1 Dirac fermions in graphene: *chiral symmetry, winding number*

📖 MOORE & MOESSNER: *chapter 2.5*

Consider a Hamiltonian $H(\boldsymbol{k})$ that has a 2×2 matrix block structure,

$$H(\boldsymbol{k}) = \begin{pmatrix} 0 & Q^{\dagger}(\boldsymbol{k}) \\ Q(\boldsymbol{k}) & \end{pmatrix}. \tag{1}$$

The complex function $Q(\boldsymbol{k})$ depends on the two-dimensional momentum $\boldsymbol{k} = (k_x, k_y)$.

(a) A Hamiltonian of this form is said to have a *chiral symmetry*, which means that it anti-commutes with some unitary matrix C. Can you find such a C?
Explain that the spectrum of H is symmetric around zero.

(b) The winding numer W of H is defined by $1/2\pi$ times net increment of the phase of Q as $\boldsymbol{k}$ varies along a closed contour Γ. Why must W be an integer? If $W \neq 0$, why must Q vanish at some point $\boldsymbol{k}_0$ inside Γ?.

c) Assume that $W = 1$. Expand Q around $\boldsymbol{k}_0$ and show that to first order in $\delta\boldsymbol{k} = \boldsymbol{k} - \boldsymbol{k}_0$ the Hamiltonian can be written in the form

$$H(\delta\boldsymbol{k}) = \sum_{i,j=x,y} v_{ij}\delta k_i \sigma_j, \tag{2}$$

with Pauli matrices σ_x and σ_y. This is called the Dirac Hamiltonian; the point $\boldsymbol{k}_0$ is called the Dirac point.

(d) Calculate the eigenvalues of the Dirac Hamiltonian. Motivate why Dirac fermions are referred to as "relativistic" particles.

(e) In graphene the function Q is given by

$$Q(\boldsymbol{k}) = t_0 \left(1 + e^{i\boldsymbol{k}\cdot\boldsymbol{n}_+} + e^{i\boldsymbol{k}\cdot\boldsymbol{n}_-}\right), \tag{3}$$

with $\boldsymbol{n}_\pm = a_0(\pm\sqrt{3}/2, 3/2)$ and real parameters t_0 and a_0 (hopping energy and lattice constant). Find two Dirac points at $\pm k_0$, with opposite winding number $W = \pm 1$. These are called the two "valleys" of the band structure.

(f) Show that the Hamiltonian in each valley has the form

$$H_\pm(\delta\boldsymbol{k}) = v\left(\delta\boldsymbol{k}_x\sigma_x \pm \delta\boldsymbol{k}_y\sigma_y\right). \tag{4}$$

How is the velocity v related to the parameters t_0 and a_0? Compare v in graphene to the speed of light. Are these really relativistic particles?

(g) If the graphene layer is placed on a substrate a chiral-symmetry-breaking term $\pm\mu\sigma_z$ is added to $H_\pm$. Show that a gap $\propto \mu$ opens at the Dirac point.

2 Chiral symmetry in 1D: *SSH chain, zero-modes*

Asbóth: *chapter 1*; Moore & Moessner: *box 4.1*

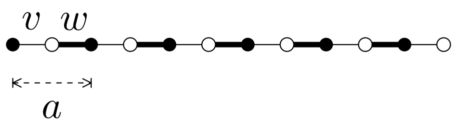
A one-dimensional (1D) lattice model with chiral symmetry has a Hamiltonian of the form

$$H(k) = \begin{pmatrix} 0 & h(k) \\ h^*(k) & 0 \end{pmatrix}, \tag{5}$$

with $h(k) = h(k + 2\pi/a)$, for a lattice constant a. Because of this periodicity we can define a closed loop even in 1D. The winding number W is then the increment of the phase of $h(k)$ as k increases by $2\pi/a$.

The SSH (Su-Schrieffer-Heeger) model has Hamiltonian

$$H_{\mathrm{SSH}}(k) = \begin{pmatrix} 0 & v + we^{-ika} \\ v + we^{ika} & 0 \end{pmatrix}, \quad v, w > 0. \tag{6}$$



(a) The operator $e^{\pm ika}$, with $k = -id/dx$, acting on a function $\psi(x)$ translates by $\pm a$: $e^{\pm ika}\psi(x) = \psi(x \pm a)$. Use this to explain why H_{SSH} describes the staggered hopping strength along a chain of atoms, as indicated in the figure.

