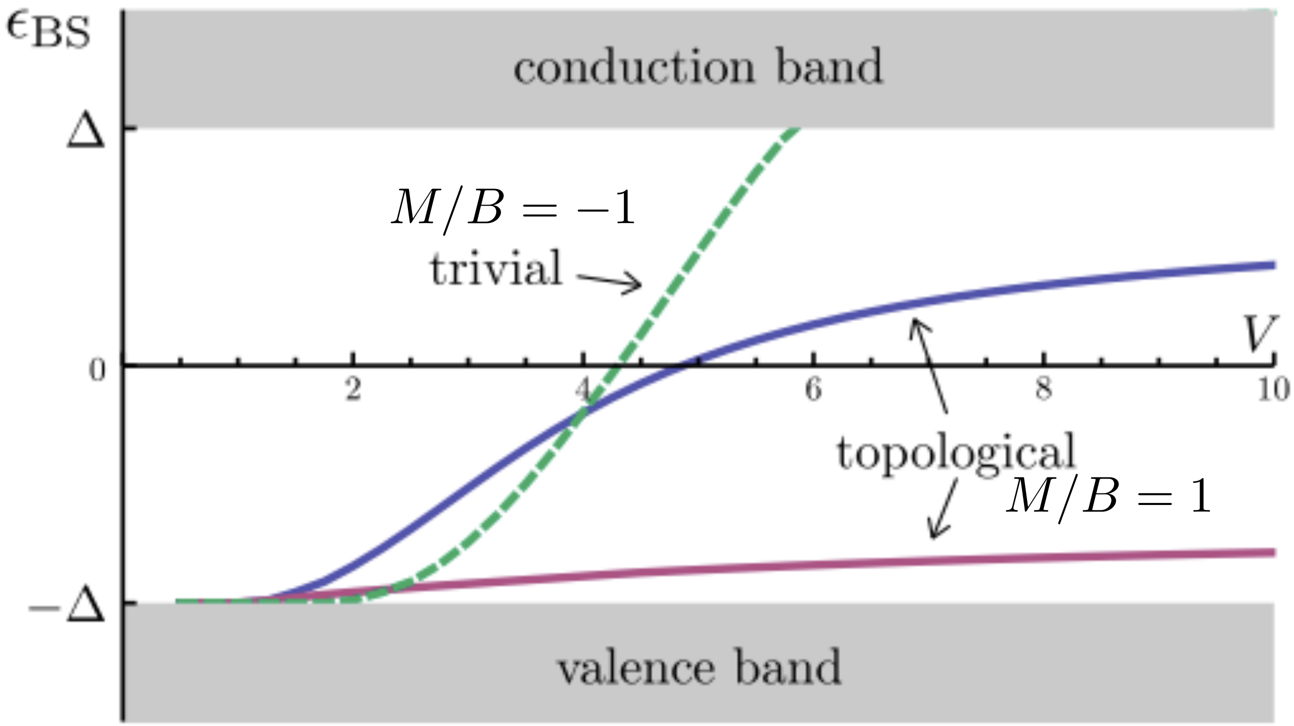
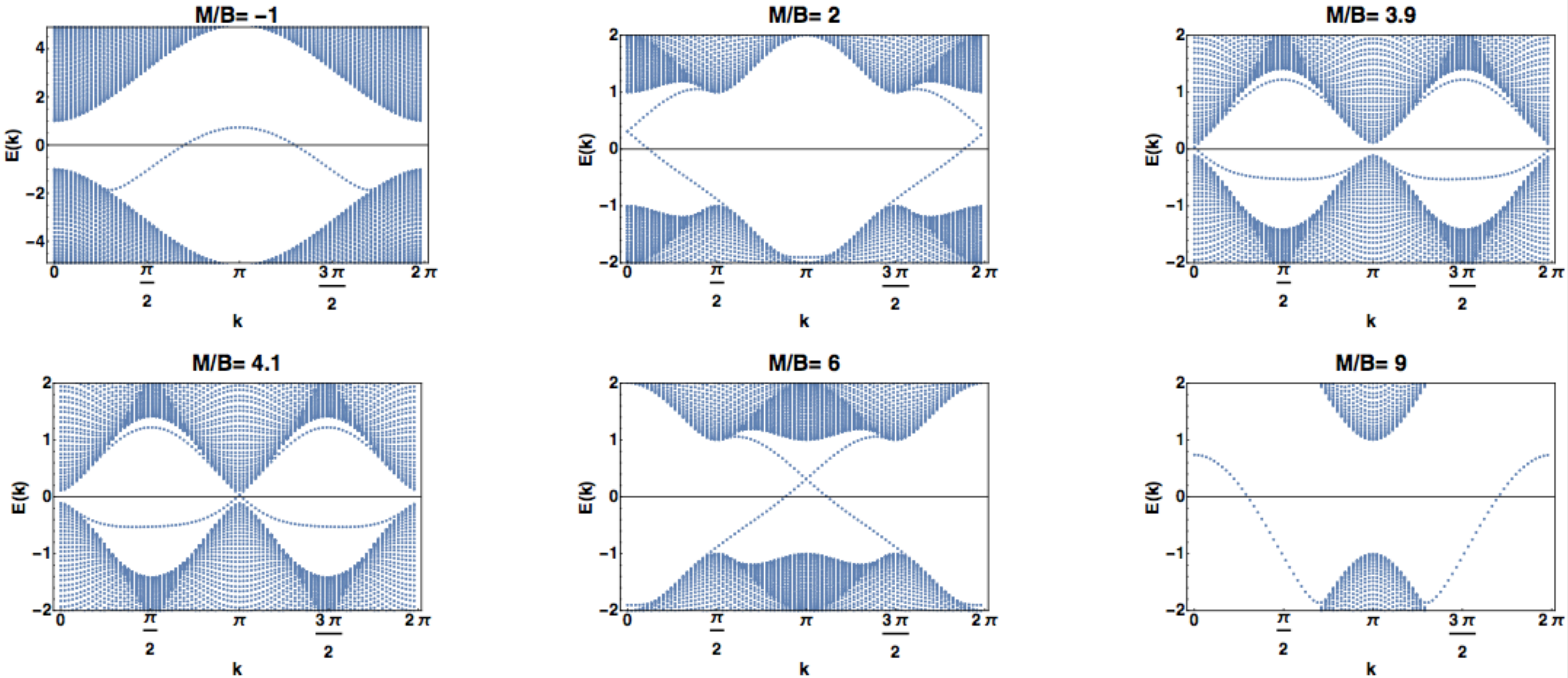


