

Journal notes on:

Introduction to topological superconductivity

by Francisco Lobo



CONTENTS

I.	Introduction to superconductivity theory	3
A.	London theory	3
B.	BCS theory	3
C.	Ginzburg-Landau theory	3
1.	Classic type II superconductors	3
2.	Josephson effect	3
D.	Time-dependent Ginzburg-Landau theory	3
II.	Introduction to topological superconductivity	3
A.	Nanowire models in 1D	3
1.	SSH model	3
2.	Kitaev model	3
3.	Oreg-Lutchyn model	7
B.	Hall effects	11
1.	Integer quantum Hall effect	11
2.	Quantum spin Hall (Kane-Mele) effect	11
3.	Quantum anomalous Hall effect	11
4.	Fraction Hall effect	11
C.	Graphene	11
1.	Monolayer graphene	11
2.	Bilayer Bernal graphene	14
3.	Haldane model	16
4.	Kekulé modulation	16
5.	Twisted bilayer graphene	16

I. INTRODUCTION TO SUPERCONDUCTIVITY THEORY

This chapter closely follows "Introduction to superconductivity" by Tinkham - Dover Publications 9780486435039.

A. London theory

B. BCS theory

C. Ginzburg-Landau theory

1. Classic type II superconductors

2. Josephson effect

D. Time-dependent Ginzburg-Landau theory

II. INTRODUCTION TO TOPOLOGICAL SUPERCONDUCTIVITY

A lot from Akhmerov's course. Not a linear story telling of topological superconductivity theory per say, more of a compilation of different models that spark interest due to their topological and superconductive properties. Each section are mostly self contained. As supplementary material for some models, there are broad strokes of a possible numerical implementation. This is always done in *Julia* using the *Quantica.jl* package by Pablo San-Jose. Check the repository and it's tutorial at <https://github.com/pablosanjose/Quantica.jl>.

A. Nanowire models in 1D

1. SSH model

The most relevant references used for this section follow:

- Asboth's "A short course on topological insulators" - arXiv:1509.02295..

2. Kitaev model

The most relevant references used for this section follow:

- Kitaev's "Unpaired Majorana fermions in quantum wires" - Phys.-Usp. 44 131
- Akhmerov's "From Kitaev chain to a nanowire" online course - <https://topocondmat.org/>

The *Kitaev chain* or *Kitaev–Majorana chain* is a toy model for a topological superconductor using a 1D hybrid (semiconductor+superconductor) nanowires featuring Majorana bound states.

The Kitaev chain model consists of a 1D linear lattice of N sites and spinless fermions at zero temperature, subjected to nearest neighbor hopping interactions. The real-space tight-binding Hamiltonian describing such model reads

$$H = \mu \sum_{i=1}^N \left(c_i^\dagger c_i - \frac{1}{2} \right) - t \sum_{i=1}^{N-1} \left(c_{i+1}^\dagger c_i + h.c. \right) + \Delta \sum_{i=1}^{N-1} \left(c_{i+1}^\dagger c_i^\dagger + h.c. \right) \quad (1)$$

with c_i^\dagger (c_i) fermionic creation (annihilation) operators, μ the chemical potential, t the hopping energy and Δ an proximity induced superconducting p -wave pairing.

The objective of this model definition is to be able to have a Majorana bound states on the edges mode. For this, let us engineering the Hamiltonian in such a special way that it is actually possible to separate two Majoranas. Foremost, we define each site n as if it has two sublattices, $s = A$ and $s = B$. We then define Majorana operators relating to the fermionic operators as

$$\gamma_i^A = c_i^\dagger + c_i \quad \text{and} \quad \gamma_i^B = i(c_i^\dagger - c_i) \quad (2)$$

or rather, in the opposite way, as

$$c_i^\dagger = \frac{1}{2}(\gamma_i^A - i\gamma_i^B) \quad \text{and} \quad c_i = \frac{1}{2}(\gamma_i^A + i\gamma_i^B) \quad (3)$$

Indeed, each site can host a fermion or, equivalently, each site hosting two Majorana modes. These Majorana operators are Hermitian $\gamma_i^s = (\gamma_i^s)^\dagger$, unitary $(\gamma_i^s)^2 = 1$ and anticommute as $\{\gamma_i^s, \gamma_j^{s'}\} = 2\delta_{ij}\delta_{ss'}$.

Substituting directly into the Hamiltonian of Eq.(1) the fermionic operators as given by Eqs.(3) we obtain

$$H = -i\mu \frac{1}{2} \sum_{i=1}^N \gamma_i^B \gamma_i^A + i \frac{1}{2} \sum_{i=1}^{N-1} (\omega_+ \gamma_i^B \gamma_{i+1}^A + \omega_- \gamma_{i+1}^B \gamma_i^A), \quad \text{with } \omega_\pm = \Delta \pm t \quad (4)$$

From it we can distinguish between two phases—trivial and topological—, corresponding, respectively, to two different ways of pairing these Majorana states— no unpaired modes or one isolated mode on both edges, both depicted in Fig.1 in blue and red respectively. This phases can be identified, respectively, in their limiting regimes where one sets $\Delta = t = 0$ and $\mu = 0$ with $\Delta = t \neq 0$.

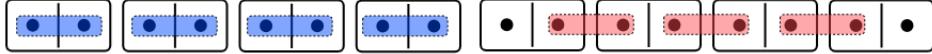


Figure 1. Kitaev chain Majorana modes pairing possibilities

Indeed, see that by setting $\Delta = t = 0$ within the Hamiltonian of Eq.(4) we obtain

$$H_{\text{trivial}} = -i\mu \frac{1}{2} \sum_{i=1}^N \gamma_i^B \gamma_i^A, \quad (5)$$

which corresponds to the "no unpaired Majorana modes" configuration. The energy cost for each fermion to be occupied is μ , with all excitations having an energy of either $\pm\mu/2$. The band structure will then have a gapped bulk and no zero energy edge states.

On the other hand, see that by setting $\mu = 0$ with $\Delta = t \neq 0$ we obtain

$$H_{\text{topological}} = it \sum_{n=1}^{N-1} \gamma_n^B \gamma_{n+1}^A \quad (6)$$

which corresponds to the "unpaired edge Majorana mode" configuration where every Majorana operator is coupled to a Majorana operator of a different kind in the next site. Note that the summation only goes up to $n = N - 1$. Moreover, see that by assigning a new fermion operator $\tilde{c}_i = 1/2 (\gamma_i^B + i\gamma_{i+1}^A)$, the Hamiltonian can be otherwise expressed as

$$H_{\text{topological}} = 2t \sum_{n=1}^{N-1} \left(\tilde{c}_i^\dagger \tilde{c}_i + \frac{1}{2} \right) \quad (7)$$

which describes a new set of $N - 1$ Bogoliubov quasiparticles with energy t . For every Majorana pair we assign an energy difference $2t$ between the empty and filled state. All states which are not at the ends of the chain have an energy of $\pm t$ and thus the bands structure has a gapped bulk. However, see that the missing mode $\tilde{c}_N = 1/2 (\gamma_N^B + i\gamma_1^A)$, which couples the Majorana operators from the two endpoints of the chain, does not appear in the Hamiltonian and does most have zero energy. This mode is called a Majorana zero mode and is highly delocalized. As the presence of this mode does not change the total energy, the ground state is two-fold degenerate. This condition is a topological superconducting non-trivial phase.