(b) Compute the winding number W of the SSH Hamiltonian. Show that $W = 1$ for $v < w$, while $W = 0$ for $v > w$. The SSH chain is called *topologically nontrivial* when $W \neq 0$.

(c) The transition from $W = 0$ to $W = 1$ is called a topological phase transition. Show that this transition is associated with a closing and reopening at $k = \pi/a$ of an energy gap of H_{SSH}.

In the extreme case $w = 1$, $v = 0$ the SSH chain in the figure has a pair of states at zero energy located at each end. This pair of "zero-modes" persists in the topologically nontrivial regime, provided that the length L of the chain is long enough.

(d) Write H_{SSH} in the form a matrix that couples sites on a 1D lattice. Compute the energy spectrum of a 20-atom chain, for $w = 1$ as a function of v. Show the appearance of a pair of states near $E = 0$ for $v < w$.

(e) An intuitive way to understand the robustness of the zero-mode, is to note that chiral symmetry enforces a $\pm E$ symmetry of the spectrum. (Why is this?) Consider a semi-infinite chain. Start from $w = 1$, $v = 0$, when there is a zero-mode. Now imagine increasing v. Why does chiral symmetry keep the zero-mode pinned at $E = 0$? How does this argument break down when v crosses w?

The winding number of the chirally symmetric Hamiltonian has an alternative interpretation that will allow us to generalize this topological invariant to systems without chiral symmetry.

(f) Show that the winding number, defined as the increment of the phase of $h(k)$, can equivalently be written as an integral

$$W = \frac{1}{2\pi i}\int_0^{2\pi/a} dk\, h^{-1}(k)\frac{d}{dk}h(k). \tag{7}$$

(g) Denote by $u(k)$ the eigenstate (normalized to unity) of the lowest band of $H(k)$. The integral

$$\gamma = i\int_0^{2\pi/a} dk\, u^*(k)\frac{d}{dk}u(k) \tag{8}$$

is a 1D Berry phase, also known as a Zak phase. The integrand is called the Berry connection. Show (by explicit calculation) that

$$W = \frac{1}{\pi}\gamma. \tag{9}$$

3 Chern insulator: *Chern number, chiral edge states, quantum Hall effect*

✍ ASBÓTH: *chapters 2.2.4 and 6*; GRUSHIN: *chapter 5 A,B,C;* FRUCHART & CARPENTIER*:* section 3

In a 2D system the Berry connection $\boldsymbol{A} = (A_x, A_y)$ has two components,

$$A_\alpha(\boldsymbol{k}) = i\left\langle u(k_x,k_y)\left|\frac{\partial}{\partial k_\alpha}\right|u(k_x,k_y)\right\rangle. \tag{10}$$

The Chern number is defined by the integral over the Brillouin zone (BZ) of the curl of $\boldsymbol{A}$ (also known as the Berry curvature),

$$C = \frac{1}{2\pi}\iint_{\mathrm{BZ}} dk_x dk_y\left(\frac{\partial A_x}{\partial k_y} - \frac{\partial A_y}{\partial k_x}\right). \tag{11}$$

Each energy band has its own Chern number. A Chern insulator has a band with a nonzero Chern number.

(a) Explain why $C = 0$ if the system obeys time reversal symmetry.

(b) The eigenstate $u(\boldsymbol{k})$ is determined up to multiplication by a phase factor $e^{i\phi(\boldsymbol{k})}$. Show that the transformation $u(\boldsymbol{k}) \mapsto e^{i\phi(\boldsymbol{k})}u(\boldsymbol{k})$ does not change the Chern number.

A simple model Hamiltonian of a Chern insulator is

$$\begin{aligned} H(\boldsymbol{k}) &= t_0\sigma_x \sin ak_x + t_0\sigma_y \sin ak_y + M(\boldsymbol{k})\sigma_z, \\ M(\boldsymbol{k}) &= M_0 - t_0\cos ak_x - t_0\cos ak_y. \end{aligned} \tag{12}$$

(c) Why does the term $\propto M$ break time reversal symmetry?

(d) Calculate the Chern number of the lowest band, as a function of M_0/t_0.

