Defects in Graphene: A Topological Description

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I. Abstract

Specific types of spatial defects or potentials can turn monolayer graphene into a topological material. These topological defects are classified by a spatial dimension D and they are systematically obtained from the Hamiltonian by means of its symbol $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$, an operator which generalises the Bloch Hamiltonian and contains all topological information. This approach, when applied to Dirac operators, allows to recover the tenfold classification of insulators and superconductors. The existence of a stable $\mathbb{Z}$-topology is predicted as a condition on the dimension D, similar to the classification of defects in thermodynamic phase transitions. Kekule distortions, vacancies and adatoms in graphene are proposed as examples of such defects and their topological equivalence is discussed.

II. Hamiltonian *vs* Symbol

Translation invariance allows one to use a Bloch Hamiltonian with a good qunatum number $\boldsymbol{k}$.

$$H\left(\partial_{\boldsymbol{r}}\right) \to \mathcal{H}\left(\boldsymbol{k}\right)$$

The spectrum of the Hamiltonian can be extracted from the spectrum of the Bloch Hamiltonian
Topological information of the system is encoded in the Bloch Hamiltonian

In the presence of defects, translation invariance is broken and a Bloch Hamiltonian can no longer be defined. However, an extension of the Bloch Hamiltonian, called the Symbol of the Hamiltonian, can be defined.

The symbol of a differential operator is its classically counterpart, intuitively obtained by replacing derivatives with respect to positions by parameters $\boldsymbol{k}$.

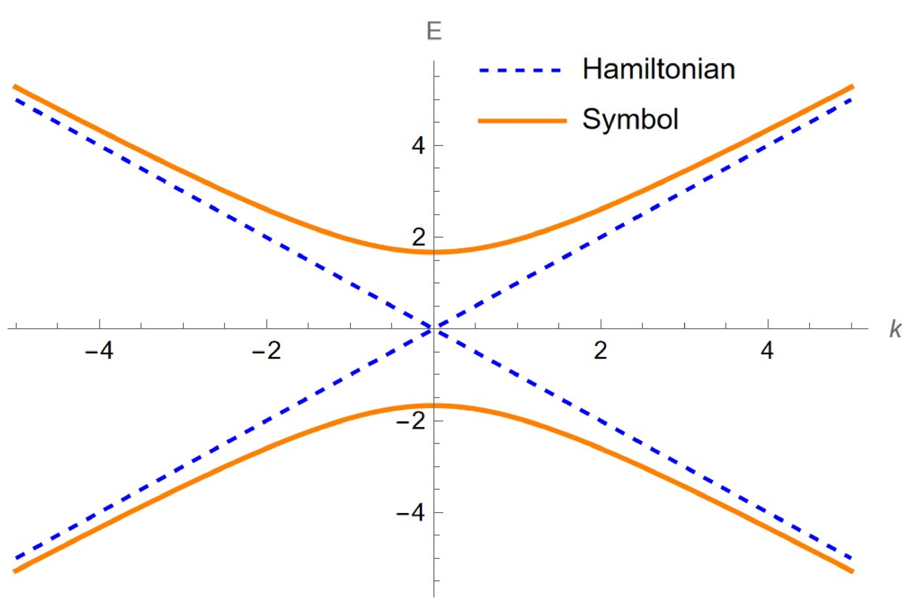
Hamiltonian $\to$ Symbol
$$H\left(\partial_{\boldsymbol{r}},\boldsymbol{r}\right) \to \mathcal{H}\left(\boldsymbol{k},\boldsymbol{r}\right)$$
$$\partial_{\boldsymbol{r}} \to \boldsymbol{k}$$
Operators $\to$ Parameters

In the presence of translation invariance the symbol of an Hamiltonian equals the Bloch Hamiltonian.

The formal definition of the symbol is with a weyl transform.