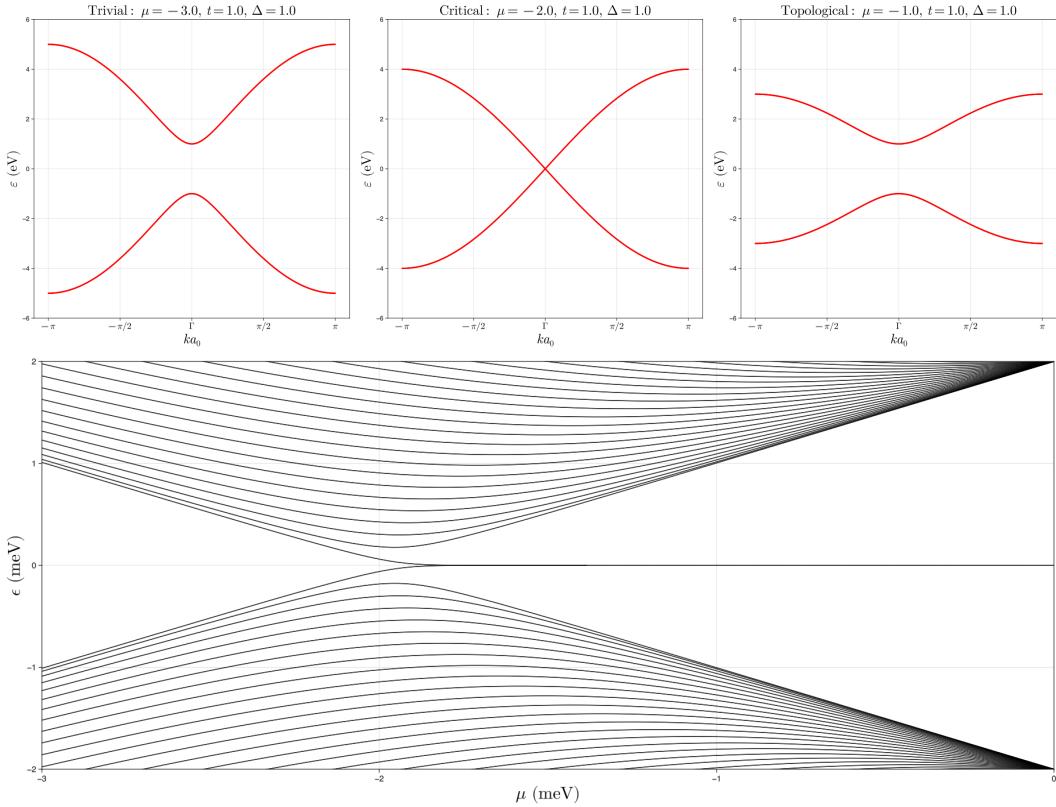


Figure 2. Kitaev chain (**top**) band structure and (**bottom**) band spectrum for a chain length of $L = 50$ with lattice spacing $a_0 = 1$ fixing $\Delta = t = 1.0$. The critical μ shifts forward to infinity as $L \rightarrow 0$.

Numerical implementation in Quantica.jl Shown below are the broad strokes of a numerical implementation of the Hamiltonian in Julia using the Quantica.jl. However, prior to this implementation,

we will be needing the Bogoliubov-de Gennes formalism. For this, we define a Nambu spinor

$$\check{c}_i^\dagger = \begin{pmatrix} c_i^\dagger & c_i \end{pmatrix} \quad \text{and} \quad \check{c}_i = \begin{pmatrix} c_i \\ c_i^\dagger \end{pmatrix} \quad (8)$$

such that that Hamiltonian in Eq.(1) reads

$$H = \mu \frac{1}{2} \sum_i \check{c}_i^\dagger \tau_z \check{c}_i - t \sum_{i=1}^{N-1} \check{c}_{i+1}^\dagger \tau_z \check{c}_i + \Delta \sum_{i=1}^{N-1} \check{c}_{i+1}^\dagger i \tau_y \check{c}_i \quad (9)$$

with τ_x, τ_y, τ_z Pauli matrices in the particle-hole subspace.

To understand why this is the case check:

$$\mu : \quad \check{c}_i^\dagger \tau_z \check{c}_i = \begin{pmatrix} c_i^\dagger & c_i \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} c_i \\ c_i^\dagger \end{pmatrix} = c_i^\dagger c_i - c_i c_i^\dagger = 2c_i^\dagger c_i - 1 \quad (10)$$

$$t : \quad \check{c}_j^\dagger \tau_z \check{c}_i = \begin{pmatrix} c_j^\dagger & c_j \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} c_i \\ c_i^\dagger \end{pmatrix} = c_j^\dagger c_i - c_j c_i^\dagger = c_j^\dagger c_i + h.c \quad (11)$$

$$\Delta : \quad \check{c}_j^\dagger i \tau_y \check{c}_i = \begin{pmatrix} c_j^\dagger & c_j \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} c_i \\ c_i^\dagger \end{pmatrix} = c_j^\dagger c_i^\dagger - c_j c_i = c_j^\dagger c_i^\dagger + h.c \quad (12)$$

where we the fermionic anti-commutation properties $\{c_i, c_j^\dagger\} = \delta_{ij}$ and $\{c_i, c_j\} = 0$, such that $c_i c_i^\dagger = 1 - c_i^\dagger c_i$, $c_j c_i^\dagger = -c_i^\dagger c_j$ and $c_j c_i = -c_i c_j$.

