Creating and Imaging Topological Materials

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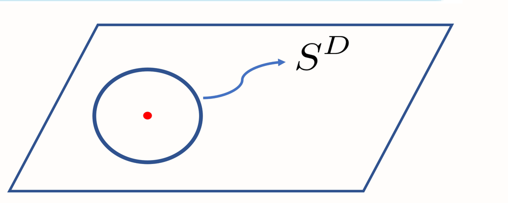
I. Abstract

The quantum Hall resistivity's robustness sparked ongoing interest in measurable topological quantities, but systematic design of topological materials remains elusive. Often, it's unclear how to access Chern or winding numbers in a given material. We demonstrate that edge states, as topological fingerprints, reflect interference patterns that translate phase information into measurable amplitude. This enables a novel method for directly reading topological numbers from interference patterns.

IV. Tenfold Classification

Class	s	T	P	C	d=0	1	2	3
A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	1	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	0	+	0	0	$\mathbb{Z}$	0	0	0
BDI	1	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	2	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	3	-	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	4	-	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	5	-	-	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	6	0	-	0	0	0	$2\mathbb{Z}$	0
CI	7	+	-	1	0	0	0	$2\mathbb{Z}$

In presence of defects, $d \to \delta = d - D$



The effective Dirac Hamiltonian for spatial coordinate r and momentum k,

$$\mathcal{H}(k,r) = h(k,r) \cdot \gamma$$

$$\nu_{d+D} = \frac{1}{S^{d+D}} \int_{S^{d+D}} d^d k \, d^D r \, J(h,d,D), \quad J = \begin{vmatrix} h_1 & \cdots & h_{d+D+1} \\ \partial_1 h_1 & \cdots & \partial_1 h_{d+D+1} \\ \vdots & \ddots & \vdots \\ \partial_{d+D} h_1 & \cdots & \partial_{d+D} h_{d+D+1} \end{vmatrix} \tag{1}$$

where γ matrices are $2^m \times 2^m$. The topological number ν_{d+D} is non-zero if,

$$2m = d + D + 1 \tag{2}$$

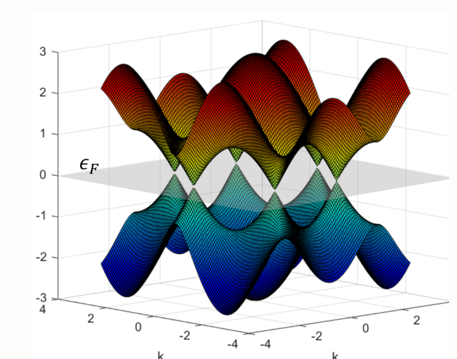
V. 2D Dirac Materials

Honeycomb lattice- Graphene

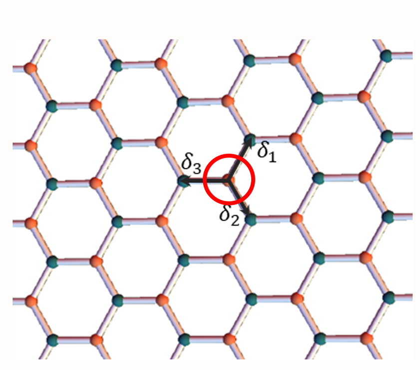
Graphene is a bipartite lattice. The tight binding Hamiltonian is,

$$H_0 = -t \sum_{\substack{i=0,1,2 \\ R \in A}} a_R^\dagger b_{R+\delta_i} + h.c.$$

Near the Fermi energy $\epsilon_F = 0$, the energy spectrum displays a linear form with two distinct Dirac cones, K and K'. Graphene is classified as BDI and lacks topological features.



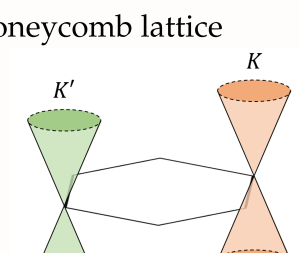
Band structure of Graphene



Honeycomb lattice

In general such materials are called Dirac materials. The Bloch Hamiltonian for each cone,

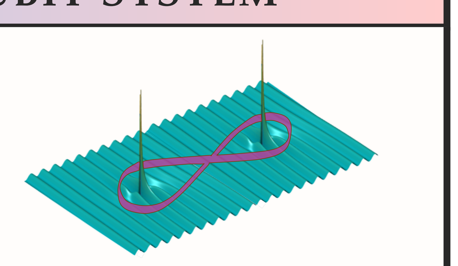
$$\mathcal{H}(\boldsymbol{k} = \boldsymbol{K} + \boldsymbol{q}) = v_F \boldsymbol{\sigma} \cdot \boldsymbol{q}.$$



Perturbations may couple the two Dirac cones.

