

NOTES

IMPERIAL COLLEGE LONDON

DEPARTMENT OF PHYSICS

Quantum Theory of Matter

Author:

Chen Huang

Email:

chen.huang23@imperial.ac.uk

Date: June 3, 2024

Contents

1	Geometry phase	4
1.1	Adiabatic quantum dynamics	4
1.1.1	Berry connection in the adiabatic limit	4
1.1.2	Example: two-level system	5
1.2	Berry curvature	6
1.2.1	Gauge degree of freedom	6
1.2.2	Two-level system revisited	7
2	Electron bands	9
2.1	Bloch's theorem	9
2.2	*Nearly free electron model	9
2.3	Tight binding model	9
2.3.1	Tight binding Hamiltonian	10
2.3.2	Energy eigenstates	10
3	Tight binding chains	11
3.1	Number and current on a lattice	11
3.2	Variations on a chain	12
3.2.1	Alternating chain	12
3.2.2	Sublattice symmetry	13
3.3	Polyacetylene and Peierls instability	14
4	Edge states on chains	17
4.1	Semi-infinite SSH chains	17
4.1.1	Fully dimerized limit	17
4.1.2	Away from isolated dimers	18
4.1.3	Exact solution for the edge state of a semi-infinite chain	18
4.1.4	Finite chains	19
4.2	Topological protection of the edge state	19
5	Adiabatic transport	21
5.1	Adiabatic cycle on a dimerized chain	21
5.1.1	Rice-Mele model	21
5.1.2	Charge pump cycle	22
5.2	Quasi-adiabatic regime	23
5.3	Thouless adiabatic current	24
5.4	First Chern number	25
6	Electrons in a vector potential	26
6.1	Gauge choice in electromagnetic	26
6.2	Current in a vector potential	27
6.3	Aharonov-Bohm effect	27
6.3.1	Adiabatic derivation	27
6.3.2	Aharonov-Bohm interferometry	29

7	Electrons in a magnetic field	30
7.1	Electrons in a uniform magnetic field	30
7.2	Classical Hall effect	31
7.3	Integer quantum Hall effect	33
7.3.1	Landau levels in an electric field	33
7.3.2	Edge states	34
7.3.3	Laughlin's gauge argument: adiabatic transport	34
7.4	Kubo formula	35
7.4.1	Linear response theory	35
7.4.2	Conductivity as linear response	36
8	Carbon and carbon allotropes	37
8.1	The carbon atom	37
8.2	Hybridization and the structure of carbon allotropes	37
8.3	Crystallography of Graphene	38
9	Electronic states in graphene	39
9.1	The tight-binding method	39
9.2	Tight-binding formulation for graphene	40
9.2.1	Nearest-neighbour approximation	41
9.2.2	Energy bands of graphene	43
9.3	Low-energy dispersion and the Dirac equation	43
9.4	Pseudospin and chirality	44
10	Symmetries of electronic states	47
10.1	Symmetry in quantum mechanics	47
10.1.1	Unitary transformations	47
10.1.2	Symmetries of Hamiltonians	47
10.2	Parity in quantum mechanics	48
10.2.1	Coordinate and momentum eigenstates	48
10.2.2	Operators under parity	48
10.2.3	Commutation with a Hamiltonian	49
10.3	Time-reversal	49
10.3.1	Time-reversal in classical mechanics	49
10.3.2	Time-reversal in quantum mechanics	50
10.3.3	More general	51
10.3.4	Anti-unitary operator	52
10.3.5	Transformations of operators	53
10.3.6	Time-reversed with spin: Kramers' degeneracy	53
10.4	Symmetries of Hamiltonians	54
10.4.1	Parity and time-reversal symmetry	55
10.4.2	Lattice symmetry	56
10.4.3	Symmetry breaking	56