Also, see that these Hamiltonian has particle-hole symmetry, i.e $\mathcal{P}H\mathcal{P}^{-1} = -\tau_x H^* \tau_x = -H$ with $\mathcal{P} = \tau_x \mathcal{K}$ and \mathcal{K} complex conjugation, as well as time reversal symmetry, i.e $\mathcal{T}H\mathcal{T}^{-1} = H^* = H$ with $\mathcal{T} = \mathcal{K}$ for this spinless case (for reference, $\mathcal{T} = i\sigma_y \mathcal{K}$ for a 1/2-spin system). Once again, to understand why this is the case check.

```

1  build_Kitaev_chain(; kw...) = build_Kitaev_chain(LatticeParams(; kw...))
2  function build_Kitaev_chain(p::LatticeParams)
3      @unpack L, a0 = p
4
5      lat = LP.linear(; a0)
6
7      model_normal = -@onsite(; μ=0.0) -> μ*tz) - @hopping(; t=0.0) -> t*tz)
8      model_anomalous = @hopping(; Δ=0.0) -> Δ*lim*ty, region = (r, dr) -> dr[1] > 0)
9      model_anomalous_dagger = @hopping(; Δ=0.0) -> -Δ*lim*ty, region = (r, dr) -> dr[1] < 0)
10     model = model_normal + model_anomalous + model_anomalous_dagger
11
12     h = lat |> hamiltonian(model, orbitals=2)
13
14     if isfinite(L) h=supercell(h, region = r -> 0 <= r[1] <= L) end
15
16     return h
17 end
18
19

```

Figure 3. Kitaev Hamiltonian expressed in Nambu orbital space. The key factor of this implementation is that it is necessary to define the p -wave pairing (Nambu) hopping with a sign difference as it hops front and backwards, otherwise it will not be an hermitian term. [Explain a bit of the code.](#)

3. Oreg-Lutchyn model

The most relevant references used for this section follow:

- Lutchyn's "Majorana Fermions and a Topological Phase Transition in Semiconductor-Superconductor Heterostructures "- Phys. Rev. Lett. 105, 077001
- Oreg's "Helical liquids and Majorana bound states in quantum wires" - Phys. Rev. Lett. 105, 177002
- Lobo's "Exponential suppression of the topological gap in self-consistent intrinsic Majorana nanowires" - arXiv:2412.15174

The Oreg-Lutchyn Majorana minimal model consists of a finite 1D semiconductor (SM) nanowire with strong spin-orbit coupling (SOC) α and a tunable chemical potential μ , in proximity of a superconductor (SC) of homogeneous pairing Δ , having a magnetic field B_z applied along its length, defined as the \hat{z} direction. The Rashba effect describes the coupling of an electric field E_x that breaks inversion symmetry breaking in the direction perpendicular to the wire, to the electron's spin, i.e $\propto (i\vec{\nabla} \times \hat{x}) \cdot \vec{\sigma} = i\sigma_y \partial_z$ with $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. The Zeeman effect described the spin splitting due to the in-plane magnetic field B_z . The pairing term describes the Cooper pairs from BCS theory than could tunnel from the SM to the SC.

The tight-binding Hamiltonian describing such system can then be decomposed as

$$H = H_K + H_{SOC} + H_Z + H_{SC} \quad (13)$$

$$H_K = (2t - \mu) \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} \quad (14)$$

$$H_{SOC} = \frac{\alpha}{2a_0} \sum_{i\sigma} (c_{i+1\bar{\sigma}}^\dagger c_{i\sigma} + h.c.) \quad (15)$$

$$H_Z = V_Z \sum_i (c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}) \quad (16)$$

$$H_{SC} = \Delta (c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger + h.c.) \quad (17)$$

with c_i^\dagger (c_i) fermionic creation (annihilation) operators, μ the chemical potential, $t = \eta/a_0^2$ the hopping energy into $\langle i,j \rangle$ nearest-neighbouring sites with a_0 the lattice constant and $\eta = \hbar^2/2m^*$ with m^* the effective mass of the electrons, $V_Z = g_J \mu_B B_z / 2$ the Zeeman potential with g_J the Landé gyromagnetic moment and μ_B Bohr's magneton, α the Rashba SOC strength and Δ proximity induced superconducting s -wave pairing.

A paragraph explaining the bands.

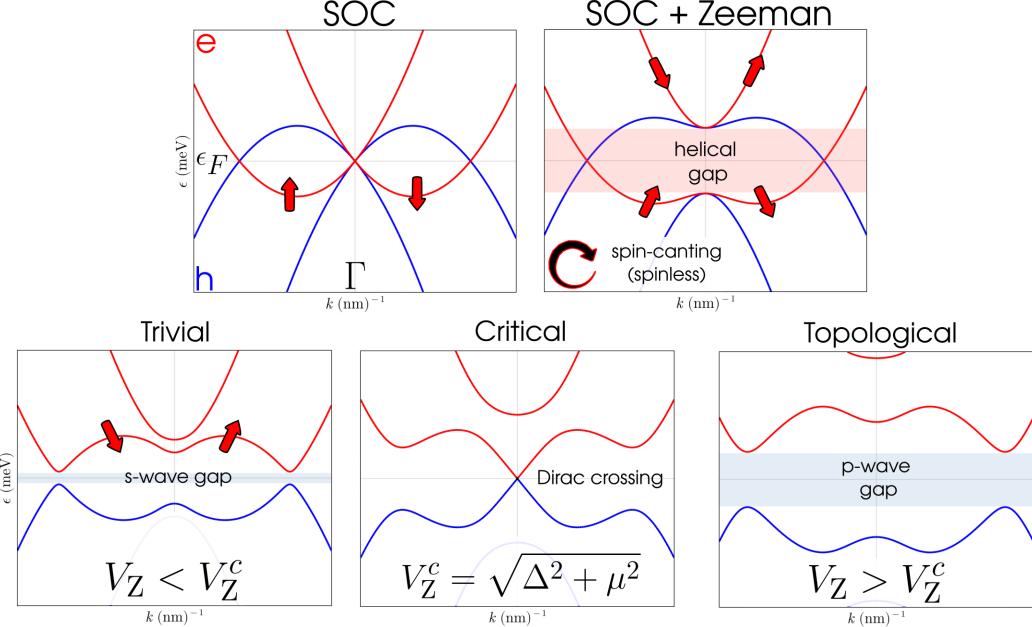


Figure 4.

A paragraph explaining the phase-diagram, pfaffian and band spectrum.

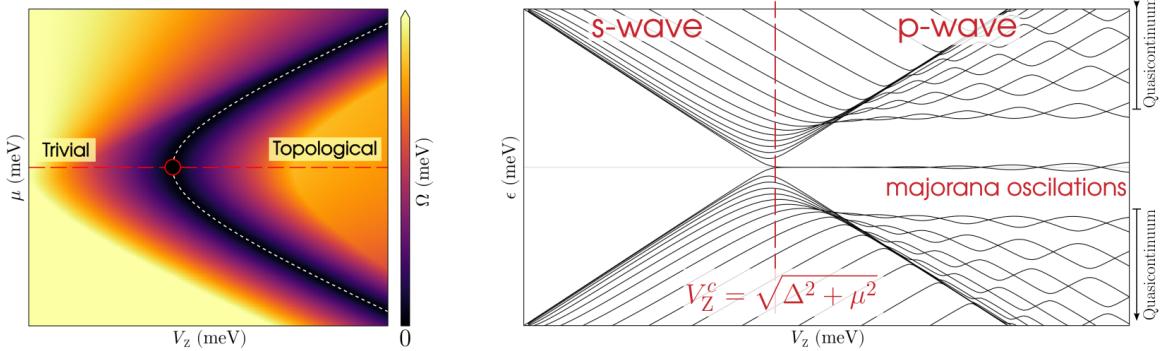


Figure 5.