A boundary of the Chern insulator can be modelled by a region in which $M/t_0 \to \infty$. Consider a boundary along the x-axis, and take $M \to \infty$ for $y > 0$ and $M/t_0 = 1$ for $y < 0$. The low-energy states are near $\boldsymbol{k} = 0$, so it makes sense to expand $H(\boldsymbol{k})$ to first order in k_x and k_y,

$$H_0 = at_0 k_x \sigma_x + at_0 k_y \sigma_y + (M(y) - 2t_0)\sigma_z. \tag{13}$$

(e) Solve the Schrödinger equation $H_0\psi = E\psi$ by searching for a solution of the form

$$\psi(x, y) = e^{ikx} \exp\left(-\int_0^y dy' \, [M(y') - 2t_0]\right) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \tag{14}$$

Check that this solution decays for $|y| \to \infty$, hence it describes a state localized at the edge of the Chern insulator. Show that this edge state propagates in the $-x$ direction. Because of this uni-directional motion it is called a *chiral* edge state.

(f) Explain that the edge state carries an electrical current $(e/h)\delta E$ along the boundary in an energy range δE around $E = 0$. What would be the electrical conductance of a Chern insulator confined to the strip $|y| < W$?

More generally, a Chern insulator with Chern number C has an electrical conductance quantized at $G = |C| \times e^2/h$. This is a manifestation of the *quantum Hall effect.* Because the quantization of the conductance arises from a topological invariant, one speaks of "topological protection".

4 Quantum spin Hall effect: *Kramers degeneracy, helical edge states, scattering matrix*

Moore & Moessner: *chapters 3.4 and 3.5*; Asbóth: *chapters 8 and 10*; Grushin: *chapter 5 D*; Fruchart & Carpentier: *section 4*

So far we encountered two topological invariants, winding number and Chern number, that can take on any integer value. A 2D system with time reversal symmetry can have a topological invariant that can take on just two values. One speaks of $\mathbb{Z}$ versus $\mathbb{Z}_2$ topological invariants.

To construct a topologically nontrivial 2D system that is time-reversally invariant, the simplest way is to couple a Chern insulator for spin-up electrons with $C = +1$ to a Chern insulator for spin-down electrons with $C = -1$. At the boundary there will then be a pair of counterpropagating edge states. The direction of motion is set by the spin direction, a property known as spin-momentum locking, or helicity. One might wonder whether scattering could cause backscattering and gap out the edge states. This is prevented by Kramers degeneracy.

A time-reversally invariant Hamiltonian of a spin-1/2 particle satisfies

$$\sigma_y H^* \sigma_y = H, \tag{15}$$

where the complex conjugation is taken in the real-space basis (so $\boldsymbol{k} = -i\hbar\nabla \mapsto -\boldsymbol{k}$).

(a) Show that this symmetry relation implies that, if ψ is an eigenstate of H at eigenvalue E, then also $\sigma_y\psi^*$ is an eigenvalue at the same energy. Can you also show that these two eigenstates are linearly independent?
(b) Suppose we add a spin-independent disorder potential $V(x, y)$ to the Hamiltonian. Explain why Kramers degeneracy prevents disorder from opening a gap in the energy spectrum of the helical edge states. What would happen if we would couple two Chern insulators with $C = \pm 2$?

To study electrical conduction it is helpful to work with the scattering matrix at a given energy, instead of the Hamiltonian. The scattering matrix $S(E)$ is a 2×2 matrix that relates incoming and outgoing amplitudes of a pair of helical edge states at energy E,

$$\begin{pmatrix} \psi_{\text{out at the left}} \\ \psi_{\text{out at the right}} \end{pmatrix} = S \begin{pmatrix} \psi_{\text{in at the left}} \\ \psi_{\text{in at the right}} \end{pmatrix}. \tag{16}$$

Particle number conservation requires that S is a unitary matrix: $S^{-1} = S^\dagger$. Time reversal symmetry requires that $S_{nm} = -S_{mn}$.

(c) Show that these two conditions imply that a wave incoming from the left is transmitted to the right with unit probability.