11 Topological materials	57
11.1 Topology and topological invariant	57
11.1.1 The Gauss-Bonnet theorem	57
11.2 Topological band theory	57
11.2.1 Two-level systems	58
11.3 Spin-orbit interaction	59
11.4 The Kane-Mele Model	59
11.5 Edge states	60
11.5.1 States at zero energy	60
11.5.2 States at non-zero energy	61
11.6 Topological character of Kane-Mele model	61

1 Geometry phase

In this chapter, we explore how quantum systems behave when they experience slow changes, a situation referred to as the **adiabatic regime**. We'll unpack two key ideas that emerge from the geometric or Berry phase: the Berry connection and the Berry curvature. To make these concepts more tangible, we will look at a straightforward example: a two-level system, like an electron with spin-half, in the presence of a magnetic field.

1.1 Adiabatic quantum dynamics

1.1.1 Berry connection in the adiabatic limit

Consider the Hamiltonian \hat{H} with parameter \mathbf{R} . The system has a discrete set of energy eigenstates, labelled by ν , then

$$\hat{H}(\mathbf{R}) |\nu, \mathbf{R}\rangle = E_\nu(\mathbf{R}) |\nu, \mathbf{R}\rangle. \quad (1)$$

Consider the slow variation in $\mathbf{R}(t)$ in time t , system prepared in state ν stays in state ν in the adiabatic regime, that is, $|\nu, \mathbf{R} + \delta\mathbf{R}\rangle \simeq |\nu, \mathbf{R}\rangle$. The eigenstates $|\nu, \mathbf{R}(t)\rangle$ are defined as **instantaneous eigenstates** at time t .

We prepare the system in an eigenstate $|\psi(t=0)\rangle = |\nu, \mathbf{R}(t=0)\rangle$. The wavefunction $|\psi\rangle$ obeys the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(\mathbf{R}(t)) |\psi(t)\rangle. \quad (2)$$

For a constant parameter \mathbf{R} , we have $|\psi(t)\rangle = \exp(-\frac{i}{\hbar} E_\nu(\mathbf{R})t) |\nu, \mathbf{R}\rangle$. So we try

$$|\psi(t)\rangle = \exp\left(-\frac{i}{\hbar} \int_0^t E_\nu(\mathbf{R}(t')) dt'\right) |\nu, \mathbf{R}(t=0)\rangle, \quad (3)$$

and we also guess $|\psi(t)\rangle$ in the adiabatic limit to be the form

$$|\psi(t)\rangle \simeq e^{i\gamma_\nu(t)} |\nu, \mathbf{R}(t)\rangle, \quad (4)$$

where $e^{i\gamma_\nu(t)}$ is a phase factor of modulus unity at all times. We substitute the form Eq.(4) into both sides of the Schrödinger equation Eq.(2):

$$\text{LHS} = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = e^{i\gamma_\nu(t)} \left(-\hbar\dot{\gamma}_\nu(t) + i\hbar\dot{\mathbf{R}}(t) \cdot \nabla_{\mathbf{R}} \right) |\nu, \mathbf{R}(t)\rangle, \quad (5)$$

$$\text{RHS} = \hat{H}(\mathbf{R}(t)) |\psi(t)\rangle = e^{i\gamma_\nu(t)} E_\nu(\mathbf{R}(t)) |\nu, \mathbf{R}(t)\rangle. \quad (6)$$

Then we have

$$E_\nu(\mathbf{R}(t)) |\nu, \mathbf{R}(t)\rangle = \left(-\hbar\dot{\gamma}_\nu + i\hbar\dot{\mathbf{R}} \cdot \nabla_{\mathbf{R}} \right) |\nu, \mathbf{R}(t)\rangle. \quad (7)$$

Taking overlap with $\langle \nu, \mathbf{R} |$, then

$$E_\nu(\mathbf{R}(t)) = -\hbar\dot{\gamma}_\nu(t) + i\hbar\dot{\mathbf{R}}(t) \cdot \langle \nu, \mathbf{R}(t) | \nabla_{\mathbf{R}} | \nu, \mathbf{R}(t) \rangle. \quad (8)$$