Numerical implementation in Quantica.jl Shown below are the broad strokes of a numerical implementation of the Hamiltonian in Julia using the Quantica.jl. However, prior to this implementation, we will be needing the Bogoliubov-de Gennes formalism. For this, need to double the degrees of freedom through the Nambu-spinor. In the so called unrotated-spin basis we define a Nambu spinor as

$$\check{c}_i^\dagger = \begin{pmatrix} c_i^\dagger & c_i \end{pmatrix} = \begin{pmatrix} c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger & c_{i\uparrow} & c_{i\downarrow} \end{pmatrix} \quad (18)$$

In this Nambu \otimes spin orbital space the Hamiltonian in Eq.(13) reads

$$H = H_K + H_{SOC} + H_Z + H_{SC} \quad (19)$$

$$H_K = (2t - \mu) \sum_i \check{c}_i^\dagger [\tau_z \otimes \sigma_0] \check{c}_i - \frac{1}{2} t \sum_{\langle i,j \rangle} \check{c}_i^\dagger [\tau_z \otimes \sigma_0] \check{c}_j \quad (20)$$

$$H_{SOC} = \frac{\alpha}{2a_0} \sum_i \check{c}_i^\dagger [\tau_z \otimes i\sigma_y] \check{c}_{i+1} \quad (21)$$

$$H_Z = V_Z \sum_i \check{c}_i^\dagger [\tau_z \otimes \sigma_z] \check{c}_i \quad (22)$$

$$H_{SC} = \frac{1}{2} \Delta \sum_i \check{c}_i^\dagger [\tau_y \otimes \sigma_y] \check{c}_i \quad (23)$$

with τ Pauli matrices in the particle-hole subspace and σ in the spin subspace.

To understand why this is the case check we show explicitly the derivation for the pairing term as an example. It reads:

$$\begin{aligned} \check{c}_i^\dagger [\tau_y \otimes \sigma_y] \check{c}_i &= \left(\begin{array}{cccc} c_\uparrow^\dagger & c_\downarrow^\dagger & c_\uparrow & c_\downarrow \end{array} \right) \left(\begin{array}{cc|cc} 0 & 0 & 0 & -1 \\ 0 & 0 & +1 & 0 \\ \hline 0 & +1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{array} \right) \left(\begin{array}{c} c_\uparrow \\ c_\downarrow \\ c_\uparrow^\dagger \\ c_\downarrow^\dagger \end{array} \right) \\ &= -c_\uparrow^\dagger c_\downarrow^\dagger + c_\downarrow^\dagger c_\uparrow^\dagger + c_\uparrow c_\downarrow - c_\downarrow c_\uparrow = 2(c_\downarrow^\dagger c_\uparrow^\dagger + \text{h.c.}) \end{aligned} \quad (24)$$

where we the fermionic anti-commutation properties $\{c_i, c_j^\dagger\} = \delta_{ij}$ and $\{c_i, c_j\} = 0$.

The remaining terms derivation is analogous but even simpler because there is will be no mixing of particle with particle-hole components; the holeonic terms will correspond to the negative of the electronic terms, meaning that one just needs to expand the space according to $\tau_z \otimes$ the respective spin matrix. For the kinetic term there is no mixing of spin so it must trivially have the spin Pauli matrix σ_0 . Similarly, for the Zeeman term there is only the same-spin mixing of the type $\uparrow\uparrow - \downarrow\downarrow$ so it must have σ_z . As for the SOC term there is spin-mixing of opposing spins, so the options are either σ_x or $i\sigma_y$ (with a i for it to be hermitian). One can check with the fermionic anti-commutation properties that it is indeed $i\sigma_y$.

Therefore, within this spin \otimes Nambu orbital space in mind, we can define the Oreg-Lutchyn Hamiltonian as:

```

1
2 build_OregLutchyn_wire(; kw...) = build_OregLutchyn_wire(Params(; kw...))
3 function build_OregLutchyn_wire(p::Params)
4     @unpack L, a0, m0 = p
5     t = ℏ²ome/(2m₀*a₀²)
6
7     lat = LP.linear(; a₀)
8
9     model_K = @onsite(; μ=0.0) -> (2*t-μ)*σ₀τ₂ - hopping(t*σ₀τ₂)
10    model_Z = @onsite(; Vz=0.0) -> Vz*σ₂τ₂
11    model_α = @hopping((r, dr; α=0.0) -> α*(im*dr[1]/(2a₀²))*σᵧτ₂)
12    model_Δ = @onsite(; Δ₀=0.0) -> Δ₀*σᵧτᵧ
13    model = model_K + model_Z + model_α + model_Δ
14
15    h = lat |> hamiltonian(model, orbitals=4)
16    if isfinite(L) h=supercell(h, region = r -> 0 <= r[1] <= L) end
17
18    return h
19 end
20

```

Figure 6. Oreg-Lutchyn Hamiltonian expressed in spin \otimes Nambu orbital space. Explain a bit of the code. Prefer the Pauli notation with the krons.

Alternative Nambu basis It is common for people to define instead the Nambu spinor in a rotated basis as such

$$\bar{c}_i^\dagger = \begin{pmatrix} c_i^\dagger & [i\sigma_y c_i] \end{pmatrix} = \begin{pmatrix} c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger \\ c_{i\downarrow} & -c_{i\uparrow} \end{pmatrix} \quad (25)$$

As also explained in section II.C.1 of the previous part, these basis' operators relate to each other as

$$\bar{c}_i = \bar{\mathcal{U}} \check{c}_i \Leftrightarrow \check{c}_i = \bar{\mathcal{U}}^\dagger \bar{c}_i \quad (26)$$

$$\bar{c}_i^\dagger = \check{c}_i^\dagger \bar{\mathcal{U}}^\dagger \Leftrightarrow \check{c}_i^\dagger = \bar{c}_i^\dagger \bar{\mathcal{U}} \quad (27)$$

and, consequently, for a generic \tilde{M} matrix,

$$\bar{M} = \bar{\mathcal{U}} \tilde{M} \bar{\mathcal{U}}^\dagger \quad (28)$$

with $\bar{\mathcal{U}}$ is a unitary matrix (i.e $\bar{\mathcal{U}}^\dagger \bar{\mathcal{U}} = \bar{\mathcal{U}} \bar{\mathcal{U}}^\dagger = \mathbb{1}$)

$$\bar{\mathcal{U}} = \begin{pmatrix} \sigma_0 & 0 \\ 0 & i\sigma_y \end{pmatrix} \quad (29)$$