VI. Topology of Two Qubit System

We examine a general two-qubit system with time-reversal symmetry only, classified under class AI. Being zero-dimensional ($d = 0$), it thus presents $\mathbb{Z}$ topology.

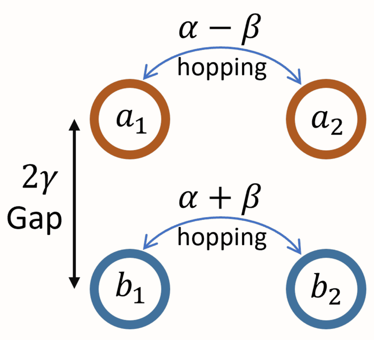


The overall non-local Hamiltonian, considering only local transformations, is

$$H_{AI} = \alpha \sigma_x \otimes \sigma_x + \beta \sigma_y \otimes \sigma_y + \gamma \sigma_z \otimes \sigma_z$$

where $\alpha, \beta, \gamma \in \mathbb{R}$.

We propose an equivalent description of H_{AI} by means of a tight-binding model of a particle on a 4-site lattice. The effective Hamiltonian,



$$\mathcal{H}(k) = \begin{pmatrix} \gamma + (\alpha - \beta)\cos k & 0 \\ 0 & -\gamma + (\alpha + \beta)\cos k \end{pmatrix}$$

Now we calculate the topological numbers (winding number) for this zero-dimensional system using (1),

$$\boldsymbol{\nu \in \{\pm 2, \pm 1, 0\} \simeq \mathbb{Z}_5}$$

II. Index Theorem

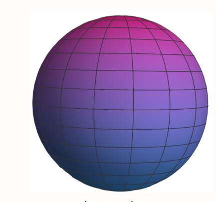
The index theorem links topology and analysis by indicating that the shape of space governs the count of particular solutions to differential equations. We define the analytical index of an operator D,

$$\text{Index } D = \dim(\ker D) - \dim(\ker D^\dagger)$$

where, $\ker D$ is the kernel i.e. the space of solutions of $D\psi = 0$.

Compact Manifold Without Boundary

Let D be an elliptic operator on a boundary-free compact manifold $\mathcal{M}$. The index theorem connects the analytical index with the topological index (curvature integral κ).

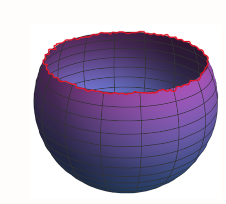


$\chi(\mathcal{M}) = 2$

$$\text{Index } D = n_+ - n_- = \int_{\mathcal{M}} \kappa = \chi(\mathcal{M})$$

Compact Manifold With Boundary

If the manifold $\mathcal{M}$ has a boundary, the integral over the curvature κ is no longer an integer and there's no index for D. To restore the index theorem, we need to add a boundary contribution to the curvature term and use non-local boundary conditions.



$\chi(\mathcal{M}) \neq 2$

$$\text{Index } D = n_+ - n_- = \int_{\mathcal{M}} \kappa - \frac{1}{2}\left(\eta(0) + h\right)$$

where h is the number of zero modes of the restriction of D to the boundary ∂M denoted by B. The eta invariant $\eta(0)$ is found by regularizing the sum,

$$\eta(s) = \sum_{\substack{n \\ \omega_n \neq 0}} \frac{\text{sign}(\omega_n)}{|\omega_n|}^s$$