More generally, consider N pairs of helical edge states. The $\mathbb{Z}_2$ topological invariant P is the parity of N: $P = 0$ if N is even and $P = 1$ if N is odd. The scattering matrix now has dimensions $2N \times 2N$; the $N \times N$ upper-left block (the reflection matric r) describes the backscattering of a wave incoming from the left. The electrical conductance is obtained from r via the Landauer formula,

$$G = \frac{e^2}{h}\left(N - \operatorname{tr} r r^\dagger\right). \tag{17}$$

(d) Derive that $\det r = 0$ if N is odd. What does this imply for the electrical conductance?

5 Topological insulators: *fermion doubling, half-integer quantum Hall effect*

Moore & Moessner: *chapter 3.6*; Grushin: *chapter 6*

In the quantum spin Hall effect we have a gapped 2D interior and gapless states at the 1D boundary, described by the Hamiltonian $H_{1D} = vk_x\sigma_x$ (for a boundary along the x-axis). This carries over to one higher dimension: a gapped 3D interior with gapless states on the 2D surface, with Hamiltonian $H_{2D} = vk_x\sigma_x + vk_y\sigma_y$ (for a surface in the x–y plane). In each case the gapless nature of the excitations is protected by time reversal symmetry. Generically, the 2D and 3D materials with an insulating interior and a gapless boundary are referred to as *topological insulators*.

A model Hamiltonian for a thin-film topological insulator is

$$\begin{aligned} &H = t_0\tau_z(\sigma_x \sin ak_x + \sigma_y \sin ak_y) + \tau_x M(k_x, k_y), \\ &M(k_x, k_y) = M_0 - M_1(2 - \cos ak_x - \cos ak_y). \end{aligned} \tag{18}$$

This Hamiltonian acts on a four-component wave function $\Psi = (\psi_{\uparrow\text{upper}}, \psi_{\downarrow\text{upper}}, \psi_{\uparrow\text{lower}}, \psi_{\downarrow\text{lower}})$, of states with spin ↑ or ↓, confined to the upper or lower surface of the thin film. The Pauli matrix σ_α acts on the spin, the Pauli matrix τ_α acts on the layer degree of freedom. The term $\propto M$ thus couples states on the upper and lower surface.

(a) Check that this Hamiltonian preserves time reversal symmetry.

(b) Show that the Hamiltonian is block diagonalized by the unitary transformation $H \mapsto UHU^\dagger$ with $U = e^{i(\pi/4)\tau_y\sigma_z}$.

The 2×2 blocks have Hamiltonian

$$H_\pm = \pm t_0(\sigma_x \sin ak_x + \sigma_y \sin ak_y) \pm M(k_x, k_y)\sigma_z. \tag{19}$$

(c) Each block separately looks like the Hamiltonian (12) of a Chern insulator. Why doesn't $H_\pm$ break time reversal symmetry?

(d) Check that for $M_0 = 0$ there is a *single* gapless Dirac cone in the Brillouin zone. In graphene we saw that Dirac cones come in pairs of opposite winding number, a consequence of time reversal symmetry known as *fermion doubling*. How does the topological insulator avoid the appearance of a second Dirac cone in the Brillouin zone?

Near $\boldsymbol{k} = 0$ we may expand to first order in $\boldsymbol{k}$. In a perpendicular magnetic field $B = dA_x/dy - dA_y/dx$ the Hamiltonian $H_\pm = \pm H_0$ is given by

$$H_0 = v(k_x - eA_x)\sigma_x + v(k_y - eA_y)\sigma_y + M_0\sigma_z, \text{ with } v = at_0. \tag{20}$$

(e) Define the operator

$$b = (2eB)^{-1/2}\Big((k_x - eA_x) + i(k_y - eA_y)\Big). \tag{21}$$

Show that this operator satisfies the canonical commutation rule

$$[b, b^\dagger] = 1. \tag{22}$$

(f) Write H_0 in terms of b and $b^\dagger$, and then obtain the eigenvalues λ_n of H_0^2,

$$\lambda_n^2 = M_0^2 + n\omega_0^2, \; n = 0, 1, 2, \ldots, \text{ with } \omega_0 = at_0\sqrt{2eB}. \tag{23}$$

Convince yourself that the eigenvalue λ_n is twofold degenerate for $n \geqslant 1$, but nondegenerate for $n = 0$. For $M_0 = 0$ the spectrum of H_0 is then given by

$$E_n = \operatorname{sign}(n)\omega_0\sqrt{|n|}, \quad n \in \mathbb{Z}. \tag{24}$$

How does this differ from the usual Landau level spectrum in a 2D semiconductor?