Rearranging this equation and we get

$$\begin{aligned} \gamma_\nu(t) &= -\frac{1}{\hbar} \int_0^t E(\mathbf{R}(t')) dt' + i \int_0^t \langle \nu, \mathbf{R} | \nabla_{\mathbf{R}} | \nu, \mathbf{R} \rangle \cdot \frac{d\mathbf{R}}{dt'} dt' \\ &= -\frac{1}{\hbar} \int_0^t E(\mathbf{R}(t')) dt' + i \int_C \langle \nu, \mathbf{R} | \nabla_{\mathbf{R}} | \nu, \mathbf{R} \rangle \cdot d\mathbf{R} \\ &= \gamma_{\nu, \text{dyn}} + \gamma_{\nu, \text{geom}}, \end{aligned} \quad (9)$$

where C is the path in parameter space from $\mathbf{R}(0)$ to $\mathbf{R}(t)$. Here, we get two phases: the **dynamic phase** and the **geometric phase**.

$$\gamma_{\nu, \text{dyn}} = -\frac{1}{\hbar} \int_0^t E(\mathbf{R}(t')) dt', \quad (10)$$

$$\gamma_{\nu, \text{geom}} = i \int_C \langle \nu, \mathbf{R} | \nabla_{\mathbf{R}} | \nu, \mathbf{R} \rangle \cdot d\mathbf{R} = \int_C \mathbf{A}_\nu(\mathbf{R}) \cdot d\mathbf{R}. \quad (11)$$

We know that $e^{i\gamma}$ is a phase factor of modulus unity at all times, which means $\langle \nu | \nabla_{\mathbf{R}} \nu \rangle$ should be purely imaginary ($\mathbf{A}_\nu(\mathbf{R})$ is purely real). Now we prove this property:

$$\nabla_{\mathbf{R}} \langle \nu, \mathbf{R} | \nu, \mathbf{R} \rangle = \langle \nabla_{\mathbf{R}} \nu | \nu \rangle + \langle \nu | \nabla_{\mathbf{R}} \nu \rangle = \langle \nu | \nabla_{\mathbf{R}} \nu \rangle^* + \langle \nu | \nabla_{\mathbf{R}} \nu \rangle = 0. \quad (12)$$

The quantity $\mathbf{A}_\nu(\mathbf{R})$ here is called **Berry connection**:

$$\mathbf{A}_\nu(\mathbf{R}) = i \langle \nu, \mathbf{R} | \nabla_{\mathbf{R}} | \nu, \mathbf{R} \rangle = -\text{Im} \langle \nu, \mathbf{R} | \nabla_{\mathbf{R}} | \nu, \mathbf{R} \rangle. \quad (13)$$

1.1.2 Example: two-level system

Consider a particle with spin $S = 1/2$ as an analogy for a two-level system. The spin in a Zeeman field with the Hamiltonian

$$\hat{H} = \mathbf{d}(t) \cdot \hat{\boldsymbol{\sigma}} = d_x \hat{\sigma}_x + d_y \hat{\sigma}_y + d_z \hat{\sigma}_z = \begin{pmatrix} d_z & d_x - id_y \\ d_x + id_y & -d_z \end{pmatrix}, \quad (14)$$

where $\mathbf{d} = (d_x, d_y, d_z) = d(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$. It shows that

$$\hat{H} = d \begin{pmatrix} \cos \theta & e^{-i\phi} \sin \theta \\ e^{i\phi} \sin \theta & -\cos \theta \end{pmatrix}. \quad (15)$$

The eigenvalues of \hat{H} are $\pm d$. Suppose the magnetic field rotates by 2π and $\phi(t) = 2\pi t/T$. d and θ are constants when the system evolves from $t = 0$ to $t = T$. The instantaneous eigenstates at given ϕ are denoted as $|\pm, \phi\rangle$:

$$E_+ = +d, \quad |+, \phi\rangle = e^{-i\phi} \cos(\theta/2) |\uparrow\rangle + \sin(\theta/2) |\downarrow\rangle, \quad (16)$$

$$E_- = -d, \quad |-, \phi\rangle = e^{-i\phi} \sin(\theta/2) |\uparrow\rangle - \cos(\theta/2) |\downarrow\rangle. \quad (17)$$