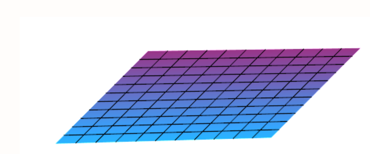
where $\{\omega_n\}$ are set of eigenvalues of B. The non-local boundary conditions,

$$f(u,y) = \sum_n f_n(u) e_n(y) \quad g(u,y) = \sum_n g_n(u) e_n(y)$$

$$f_n(0) = 0 \quad \text{for } \omega_n \geq 0, \qquad g_n(0) = 0 \quad \text{for } \omega_n < 0$$

Non- Compact Manifold

Callias formulated an index theorem for infinite spaces using phase shifts. With no boundary present, only L_2 (scattering) boundary conditions are necessary.



$$\text{Index } D = n_+ - n_- = \int_{\mathcal{M}} \kappa + \frac{1}{\pi}\left(\delta_k^+ - \delta_k^-\right)$$

where $\delta_k^\pm$ denotes the left (right) handed phase shifts of the operators $D^\dagger D$ ($DD^\dagger$).

VII. Imaging Topology

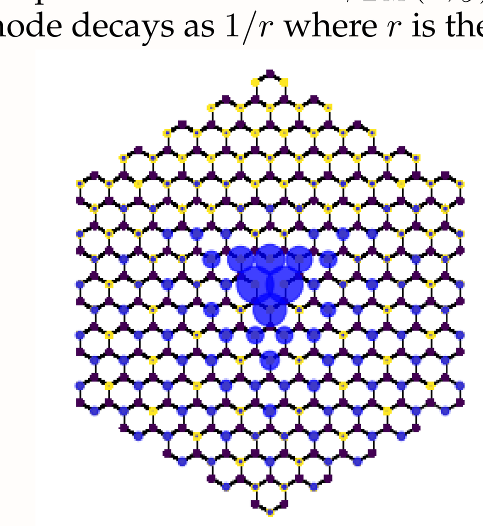
Graphene with vacancy

A vacancy is created by removing the atom and the bonds of a site. We do not break any symmetries so we remain in the same class BDI but move in effective dimensions from 2 to 1 because of the vacancy and thus have $\mathbb{Z}$ topology. The effective Hamiltonian,

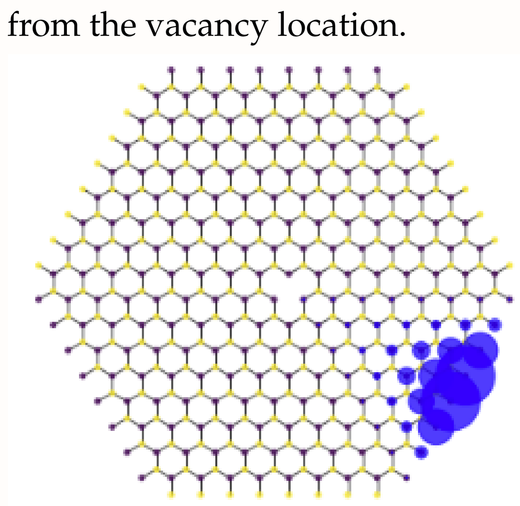
$$\mathcal{H}(k,r) = \begin{pmatrix} 0 & 0 & k_x - ik_y & he^{i\phi} \\ 0 & 0 & he^{-i\phi} & k_x + ik_y \\ k_x + ik_y & he^{i\phi} & 0 & 0 \\ he^{-i\phi} & k_x - ik_y & 0 & 0 \end{pmatrix}$$

Numerical results

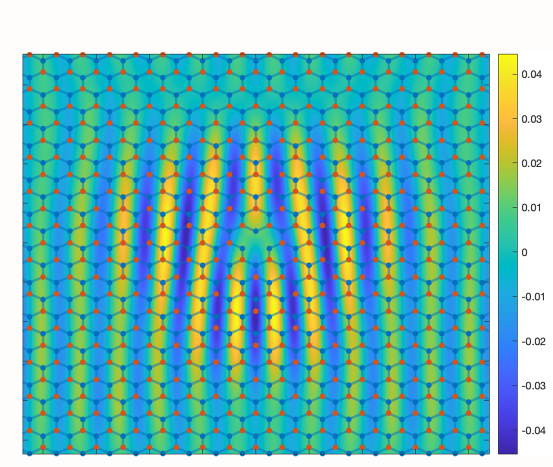
We plot the zero mode $\psi_{ZM}(x,y)$ of the Hamiltonian on the lattice. The zero mode decays as $1/r$ where r is the radius from the vacancy location.