(g) Explain the half-integer quantum Hall effect from a single surface of the topological insulator. This is also referred to as the *anomalous* quantum Hall effect — to be distinguished from the *quantum anomalous* Hall effect, which is the quantum Hall effect at zero magnetic field.

6 Topological superconductors: *Kitaev chain, Majorana fermions*

Moore & Moessner: *chapter 9.4, box 9.2*; Grushin: *chapter 4.I*

The Kitaev chain is the superconducting counterpart of the SSH chain: the role of chiral symmetry to stabilize the zero-modes is taken over by particle-hole symmetry.

Consider spin-polarized fermions on a chain of N sites with Hamiltonian

$$H = \sum_{j=1}^{N-1}\left[-t(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) + \Delta(a_j a_{j+1} + a_{j+1}^\dagger a_j^\dagger)\right] - \mu\sum_{j=1}^{N}\left(a_j^\dagger a_j - \tfrac{1}{2}\right), \tag{25}$$

where t is the hopping amplitude between neighbouring sites, μ is the chemical potential, and Δ is the superconducting pair potential. The operators $a_i, a_i^\dagger$ are the fermion annihilation and creation operators on site i, with anticommutation relations

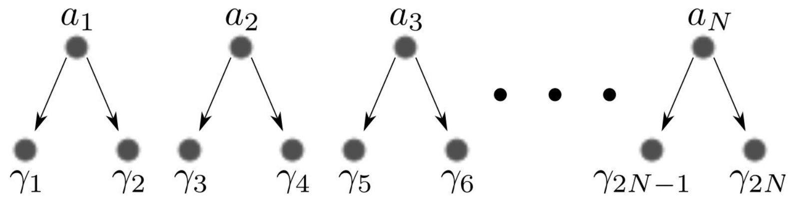
$$\begin{aligned} &a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij}, \\ &a_i a_j + a_j a_i = 0, \;\; a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0. \end{aligned} \tag{26}$$

Notice that H does not conserve the number of particles, but it does conserve the parity of the particle number: The term $\propto \Delta$ changes the number of particles by ± 2. The pair of fermions is called a Cooper pair.

We make the transformation

$$\gamma_{2j-1} = a_j + a_j^\dagger \text{ and } \gamma_{2j} = -i(a_j - a_j^\dagger).$$

indicated in the figure. The γ operators are called "Majorana operators" and the quasiparticles they represent are called "Majorana fermions".



(a) Compute $\gamma_n^\dagger$ and compare it to γ_n. Explain why it is said that a Majorana fermion "is its own antiparticle".

(b) What are the commutation relations of the operators γ_j ? Evaluate γ_j^2.

(c) Rewrite the Hamiltonian in terms of the Majorana operators.

(d) Consider the special case $\Delta = t$, $\mu = 0$. Show that γ_1 and γ_{2N} are absent from the Hamiltonian of the Kitaev chain. These play the role of the zero-modes of the SSH chain.

To consider the more general case of arbitrary t, μ, Δ, we need a formalism that can deal with the absence of particle-number conservation. This has been developed by Bogoliubov and De Gennes. Include all the fermion operators in a vector Ψ of length $2N$, composed of two vectors u, v of length N:

$$\Psi = (u, v),\ \ u = (a_1, a_2, \dots a_N),\ \ v = (a_1^\dagger, a_2^\dagger, \dots a_N^\dagger). \tag{27}$$

The Pauli matrices τ_x, τ_y, τ_y act on the u and v vectors,

$$\tau_x \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} v \\ u \end{pmatrix},\ \ \tau_y \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} -iv \\ iu \end{pmatrix},\ \ \tau_z \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u \\ -v \end{pmatrix}. \tag{28}$$

The operator $|j\rangle\langle j|$ projects onto site number j of the chain. With this notation we can rewrite the Hamiltonian (25) as a combination of Pauli matrices,

$$H = \tfrac{1}{2}\Psi^\dagger \mathcal{H} \Psi,\ \ \mathcal{H} = -\sum_{j=1}^{N-1} \Big[(t\tau_z + i\Delta\tau_y)|j\rangle\langle j+1| + \text{H.c.} \Big] - \mu\tau_z \sum_{j=1}^{N} |j\rangle\langle j|. \tag{29}$$

(The abbreviation H.c. means "Hermitian conjugate".) The matrix operator $\mathcal{H}$ is called the Bogoliubov-De Gennes Hamiltonian.