If we prepare the system in the state $|+\rangle$, after one full 2π -rotation of \mathbf{d} , the phases are

$$\gamma_{+, \text{dyn}} = -\frac{1}{\hbar} \int_0^T E_+ dt = -\frac{d}{\hbar} T, \quad (18)$$

$$\gamma_{+, \text{geom}} = i \int_0^{2\pi} \langle +, \phi | \partial_\phi | +, \phi \rangle d\phi = i \int_0^{2\pi} (-i) \cos^2(\theta/2) d\phi = \pi(1 + \cos \theta). \quad (19)$$

Similarly, if we prepare the system in the state $|-\rangle$, after one full 2π -rotation of \mathbf{d} , the phases are

$$\gamma_{-, \text{dyn}} = -\frac{1}{\hbar} \int_0^T E_- dt = \frac{d}{\hbar} T, \quad (20)$$

$$\gamma_{-, \text{geom}} = i \int_0^{2\pi} \langle -, \phi | \partial_\phi | -, \phi \rangle d\phi = i \int_0^{2\pi} (-i) \sin^2(\theta/2) d\phi = \pi(1 - \cos \theta). \quad (21)$$

The Berry phase $\gamma_{\nu, \text{geom}}$ depends on how the instantaneous eigenstates $|\nu, \mathbf{R}\rangle$ are defined. If we choose $\hat{\sigma}_z$ as the quantization axis, i.e., $\theta = \pi/2$. So the geometric phase of $|\pm\rangle$ is $\gamma_{\pm, \text{geom}} = \pi$.

1.2 Berry curvature

1.2.1 Gauge degree of freedom

The instantaneous eigenstates $|\nu, \mathbf{R}\rangle$ are chosen to be single-valued and differentiable. If we change instantaneous eigenstates by a single-valued, differentiable phase factor $e^{i\chi(\mathbf{R})}$:

$$|\nu, \mathbf{R}\rangle \rightarrow e^{i\chi(\mathbf{R})} |\nu, \mathbf{R}\rangle. \quad (22)$$

We call the choice of $\chi(\mathbf{R})$ a **gauge choice**. Then we find the Berry connection $\mathbf{A}_\nu(\mathbf{R})$ will be changed as well

$$\begin{aligned} \mathbf{A}_\nu(\mathbf{R}) &= i \langle \nu, \mathbf{R} | \nabla_{\mathbf{R}} | \nu, \mathbf{R} \rangle \rightarrow i \langle \nu, \mathbf{R} | e^{-i\chi(\mathbf{R})} \nabla_{\mathbf{R}} e^{i\chi(\mathbf{R})} | \nu, \mathbf{R} \rangle \\ &= i \langle \nu, \mathbf{R} | (i \nabla_{\mathbf{R}} \chi + \nabla_{\mathbf{R}}) | \nu, \mathbf{R} \rangle \\ &= \mathbf{A}_\nu(\mathbf{R}) - \nabla_{\mathbf{R}} \chi(\mathbf{R}). \end{aligned} \quad (23)$$

For a closed path C over parameter space, the geometry phase becomes

$$\gamma_{\text{geom}} = \oint_C \mathbf{A}_\nu(\mathbf{R}) \cdot d\mathbf{R} \rightarrow \oint_C \mathbf{A}_\nu(\mathbf{R}) \cdot d\mathbf{R} - [\chi(\mathbf{R}(T)) - \chi(\mathbf{R}(0))]. \quad (24)$$

$\Delta\chi=2\pi n$

Therefore, as the geometric phase $\gamma_{\nu, \text{geom}}$ changes, the geometric phase factor $e^{i\gamma_{\nu, \text{geom}}}$ is gauge-invariant.