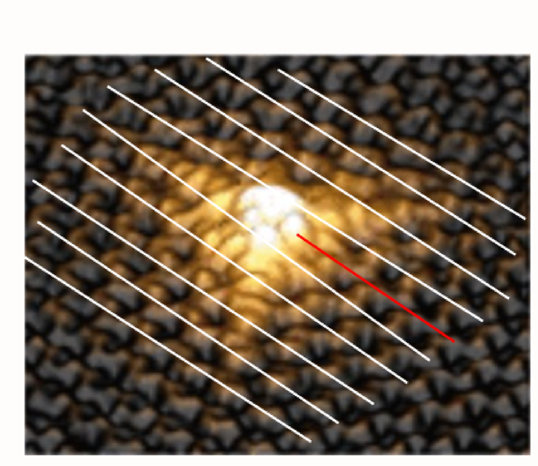
Armchair: $|\psi_{ZM}(x,y)|^2$



Bearded: $|\psi_{ZM}(x,y)|^2$



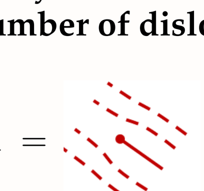
Dislocation in $\psi_{ZM}(x,y)$



Measurement results from Ugeda, et al

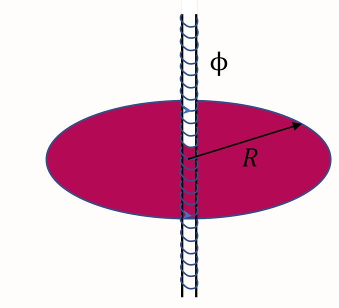
The Hamiltonian has a single zero mode (analytical index). The **winding number** (1) (topological index) is equal to the **number of dislocations**,

$$\text{Index } D = \nu_3 = 1 =$$



III. Aharonov-Bohm Flux on a Disc

We study a finite disc with radius R, with a central thin Aharonov-Bohm flux line of magnetic flux ϕ. We aim to investigate the index theorem's applicability with boundaries and its relation to the non-compact index theorem as $R \to \infty$. The Hamiltonian,



$$H = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial}{\partial \theta} + i\phi\right)^2\right]$$

Compact case with boundary

Rewrite the Hamiltonian,

$$H = DD^\dagger, \quad D = e^{i\theta}\left(\partial_r + \frac{1}{r}\left(\frac{1}{i}\partial_\theta + \phi\right)\right), \quad B = \frac{1}{R}\left(\frac{1}{i}\partial_\theta + \phi\right)$$

$$f = \sum_{n=-\infty}^{\infty} c_n r^{n-\phi} e^{i\theta n} \quad g = \sum_{n=-\infty}^{\infty} c_n r^{\phi - n} e^{i\theta n}$$

Applying non-local boundary conditions,

$$\text{Index } D = n_+ - n_- = [\phi]$$

Assuming the flux pinned within a hole of radius δ and considering the limit $\delta \to 0$, the eta invariant,

$$\eta_R(0) = 2\{\phi(R)\} - 1, \quad \eta_\delta(0) = 1 - 2\{\phi(\delta)\}$$

The index theorem with boundary is verified,

$$[\phi] = \phi - \{\phi\}$$

Non-Compact case

We find phase shifts for $DD^\dagger$ and $D^\dagger D$. The solutions are given by Bessel functions $J_{|n+\phi|}(kr)$, and looking at their asymptotic behaviour,

$$J_{|n+\alpha|}(kr) \sim (2/\pi kr)^{1/2} \cos\left(kr - \frac{1}{2}|n+\phi|\pi - \frac{\pi}{4}\right)$$