Making use of Pauli matrices' property

$$\sigma_\alpha \sigma_\beta = \sigma = \sigma_0 \delta_{\alpha\beta} + i\varepsilon_{\alpha\beta\gamma} \sigma_\gamma \quad (30)$$

one can check that

$$H_K : \bar{\mathcal{U}} [\tau_z \otimes \sigma_0] \bar{\mathcal{U}}^\dagger = [\tau_z \otimes \sigma_0] \quad (31)$$

$$H_{\text{SOC}} : \bar{\mathcal{U}} [\tau_z \otimes i\sigma_y] \bar{\mathcal{U}}^\dagger = [\tau_z \otimes i\sigma_y] \quad (32)$$

$$H_Z : \bar{\mathcal{U}} [\tau_z \otimes \sigma_z] \bar{\mathcal{U}}^\dagger = [\tau_z \otimes \sigma_z] \quad (33)$$

$$H_{\text{SC}} : \bar{\mathcal{U}} [\tau_y \otimes \sigma_y] \bar{\mathcal{U}}^\dagger = [\tau_x \otimes \sigma_0] \quad (34)$$

meaning that, in this the rotated basis, only the pairing Hamiltonian has it's Pauli matrices changed. Concretely,

$$H_{\text{SC}} = \frac{1}{2} \Delta \sum_i \bar{\mathbf{c}}_i^\dagger [\tau_x \otimes \sigma_0] \bar{\mathbf{c}}_i \quad (35)$$

B. Hall effects

1. Integer quantum Hall effect
2. Quantum spin Hall (Kane-Mele) effect
3. Quantum anomalous Hall effect
4. Fraction Hall effect

C. Graphene

1. Monolayer graphene

Hexagonal boron nitride (hBN) is a 2D material composed of a simple layer of alternating boron and nitrogen atoms disposed in a planar honeycomb lattice, as shown in Fig.(8)(a). The Bravais lattice

$$\mathbf{r}_i = n_{i1}\mathbf{a}_1 + n_{i2}\mathbf{a}_2, \quad n_{i1}, n_{i2} \in \mathbb{Z} \quad (36)$$

is generated by the real vectors basis

$$\mathbf{a}_1 = a_0 \begin{bmatrix} +\sin(30^\circ) \\ +\cos(30^\circ) \end{bmatrix} \text{ and } \mathbf{a}_2 = a_0 \begin{bmatrix} +\sin(30^\circ) \\ -\cos(30^\circ) \end{bmatrix}. \quad (37)$$

where $\sin(30^\circ) = 1/2$ and $\cos(30^\circ) = \sqrt{3}/2$. In each diamond shaped Wigner-Seitz primitive cell (depicted in yellow), we have one boron atom and one nitride atom, which we designate as sub-lattices A (depicted in red) and B (depicted in blue) respectively. The atoms within the central primitive cell are located at

$$\mathbf{s}_A = \frac{a_0}{\sqrt{3}} \begin{bmatrix} 0 \\ -1/2 \end{bmatrix} \text{ and } \mathbf{s}_B = \frac{a_0}{\sqrt{3}} \begin{bmatrix} 0 \\ +1/2 \end{bmatrix}. \quad (38)$$

where the origin is defined at the midpoint between the atoms. For each site A , the position of the nearest-neighbors (NN) in the sites B are given by

$$\boldsymbol{\delta}_1 = \frac{a_0}{\sqrt{3}} \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \boldsymbol{\delta}_2 = \frac{a_0}{\sqrt{3}} \begin{bmatrix} +\sin(60^\circ) \\ -\cos(60^\circ) \end{bmatrix} \text{ and } \boldsymbol{\delta}_3 = \frac{a_0}{\sqrt{3}} \begin{bmatrix} -\sin(60^\circ) \\ -\cos(60^\circ) \end{bmatrix}. \quad (39)$$

where $\sin(60^\circ) = \sqrt{3}/2$ and $\cos(60^\circ) = 1/2$. All these vectors are shown in Fig.(8)(a) within the real space lattice. Furthermore, from the real lattice basis vectors, in order to fulfill $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$, the reciprocal lattice basis vectors follow as

$$\mathbf{b}_1 = \frac{2\pi}{a_0} \begin{bmatrix} +\cos(30^\circ) \\ -\sin(30^\circ) \end{bmatrix} \text{ and } \mathbf{b}_2 = \frac{2\pi}{a_0} \begin{bmatrix} +\cos(30^\circ) \\ +\sin(30^\circ) \end{bmatrix}. \quad (40)$$

These are also shown in Fig.(8)(b) together with the first zone of Brillouin, formed by the area enclosed by the intersection of their bisectrices. The high-simmetry points are Γ , the origin, the Dirac points K_{\pm} and M read as

$$\Gamma = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad K_{\pm} = \pm \frac{4\pi}{3a_0} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ and } M = \frac{2\pi}{a_0} \begin{bmatrix} +\cos(30^\circ)/2 \\ +\sin(30^\circ)/2 \end{bmatrix} \quad (41)$$

where the K point is found such that $(\mathbf{M} + K_{k_x} \hat{\mathbf{M}}_{\perp})_{k_y} = 0$, with $\hat{\mathbf{M}}_{\perp}$ the unit vector in the perpendicular direction to \mathbf{M} . In far right side of Fig.(7), we make a note that the discretized grid it's in the Bloch momentums basis $\{\phi_1, \phi_2\}$, i.e in the direction of the reciprocal lattice vectors, and not simply in the reciprocal space $\{k_x, k_y\}$. In the Bloch momentums basis the Dirac points would reads as $K_{\pm} = 2\pi/3a_0 [\pm 1, \mp 1]$.

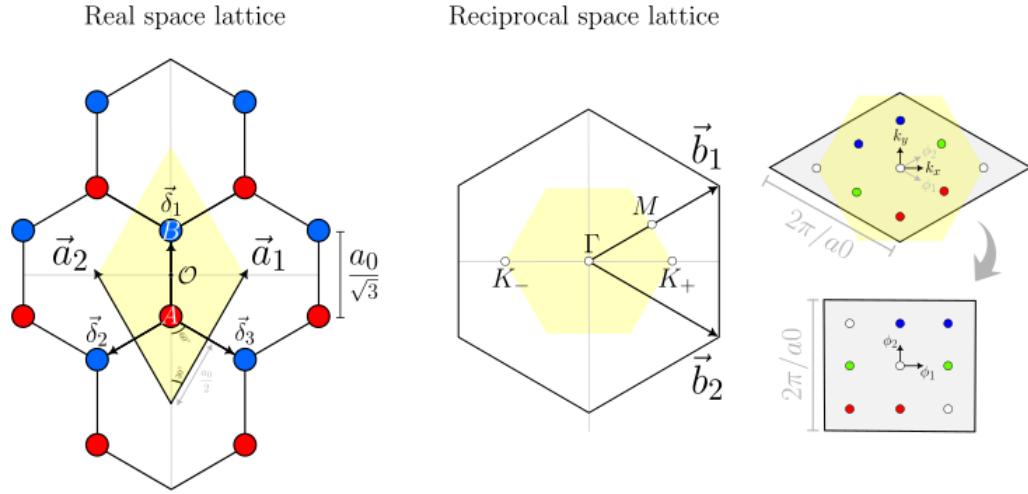


Figure 7.