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \int_{-\infty}^{\infty} d\boldsymbol{r}' e^{-i\boldsymbol{k}\cdot\boldsymbol{r}'} \left\langle \boldsymbol{r}+\frac{\boldsymbol{r}'}{2} \middle| H \middle| \boldsymbol{r}-\frac{\boldsymbol{r}'}{2} \right\rangle$$

The spectrum of the Hamiltonian CANNOT be extracted from the spectrum of the Symbol
Topological information of the system is STILL encoded in the Symbol



A gapless Hamiltonian may have a gapped symbol $\Longrightarrow$ Possible topology!

III. The Tenfold classification

Class	s	T	P	C	$\delta=0$	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	$2\mathbb{Z}$

Tenfold classification. The first five columns display the 10 symmetry classes labeled by s and defined by their antiunitary symmetries T, P and chirality C.

"+" ("−") means that the relevant operator is a symmetry which squares to 1 (-1) and "0" the absence thereof .

The last 4 columns indicate possible topological classes $(0,\mathbb{Z},\mathbb{Z}_2)$ as a function of the reduced dimension $\delta = d - D$.

Dirac symbol representative

A Dirac symbol representative for each class can be defined using Dirac matrices and $\boldsymbol{k},\boldsymbol{r}$ dependent coefficients:

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \boldsymbol{h}_s\cdot\boldsymbol{\gamma}_s + \boldsymbol{h}_a\cdot\boldsymbol{\gamma}_a$$

$$\boldsymbol{h}_s = (h_{s,0},\dots,h_{s,q}), \quad \boldsymbol{h}_a = (h_{a,1},\dots,h_{a,p}), \quad s = p-q \mod 8$$

In this Clifford representation γ_s and γ_a anti-commute:

$$\{\gamma_i,\gamma_j\} = \delta_{ij},$$

Where $\boldsymbol{h}_s(k,r) = \boldsymbol{h}_s(-k,r), \quad \boldsymbol{h}_a(k,r) = -\boldsymbol{h}_a(-k,r).$

Symmetry Relations

The symmetry relations are:

$$T\mathcal{H}\left(\boldsymbol{k},\boldsymbol{r}\right)T^{-1} = \mathcal{H}\left(-\boldsymbol{k},\boldsymbol{r}\right)$$
$$P\mathcal{H}\left(\boldsymbol{k},\boldsymbol{r}\right)P^{-1} = -\mathcal{H}\left(-\boldsymbol{k},\boldsymbol{r}\right)$$
$$C\mathcal{H}\left(\boldsymbol{k},\boldsymbol{r}\right)C^{-1} = -\mathcal{H}\left(\boldsymbol{k},\boldsymbol{r}\right)$$

For Dirac symbols this translates into:

$$T\gamma_s T^{-1} = \gamma_s, \quad T\gamma_a T^{-1} = -\gamma_a$$
$$P\gamma_s P^{-1} = -\gamma_s, \quad P\gamma_a P^{-1} = \gamma_a$$

Spatial Dimension and Defects

Kitaev and Schnyder et al extended the initial Altland-Zirnbauer classification to higher space dimension d. This is the dimension of the Brilouin zone T^d. Teo and Kane then extended the table to include defects by introducing $\delta = d - D$, where D is the dimension of a sphere S^D surrounding the defect. The entries of the tenfold classification depend on the difference $s-\delta$.

IV. Index theorem

Atiyah-Singer index theorem

Index$H$ $\qquad H = \begin{pmatrix} 0 & \mathcal{Q} \\ \mathcal{Q}^\dagger & 0 \end{pmatrix}$

"The analytical index of an elliptic differential operator on a compact manifold, equals the topological index of its symbol"

S^{d+D} $\qquad \nu_{d+D}$

Analytical index

$$\text{Index}\, H \equiv \dim\text{Ker}\,\mathcal{Q} - \dim\text{Ker}\,\mathcal{Q}^\dagger$$

Topological index (Chern or winding number)