Comparing with the $\phi = 0$ case, we obtain the phase shifts,

$$\delta_k^+ = \frac{\pi}{2}(|k| - |k+\phi|)$$

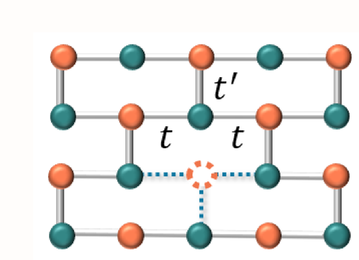
Similarly, we find δ_k^- and sum the telescoping series,

$$\frac{1}{\pi}\sum_k \left(\delta_k^+ - \delta_k^-\right) = -\{\phi\}$$

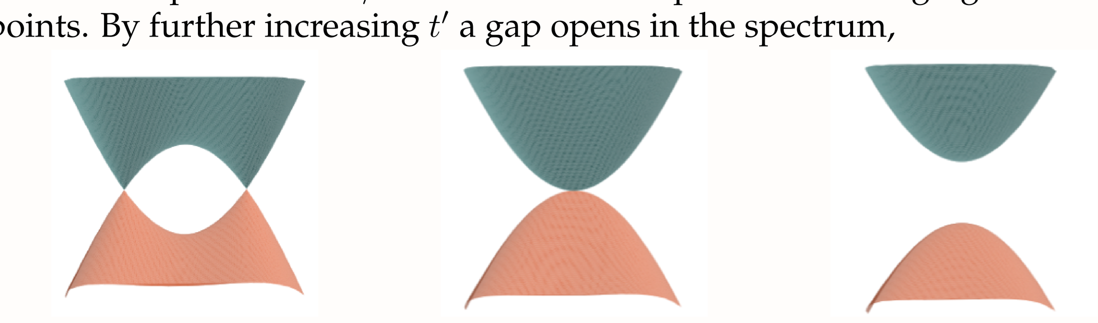
VIII. Topological Phase Transition

Brickwall with vacancy

We examine a brickwall lattice with a vacancy, focusing on anisotropic hopping. A topological phase transition occurs as the t'/t hopping ratio varies smoothly.



The critical point is at $t'/t = 2$ and it corresponds to a merging of the Dirac points. By further increasing t' a gap opens in the spectrum,



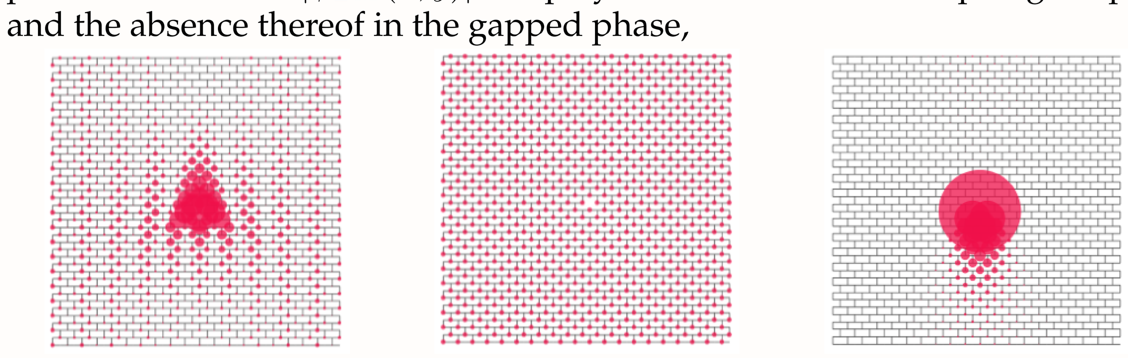
$t'/t = 1.5$ $\quad$ $t'/t = 2$ $\quad$ $t'/t = 2.3$

The effective Dirac Hamiltonian before and after the merging are,

$$\mathcal{H}_{\text{before}}(k,r) = \sqrt{1 - \frac{t'}{2t}} k_x \sigma_x \otimes \tau_z + \frac{t'}{2t} k_y \sigma_y \otimes \mathbb{I} + \text{defect terms}$$

$$\mathcal{H}_{\text{after}}(k,r) = \phi(r)\left(\left(1 - \frac{t'}{2t} + \frac{1}{2}k_x^2\right)\sigma_x + \frac{t'}{2t}k_y\sigma_y\right)$$

Before merging, the topological condition (2) holds, but it does not hold afterward, indicating a **phase transition from topological to non-topological**. The plotted zero mode $|\psi_{ZM}(x,y)|^2$ display a dislocation in the topological phase and the absence thereof in the gapped phase,



$t'/t = 1.5$ $\quad$ $t'/t = 2$ $\quad$ $t'/t = 2.3$

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