Let us consider the nearest-neighbors (NN) tight-binding model, written in real space as

$$H_{\text{TB}}(\mathbf{R}) = \sum_i \epsilon_A a_{\mathbf{r}_i}^\dagger a_{\mathbf{r}_i} + \sum_i \epsilon_B b_{\mathbf{r}_i}^\dagger b_{\mathbf{r}_i} - t \sum_{\langle i,j \rangle} (a_{\mathbf{r}_i}^\dagger b_{\mathbf{r}_i+\delta_j} + b_{\mathbf{r}_j}^\dagger a_{\mathbf{r}_i-\delta_j}), \quad (42)$$

where the operators $a_{\mathbf{r}_i}^\dagger (a_{\mathbf{r}_i})$ create (annihilate) an electron in the sub-lattice A in a given Bravais lattice site \mathbf{r}_i , the operators $b_{\mathbf{r}_i}^\dagger (b_{\mathbf{r}_i})$ the same but for sub-lattice B , ϵ_A and ϵ_B are the onsite energies of site A and B respectively, and t is the hopping strength between nearest-neighbouring sites A and B and back, denoted with $\langle i,j \rangle$.

Expressing the creation/annihilation operators as their Fourier counterparts,

$$a_{\mathbf{R}_i} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{+i\mathbf{k}\cdot(\mathbf{R}_i+\mathbf{s}_A)} a_{\mathbf{k}} \quad \text{and} \quad b_{\mathbf{R}_i} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{+i\mathbf{k}\cdot(\mathbf{R}_i+\mathbf{s}_B)} b_{\mathbf{k}}, \quad (43)$$

and using the identity $\delta(\mathbf{k} - \mathbf{k}') = 1/N \sum_i e^{-i\mathbf{R}_i \cdot (\mathbf{k} - \mathbf{k}')}$, we obtain the Hamiltonian in reciprocal space,

$$H_{\text{TB}}(\mathbf{R}) = \sum_{\mathbf{k}} \epsilon_A a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}} \epsilon_B b_{\mathbf{k}}^\dagger b_{\mathbf{k}} - t \sum_{\mathbf{k}} (\gamma_{\mathbf{k}} a_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \gamma_{\mathbf{k}}^\dagger b_{\mathbf{k}}^\dagger a_{\mathbf{k}}), \quad (44)$$

where $\gamma_{\mathbf{k}} = \sum_{\langle j \rangle} \exp(+i\mathbf{k} \cdot \boldsymbol{\delta}_j)$ is complex number. If we now define a row vector $c_{\mathbf{k}}^\dagger = [a_{\mathbf{k}}^\dagger \ b_{\mathbf{k}}^\dagger]$ we can rewrite the system's Hamiltonian as $H_{\mathbf{R}}^{\text{TB}} = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger H_{\mathbf{k}}^{\text{TB}} c_{\mathbf{k}}$ with

$$H_{\text{TB}}(\mathbf{k}) = \begin{bmatrix} \epsilon_A & -t\gamma_{\mathbf{k}} \\ -t\gamma_{\mathbf{k}}^\dagger & \epsilon_B \end{bmatrix}. \quad (45)$$

Within this simplified tight-binding model, the expression for the electronic two-band structure can easily be obtained analytically by diagonalizing the matrix in Eq.(45), yielding

$$E_{\text{TB}}^\pm(\mathbf{k}) = \pm \sqrt{\epsilon^2 + t^2 \left[3 + 2 \cos(a_0 k_x) + 4 \cos\left(\frac{a_0 \sqrt{3}}{2} k_y\right) \cos\left(\frac{a_0}{2} k_x\right) \right]}, \quad (46)$$

having defined the zero point energy at $(\epsilon_A + \epsilon_B)/2$ and defined $\epsilon \equiv (\epsilon_A - \epsilon_B)/2$ at the middle of the gap such that $\epsilon_A = \epsilon$ and $\epsilon_B = -\epsilon$. The valence band corresponds to the $E_{\text{TB}}^-(\mathbf{k})$ dispersion while the $E_{\text{TB}}^+(\mathbf{k})$ corresponds to the conduction band, as shown in Fig.(8)(c). The band structure is accompanied by the density of states $\text{DoS}(E) = \sum_{\mathbf{k}} \delta(E - E(\mathbf{k}))$.

Notice that, if $\epsilon_A = \epsilon_B$, as is the case for graphene, we obtain $\epsilon = 0$ and the band dispersion closes in a linear fashion at the so called Dirac points. In hBN, the electronic band dispersion is also at its minimum near these points but has instead a parabolic shape. In either case, these points represent a fundamental symmetry of the system, called valley parity. To see why the dispersion is parabolic at these valley points, we Taylor series expand the exponential of $\gamma_{\mathbf{k}}$ in Eq.(??) near $\mathbf{k} \rightarrow \mathbf{K} + \mathbf{p}$ with $\mathbf{p} \rightarrow 0$. We obtain $\exp(+i\mathbf{p} \cdot \boldsymbol{\delta}_j) \approx 1 + i\mathbf{p} \cdot \boldsymbol{\delta}_j$. Now, since $\sum_{\langle j \rangle} \exp(+i\mathbf{K} \cdot \boldsymbol{\delta}_j) = 0$ we are left with $\gamma_{\mathbf{K}+\mathbf{p}} \simeq i\mathbf{p} \cdot \sum_{\langle j \rangle} \exp(+i\mathbf{K} \cdot \boldsymbol{\delta}_j) \boldsymbol{\delta}_j = -\sqrt{3}a_0/2(p_x - ip_y)$. Invoking the Pauli matrices definitions, from Eq.(45) we can write the TB Hamiltonian $H_{\text{TB}}^{\mathbf{k}}$ in this low-energy regime as

$$H_{\text{TB}}(\mathbf{K} + \mathbf{p}) = \epsilon \sigma_z + t \frac{\sqrt{3}a_0}{2} (\mathbf{p} \cdot \boldsymbol{\sigma}), \quad (47)$$

which clearly resembles the 2D Dirac Hamiltonian, $H_{\text{Dirac}} = \sigma_z mc^2 + c(\mathbf{p} \cdot \boldsymbol{\sigma})$ with ϵ taking the role of the rest mass energy mc^2 and instead with a velocity $v_F = t\sqrt{3}a_0/2$, termed the *Fermi velocity*, as a replacement to the velocity of light c . Notice that, for the case of graphene, since $\epsilon = 0$, the electrons would behave as if they are massless. In this limit, the hBN low-energy dispersion can be written as the typical relativistic dispersion relation

$$E_{\text{TB}}(\mathbf{K} + \mathbf{p}) = \pm \sqrt{p^2 v_F^2 + m_{\text{eff}}^2 v_F^4}. \quad (48)$$

where m_{eff} is the effective mass of the electron at a given point near the valleys.