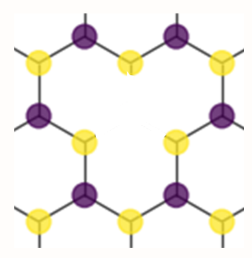
For a Dirac symbol $\mathcal{H}\left(\boldsymbol{k},\boldsymbol{r}\right) = \boldsymbol{h}\left(\boldsymbol{k},\boldsymbol{r}\right)\cdot\boldsymbol{\gamma}$

$$\nu_{d+D} = \tfrac{1}{S_{d+D}} \int_{S^{d+D}} d^d k\, d^D r\, J(\boldsymbol{h},d,D)$$

$$J(\boldsymbol{h},d,D) = \begin{vmatrix} h_1 & h_2 & \cdots & h_{d+D+1} \\ \partial_1 h_1 & \partial_1 h_2 & \cdots & \partial_1 h_{d+D+1} \\ \vdots & \vdots & \ddots & \vdots \\ \partial_{d+D} h_1 & \partial_{d+D} h_2 & \cdots & \partial_{d+D} h_{d+D+1} \end{vmatrix}$$

V. Graphene with defects

Graphene with a vacancy



$$\mathcal{H}_V(\boldsymbol{k},\boldsymbol{r}) = k_x\,\sigma_x\otimes\tau_z + k_y\,\sigma_y\otimes\mathbf{1} + \phi_1\left(\boldsymbol{r}\right)\sigma_x\otimes\tau_x + \phi_2\left(\boldsymbol{r}\right)\sigma_x\otimes\tau_y$$
$$\boldsymbol{\phi}(\boldsymbol{r}) \equiv \phi_1 + i\phi_2 = \phi(r)\,e^{i\theta}$$

$$T = \mathbf{1}\otimes\sigma_x K,\ P = \sigma_z\otimes\sigma_x K$$

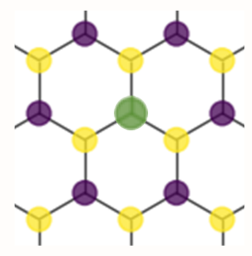
The vacancy does not break time reversal and particle hole symmetries

$$\begin{matrix} \delta = d - D = 2-1 = 1 \\ s = p - q = 2 - 1 = 1 \end{matrix} \Longrightarrow \mathbb{Z}$$

$$\nu_3 = \frac{1}{2\pi}\int dr\,\frac{1}{\phi_1^2+\phi_2^2}\begin{vmatrix} \phi_1 & \phi_2 \\ \partial_r\phi_1 & \partial_r\phi_2 \end{vmatrix} = \int\frac{d\theta}{2\pi} = 1$$

Graphene with a vacancy is topological!

Graphene with an adatom



$$\mathcal{H}_A(\boldsymbol{k},\boldsymbol{r}) = h_1(\boldsymbol{k})\,\sigma_x + h_2(\boldsymbol{k})\,\sigma_y + m(\boldsymbol{r})\,\sigma_z$$
$$h_1 - ih_2 = 1 + e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_1} + e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_2}$$

$$T = K$$

The adatom does not break time reversal symmetry but it does break particle hole symmetry

$$\begin{matrix} \delta = d - D = 2-1 = 1 \\ s = p - q = 1 - 1 = 0 \end{matrix} \Longrightarrow 0$$

Graphene with an adatom is not topological!

Graphene with a vacancy and an adatom

$$\mathcal{H}_{A+V}\left(\boldsymbol{k},\boldsymbol{r},\boldsymbol{r}'\right) = \mathcal{H}_V\left(\boldsymbol{k},\boldsymbol{r}\right) + m(\boldsymbol{r}')\sigma_z\otimes\mathbf{1}$$

$$T = \mathbf{1}\otimes\sigma_x K$$

$$\begin{matrix} \delta = d - D = 2-2 = 0 \\ s = p - q = 2 - 2 = 0 \end{matrix} \Longrightarrow \mathbb{Z}$$

$$\mathcal{C}_2 \propto \int dr dr' \frac{\partial_{r'} m}{(\phi_1^2+\phi_2^2+m^2)^{3/2}}\begin{vmatrix} \phi_1 & \phi_2 \\ \partial_r\phi_1 & \partial_r\phi_2 \end{vmatrix} = 1$$

The adatom does not disrupt the topology of the vacancy!