(e) Derive this expression for $\mathcal{H}$. Verify the particle-hole symmetry relation

$$\tau_x \mathcal{H}^* \tau_x = -\mathcal{H} \tag{30}$$

and explain why the spectrum of $\mathcal{H}$ must be $\pm E$ symmetric.

(f) Show that $\mathcal{H}$ for $\Delta = t$, $\mu = 0$ has a pair of eigenvalues $E = 0$. Where are the corresponding eigenfunctions of $\mathcal{H}$ located on the chain? These two eigenstates are called "Majorana zero-modes".

(g) Calculate numerically the spectrum of $\mathcal{H}$ for $N = 20$, $t = 1$ as a function of Δ and μ. Check the stability of the Majorana zero-modes and explain how this follows from particle-hole symmetry.

7 Weyl semimetals: *Berry flux, Fermi arcs, chiral magnetic effect*

Moore & Moessner: *chapter 7.2*; GRUSHIN: *chapter 7*

A Weyl semimetal is the 3D generalization of 2D graphene. As in graphene the excitations are massless particles, but instead of being confined to a plane they move in all three directions. The move from 2D to 3D changes the physics in a qualitative way, as we will see.

(a) The 2D Dirac cone, with Hamiltonian $H_{2D} = vp_x\sigma_x + vp_y\sigma_y$, can be gapped by a mass term $\propto \sigma_z$. Explain that the 3D Hamiltonian

$$H_{3D} = vp_x\sigma_x + vp_y\sigma_y + vp_z\sigma_z \tag{31}$$

cannot be gapped in any way. To emphasise this qualitative difference one uses a different name in 3D: a Weyl cone for Weyl fermions.

(b) Calculate the eigenfunction u of the *lowest* energy band of H_{3D}, then find the Berry connection $\boldsymbol{A} = i\langle u|\partial/\partial\boldsymbol{p}|u\rangle$ and the Berry curvature $\boldsymbol{B} = (\partial/\partial\boldsymbol{p}) \times \boldsymbol{A}$. The result is

$$\boldsymbol{B} = \tfrac{1}{2}\frac{\boldsymbol{p}}{|\boldsymbol{p}|^3}. \tag{32}$$

This is the same vector field as the magnetic field of a monopole. One says that a Weyl point is a “monopole for Berry curvature”. The flux through a sphere enclosing the Weyl point is quantized at 2π.

(c) Explain that the Hamiltonian $-H_{3D}$ has a flux of Berry curvature equal to -2π in the *highest* energy band. The $\pm$ sign of the Berry curvature is called the chirality of the Weyl fermions. Can you explain why it is not possible to associate a chirality to H_{2D}?

On a lattice the Berry curvature should be a periodic function of momentum, so the net flux through the Brillouin zone should vanish and Weyl cones should appear in pairs of opposite chirality. A simple lattice model of a Weyl semimetal is

$$\begin{aligned} H(\boldsymbol{k}) &= t\sigma_x \sin ak_x + t\sigma_y \sin ak_y + m(\boldsymbol{k})\sigma_z, \\ m(\boldsymbol{k}) &= t(\cos\beta - \cos ak_z) + t'(2 - \cos ak_x - \cos ak_y). \end{aligned} \tag{33}$$

The momentum $\boldsymbol{k}$ varies over the Brillouin zone $|k_\alpha| < \pi/a$ of a simple cubic lattice.

(d) Show that $H(\boldsymbol{k})$ has two Weyl points of opposite chirality, at the momenta $\boldsymbol{k} = (0,0,\pm K)$.

In a finite system a surface state appears that connects the two Weyl points, a socalled “Fermi arc”. To see this, we take a slab geometry, unbounded in the y–z plane and confined in the x-direction between $x = 0$ and $x = W$. We impose the following boundary condition on the wave function ψ,

$$\sigma_y\psi = \begin{cases} -\psi & \text{at } x = 0, \\ +\psi & \text{at } x = W. \end{cases} \tag{34}$$

This boundary condition corresponds to a mass term $m_0(x)\sigma_z$ in H that vanishes inside the slab and tends to $+\infty$ outside.