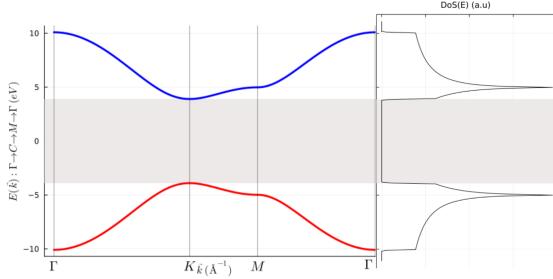


Figure 8. hBN electronic band structure from a nearest-neighbor tight-binding model accompanied by the density of the states. The dispersion goes along the symmetry path $\mathbf{k} : \Gamma \rightarrow K \rightarrow M \rightarrow \Gamma$ and was calculated using $\epsilon_g = 7.8\text{eV}$ for the energy gap, $t = 3.1\text{eV}$ for the hopping parameter and $a_0 = 1.42\sqrt{3}\text{\AA}$ for the honeycomb lattice length.

```

1 build_OregLutchyn_wire(; kw...) = build_OregLutchyn_wire(Params(; kw...))
2 function build_OregLutchyn_wire(p::Params)
3     @unpack L, a0, m0 = p
4     t = ℏ²ome/(2m0*a0^2)
5
6     lat = LP.linear(; a0)
7
8     model_K = @onsite(; μ=0.0) -> (2*t-μ)*σ₀τz - hopping(t*σ₀τz)
9     model_Z = @onsite(; Vz=0.0) -> Vz*σzτz
10    model_α = @hopping((r, dr; α=0.0) -> α*(im*dr[1]/(2a0^2))*σyτz)
11    model_Δ = @onsite(; Δθ=0.0) -> Δθ*σyτy
12    model = model_K + model_Z + model_α + model_Δ
13
14    h = lat |> hamiltonian(model, orbitals=4)
15    if isfinite(L) h=supercell(h, region = r -> 0 <= r[1] <= L) end
16
17    return h
18
19 end
20

```

Figure 9. Explain a bit of the code. Prefer the Pauli notation with the kron.

Numerical implementation in Quantica.jl

2. Bilayer Bernal graphene

Consider a bilayer graphene model depicted in Fig.(10).

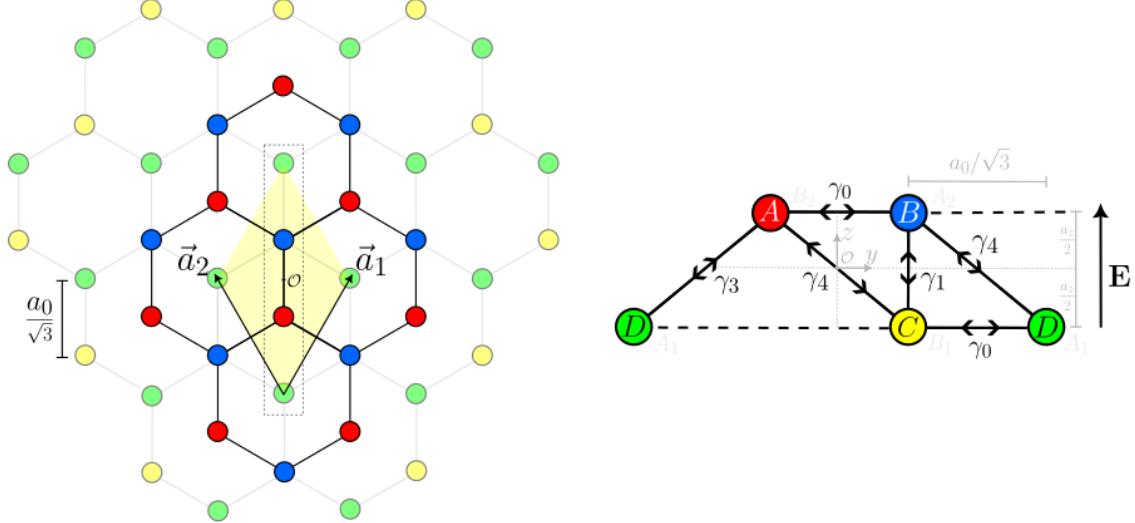


Figure 10. (a) Top view of the bilayer graphene (b) Side view of the dotted region in (a)

The tight-binding Hamiltonian of such a model reads

$$\begin{aligned}
H_{\text{BLG}} &= H_{\text{intralayer}} + H_{\text{interlayer}} = (H_{\text{top}} + H_{\text{bot}}) + (H_{\gamma_1} + H_{\gamma_3} + H_{\gamma_4}) \\
H_{\text{top}} &= \sum_i (\epsilon_A - \mu) c_i^\dagger a_i + \sum_i (\epsilon_B - \mu) b_i^\dagger b_i - \gamma_0 \sum_{\langle i,j \rangle} (a_i^\dagger b_j + h.c.) \\
H_{\text{bot}} &= \sum_i (\epsilon_C - \mu) c_i^\dagger c_i + \sum_i (\epsilon_D - \mu) d_i^\dagger d_i - \gamma_0 \sum_{\langle i,j \rangle} (c_i^\dagger d_j + h.c.) \\
H_{\gamma_1} &= +\gamma_1 \sum_{\langle i,j \rangle} (b_i^\dagger c_j + h.c.) \\
H_{\gamma_3} &= -\gamma_3 \sum_{\langle i,j \rangle} (a_i^\dagger d_j + h.c.) \\
H_{\gamma_4} &= +\gamma_4 \sum_{\langle i,j \rangle} (b_i^\dagger d_j + h.c.) + t_4 \sum_{\langle i,j \rangle} (a_i^\dagger C_j + h.c.)
\end{aligned}$$