VI. Topological edge states

A vacancy leads to a single chiral zero mode

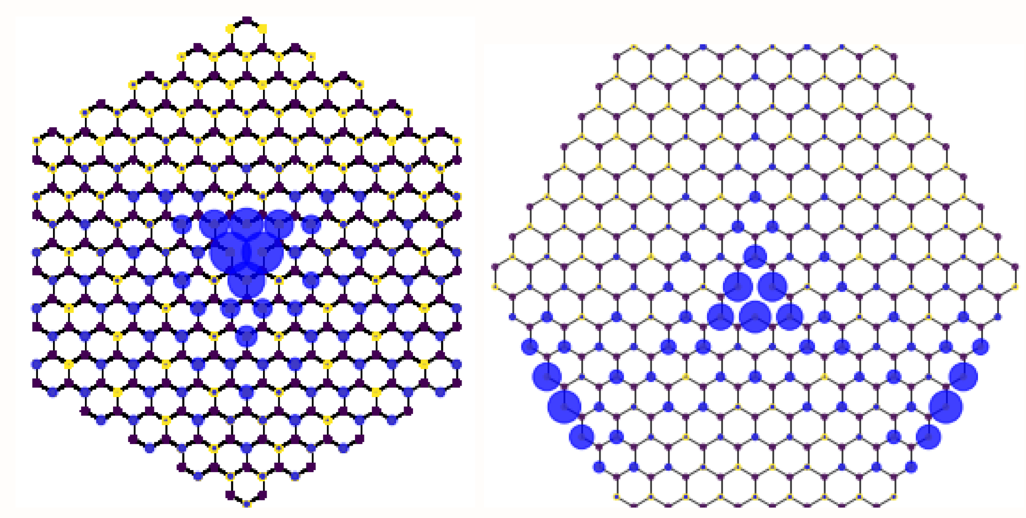
$$\text{Index}\, H \equiv \dim\text{Ker}\,\mathcal{Q} - \dim\text{Ker}\,\mathcal{Q}^\dagger = 1$$

A vacancy also leads to a winding number

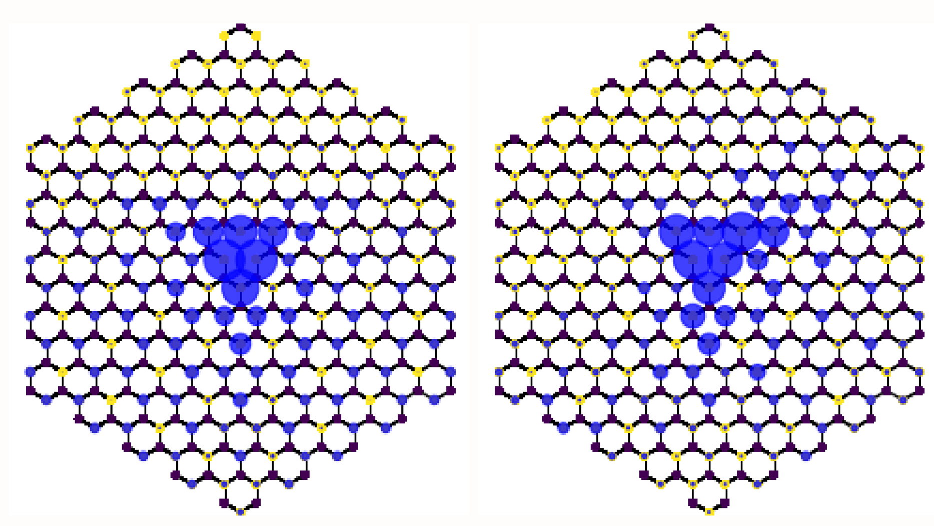
$$\nu_3 = 1$$

$$\text{Index}\, H = \nu_3$$

There is an index theorem for graphene with vacancy
Bulk-Edge correspondence, the topological zero modes are edge states



For any boundary the zero mode is localized on the edge of the lattice, vacancy location or both
The vacancy induces an additional edge to the lattice



The zero modes are topologically protected in the sense that they are insensitive to disorder

VII. Future work

$$\text{Index}H = |V_A - V_B| = \nu_3$$

For any number of vacancies

References

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