The Schrödinger equation $H\psi = E\psi$ can be solved analytically in the low-energy regime by linearizing in k_x and substituting $k_x \mapsto -i\partial/\partial x$. Integration of the resulting first-order differential equation in x gives

$$\psi(x) = e^{ix\Xi}\psi(0), \;\; \Xi = \frac{1}{t}\sigma_x[E - H(0,k_y,k_z)]. \tag{35}$$

To ensure that an eigenstate of H satisfies the boundary condition (34), we require that

$$\langle -|e^{iW\Xi}|-\rangle = 0, \;\; |\pm\rangle = \begin{pmatrix} 1 \\ \pm i \end{pmatrix}, \;\; \sigma_y|\pm\rangle = \pm|\pm\rangle. \tag{36}$$

(e) Show that this procedure gives the following dispersion relation for $E(k_y, k_z)$:

$$E^2 - t^2 \sin^2 ak_y - m(0,k_y,k_z)^2 = q^2, \tag{37}$$

with transverse wave number q given by

$$\frac{m(0,k_y,k_z)}{q}\tan(Wq/t) + 1 = 0. \tag{38}$$

Can you plot the dispersion relation? For example, plot E as a function of k_z for $k_y = 0.01$, for parameters $W = 40$, $\beta = 1.5$, $a = t = t' = 1$. (On Mathematica I use the command `ContourPlot` for that purpose.)

(f) The Fermi arcs have a purely imaginary $q = im$. Show that this solves Eq. (38) in the large-W limit if $m < 0$. The corresponding dispersion relation is

$$E_{\text{Fermi arc}} = \pm t \sin ak_y, \;\; |k_z| < \beta. \tag{39}$$

The $\pm$ sign distinguishes the Fermi arcs on opposite surfaces ($-$ at $x = 0$ and $+$ at $x = W$). Draw the trajectory along the surface of the slab of an electron in a Fermi arc state.

(g) Consider a single Weyl cone in a magnetic field, say in the z-direction. The Hamiltonian is

$$H_{3D} = vp_x\sigma_x + v(p_y + eBx)\sigma_y + vp_z\sigma_z. \tag{40}$$

Recall from exercise 5 that for $p_z = 0$ this Hamiltonian has a nondegenerate Landau level at $E = 0$. Why must this state be an eigenstate of σ_z? Plot the dispersion relation $E(p_z)$ of this zeroth Landau level.

(g) Take a look at `http://www.condmatjclub.org/uploads/2015/05/JCCM_MAY_2015_03.pdf` and explain what is meant by the *chiral magnetic effect* in a Weyl semimetal.

8 Symmetry classification: *ten-fold way, topological invariants*

We can classify the Hamiltonian based on the presence or absence of time-reversal symmetry (T) and particle-hole symmetry (P). This classification is known as the "ten-fold way", because it turns out there are 10 classes if we also distinguish $T^2 = \pm 1$ and $P^2 = \pm 1$.

(a) A first count only gives 9 classes: For T and P we have 3 possibilities each (no symmetry or a symmetry squaring to $+1$ or -1), and $3 \times 3 = 9$. Do you have an idea where the 10th class comes from? *Hint: consider the product PT.*

(b) How would you classify the SSH chain and how the Kitaev chain? What about the quantum Hall effect and the quantum spin Hall effect?

In a wire geometry a topologically nontrivial phase is characterized by the presence of zero-modes at the end points of the wire. The number Q of zero-modes at one end point is a topological invariant. This number can be associated with an *algebraic* invariant of the reflection matrix r for waves incident at zero energy on one end of the wire. Assuming that the wire is gapped inside, and is sufficiently long, there will be no transmission to the other end, so the reflection matrix is unitary.

(c) If the wire is a Kitaev chain, the particle-hole symmetry relation (30) requires that

$$r = \tau_x r^* \tau_x. \tag{41}$$

In the Kitaev chain the matrix r is 2×2, but this relation holds more generally for higher-dimensional matrices.
Prove that the determinant of r equals ± 1. We thus obtain the $\mathbb{Z}_2$ topological invariant $Q = \det r$. Which of the two values ± 1 do you think signals the presence of a Majorana zero-mode?