Here, a site located at \mathbf{r}_i is indexed by the side index i and its next nearest neighbors located at \mathbf{r}_j are indexed with the site index j . Of course, \mathbf{r}_j depends on the kind of hopping in question: for γ_0 it's $\mathbf{r}_j = \mathbf{r}_i + \boldsymbol{\delta}_j$ with $j = 1, 2, 3$, for γ_1 it's $\mathbf{r}_j = \mathbf{r}_i \pm a_z \hat{\mathbf{z}}$, and for γ_3 and γ_4 it's $\mathbf{r}_j = \mathbf{r}_i + \boldsymbol{\delta}_j \pm a_z \hat{\mathbf{z}}$. Moreover, let us consider an electric field \mathbf{E} uniform in the plane xOy and growing along the $\hat{\mathbf{z}}$, described by the tight-binding Hamiltonian

$$H_E = \sum_i E_i (f_{i\uparrow}^\dagger f_{i\uparrow} - f_{i\downarrow}^\dagger f_{i\downarrow})$$

where $E_i = E \times z_i$ is the amplitude of the electric field at position \mathbf{r}_i , only really dependent on z_i , and $f_i^\dagger = [f_{i\uparrow}^\dagger \ f_{i\downarrow}^\dagger]$ is a generic fermionic operator. Since in our bilayer model the bottom layer is situated at $z = 0$ we redefine $E(a_z) = E$, such that

$$H_{\text{BLG}+} = E \sum_i \left\{ (a_{i\uparrow}^\dagger a_{i\uparrow} - a_{i\downarrow}^\dagger a_{i\downarrow}) + (b_{i\uparrow}^\dagger b_{i\uparrow} - b_{i\downarrow}^\dagger b_{i\downarrow}) \right\}$$

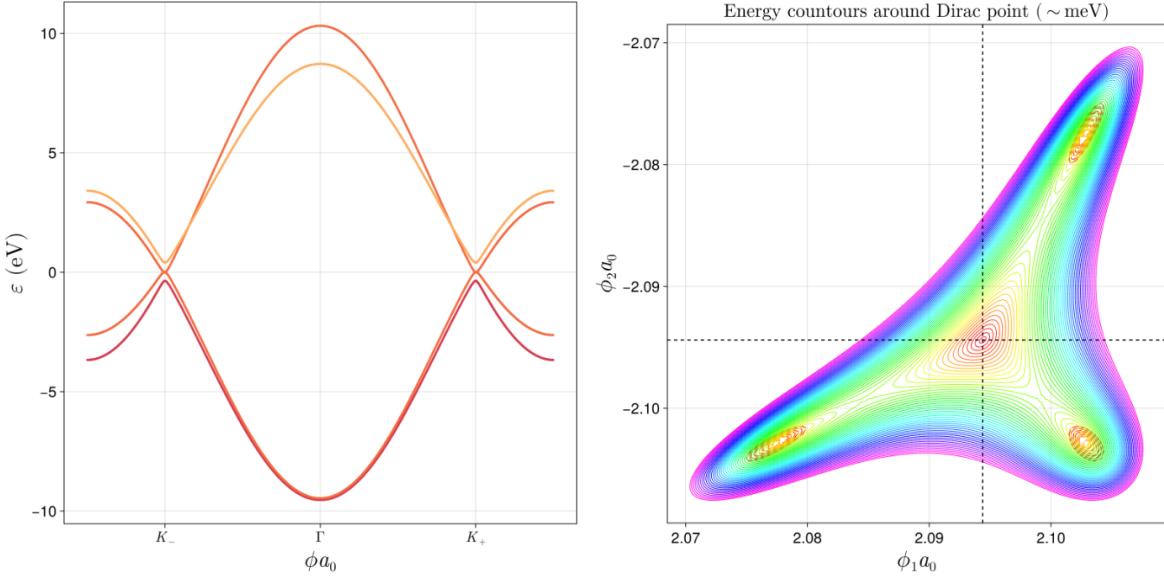


Figure 11. (a, b) Bandstructure along symmetry path $\Gamma \rightarrow K_+ \rightarrow M$ and (c) trigonal warping of BLG around the Dirac point K_+ .

```

25 build_meanfield_bilayergraphene(; kw...) = build_meanfield_bilayergraphene(LatticeParams(; kw...))
26     function build_meanfield_bilayergraphene(p::LatticeParams)
27         @unpack a0, az, nv, ε0, εC, εB, εA, θ0, γ1, γ3, γ4 = p
28
29         # building bilayer graphene lattice
30         lat_top = LP.honeycomb(; a0, names = (:A, :B), dim=3) |> translate([0, 0, az])
31         lat_bot = LP.honeycomb(; a0, names = (:C, :D), dim=3) |> translate([0, a0/3, 0])
32         lat = <combine>(lat_top, lat_bot) |> supercell(Int(nv*3), 2)
33
34         # building tight-binding model (top + bottom = join); kinetics + zeman
35         model_t = @onsite(; μ=0.0) >> (εB μ)*kron(tz, a0), sublats=:B) + @onsite(; μ=0.0) >> (εA μ)*kron(tz, θ0), sublats=:A) -> hopping(y0*kron(tz, a0); range=a0/3, sublats = (:B, :A) .=> (:A, :B))
36         model_b = @onsite(; μ=0.0) >> (εB μ)*kron(tz, a0), sublats=:D) + @onsite(; μ=0.0) >> (εC μ)*kron(tz, θ0), sublats=:C) -> hopping(y0*kron(tz, a0); range=a0/3, sublats = (:D, :C) .=> (:C, :B))
37         model_j1 = hopping(y1*kron(tz, θ0); range=az, sublats = (:B, :C) .=> (:C, :B))
38         model_j3 = -hopping(y3*kron(tz, a0); range=hypot(a0/3, az), sublats = (:D, :A) .=> (:A, :D))
39         model_j4 = hopping(y4*kron(tz, a0); range=hypot(a0/3, az), sublats = (:D, :B) .=> (:B, :D)) + hopping(y4*kron(tz, θ0); range=hypot(a0/3, az), sublats = (:C, :A) .=> (:A, :C))
40         model_Ez = @onsite((r; Ez=0.0) -> Ez*r[3]*kron(tz, oz))
41         model_Δ = @onsite((; Δ=0.0) -> Δ*kron(ty, oy)) # [essential that ΔSM = 0, just for structure]
42         model_0 = model_t + model_b + model_j1 + model_j3 + model_j4 + model_Ez + model_Δ
43
44         # hartree and fock meanfield self-energies w/ finite-range interactions
45         ZHartree = @onsite((i; Σ=zerofield) -> Σ[i])
46         ZFock = @hopping((i, j; Σ=zerofield) -> Σ[i, j]; range=nv*a0)
47         model = model_0 + ZHartree + ZFock
48
49         # building (and clipping) hamiltonian
50         h = hamiltonian(lat, model; orbitals=4)
51
52         return h
53     end

```

Figure 12. Remove all unnecessary mean-field stuff. Reorganize the code to make it more visible. Remove all code comments, explain it instead within this caption.

*Numerical implementation in Quantica.jl
Armchair and Zigzag configurations*

3. Haldane model

4. Kekulé modulation

5. Twisted bilayer graphene