Tight Binding (60 x 90 array) Line Impurity

$0 < M/B < 4d$ =8



$\mathbf{V}_0/B = -6 \times \mathbf{1}$

Tight Binding (60 x 90 array) Line Impurity

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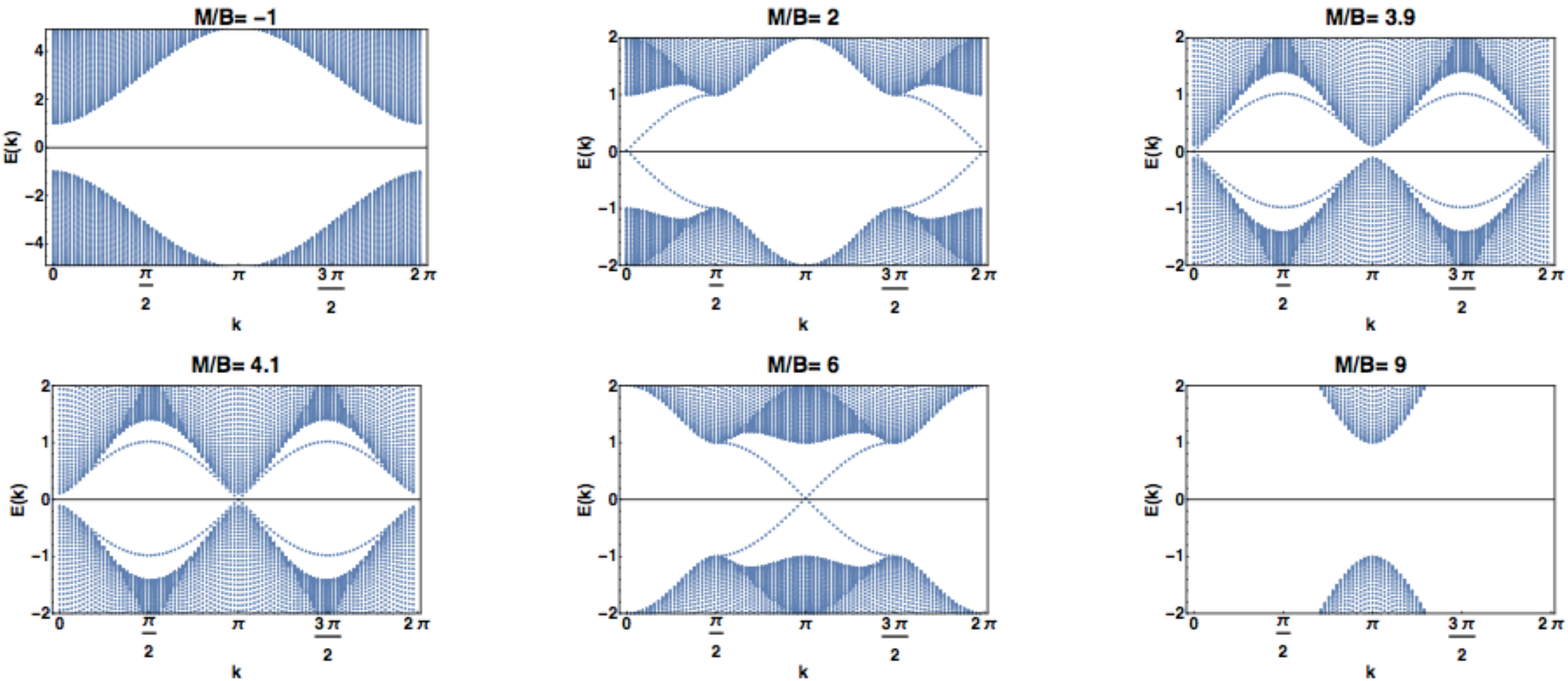

$$\mathbf{V}_0/B = -100\times\mathbf{1}$$

Conclusions

- Impurities induce local signature of topological insulator
- Experimental signature: probe by applying a gate voltage
  - Normal insulator has an in-gap state for specific voltages
  - TI's will **always** have in-gap state