(d) If the wire is an SSH chain, the combination of time-reversal symmetry and chiral symmetry requires that

$$r = \sigma_z r^\dagger \sigma_z. \tag{42}$$

Again, this relation holds for any dimension of r.
Prove that this implies that the trace of $\sigma_z r$ is equal to an integer. We thus obtain the $\mathbb{Z}$ topological invariant $Q = \mathrm{tr}\,\sigma_z r$.

(e) There exists a third algebraic invariant, known as the Pfaffian, which is the signed square root of the determinant of an antisymmetric matrix. Which combination of symmetries might allow for the Pfaffian to be a topological invariant?

9 Topological quantum computation: *Majorana qubits, braiding*

Moore & Moessner: *box 5.2, chapter 9.7*

Recall from section 6 that Majorana operators γ_n are Hermitian operators ($\gamma_n = \gamma_n^\dagger$) which satisfy the anticommutation relation

$$\{\gamma_n, \gamma_m\} \equiv \gamma_n\gamma_m + \gamma_m\gamma_n = 2\delta_{nm}. \tag{43}$$

From four Majorana operators $\gamma_1, \gamma_2, \gamma_3, \gamma_4$ we can construct a pair of Dirac operators

$$a_1 = \frac{\gamma_1 + i\gamma_2}{2}, \;\; a_2 = \frac{\gamma_3 + i\gamma_4}{2}. \tag{44}$$

These satisfy the usual fermion anticommutation relations

$$\{a_n, a_m^\dagger\} = \delta_{nm}. \tag{45}$$

(a) Explain why the *most general* Hermitian operator that couples Majoranas n and m equals a constant times $i\gamma_n\gamma_m$.
(b) Check that the operator

$$\mathscr{P}_{nm} = i\gamma_n\gamma_m \tag{46}$$

has eigenvalues ± 1. Why is this quantum number called "fermion parity"?

We denote by $|s, s\rangle$, $s, s' \in \{0, 1\}$, an eigenstate of $\mathscr{P}_{12}$ and $\mathscr{P}_{34}$ with eigenvalues $(-1)^s$ and $(-1)^{s'}$, respectively.

(c) Explain why transitions are forbidden between states with different $s + s'$ modulo 2.
Hint: Consider the global fermion parity operator $\mathscr{P}_{12}\mathscr{P}_{34}$.

(d) The two states $|0\rangle \equiv |0, 0\rangle$ and $|1\rangle \equiv |1, 1\rangle$ define a bit of quantum information stored in a pair of Majorana zero-modes; one speaks of a *Majorana qubit*. Show that the NOT operation σ_x (being the Pauli matrix that interchanges $|0\rangle$ and $|1\rangle$) is obtained by

$$\sigma_x = -i\gamma_2\gamma_3. \tag{47}$$

The other Pauli matrices can be obtained similarly by coupling other pairs of Majoranas,

$\sigma_y = i\gamma_1\gamma_3$, $\sigma_z = -i\gamma_1\gamma_2$.

The exchange of Majoranas 1 and 2 transforms $\gamma_1 \mapsto e^{i\alpha}\gamma_2$, $\gamma_2 \mapsto e^{i\beta}\gamma_1$. To maintain Hermitian operators the phases α, β are restricted by $\alpha, \beta \in \{0, \pi\}$.

(e) Conservation of fermion parity requires that the operator $\mathscr{P}_{12}$ remains unchanged. Argue that this requires either $\alpha = 0, \beta = \pi$ or $\alpha = \pi, \beta = 0$.
(f) Assume $\alpha = 0$, $\beta = \pi$. Show that the exchange is a unitary transformation $\gamma_n \mapsto U^\dagger\gamma_n U$ with

$$U = \frac{1}{\sqrt{2}}(1 + \gamma_1\gamma_2). \tag{48}$$

(g) Check that U can also be written as

$$U = e^{i(\pi/4)\sigma_z}, \tag{49}$$

which has the form of a $\pi/2$ rotation of the qubit around the z-axis on the Bloch sphere. Rotations by $\pi/2$ around other axes can be obtained by exchanging other pairs of Majoranas. These operations are called *topological* because the angle of rotation is exactly $\pi/2$, irrespective of the details of the exchange operation (which is called *braiding*). If one repeats the entire braiding operation, the Majoranas 1 and 2 have returned to their original positions but the final state differs from the initial state by a unitary operator and not just by a phase factor. That is called *non-Abelian statistics*.