We can then learn from the magnetic analogy where \mathbf{A}_ν is a vector potential - the magnetic flux density $\mathbf{B} = \nabla \times \mathbf{A}$ is gauge invariant. Similarly, we can define

$$\mathbf{B}_\nu = \nabla_{\mathbf{R}} \times \mathbf{A}_\nu(\mathbf{R}) \quad (25)$$

as a gauge invariant. This is called the **Berry curvature**. By using the Einstein summation convention

$$B_i = \varepsilon_{ijk} \partial_j A_k = i \varepsilon_{ijk} \partial_j \langle \nu | \partial_k \nu \rangle = i \varepsilon_{ijk} (\langle \partial_j \nu | \partial_k \nu \rangle + \langle \nu | \partial_j \partial_k \nu \rangle) = i \varepsilon_{ijk} \langle \partial_j \nu | \partial_k \nu \rangle, \quad (26)$$

the Berry curvature can be expressed as

$$\mathbf{B}_\nu = i \langle \nabla_{\mathbf{R}} \nu | \times | \nabla_{\mathbf{R}} \nu \rangle. \quad (27)$$

Now we use non-degenerate perturbation theory to find $| \nabla_{\mathbf{R}} \nu \rangle$. Consider a small variation $\delta \mathbf{R}$

$$\begin{aligned} |\nu, \mathbf{R} + \delta \mathbf{R}\rangle &\simeq |\nu, \mathbf{R}\rangle + \delta \mathbf{R} \cdot \sum_{\mu \neq \nu} |\mu, \mathbf{R}\rangle \frac{\langle \mu, \mathbf{R} | (\nabla_{\mathbf{R}} \hat{H}) | \nu, \mathbf{R} \rangle}{E_\nu(\mathbf{R}) - E_\mu(\mathbf{R})} \\ &= |\nu, \mathbf{R}\rangle + \delta \mathbf{R} \cdot \nabla_{\mathbf{R}} |\nu, \mathbf{R}\rangle. \end{aligned} \quad (28)$$

Then we have

$$| \nabla_{\mathbf{R}} \nu \rangle = \sum_{\mu \neq \nu} |\mu, \mathbf{R}\rangle \frac{\langle \mu, \mathbf{R} | (\nabla_{\mathbf{R}} \hat{H}) | \nu, \mathbf{R} \rangle}{E_\nu(\mathbf{R}) - E_\mu(\mathbf{R})}. \quad (29)$$

Therefore, the Berry curvature can also be expressed as

$$\mathbf{B}_\nu = i \sum_{\mu \neq \nu} \frac{\langle \nu | (\nabla_{\mathbf{R}} \hat{H}) | \mu \rangle \times \langle \mu | (\nabla_{\mathbf{R}} \hat{H}) | \nu \rangle}{(E_\nu(\mathbf{R}) - E_\mu(\mathbf{R}))^2}. \quad (30)$$

It should be noted that

$$\mathbf{B}_\nu = \nabla_{\mathbf{R}} \times \mathbf{A}_\nu \quad \leftrightarrow \quad \oint_C \mathbf{A}_\nu \cdot d\mathbf{R} = \int_D \mathbf{B}_\nu \cdot d\mathbf{S}, \quad (31)$$

where D is a surface constructed by the closed contour C . The geometry phase can also be expressed as

$$\gamma_{\nu, \text{geom}} = \oint_C \mathbf{A}_\nu \cdot d\mathbf{R} = \int_D \mathbf{B}_\nu \cdot d\mathbf{S}. \quad (32)$$

1.2.2 Two-level system revisited

Recall the situation that a spin-half electron in a magnetic field \mathbf{d} we just discussed in the Sec. 1.1.2, the Zeeman Hamiltonian is

$$\hat{H} = \mathbf{d} \cdot \hat{\boldsymbol{\sigma}}, \quad (33)$$

which associate with the eigenfunctions

$$\hat{H} |\pm, \mathbf{d}\rangle = \pm |\mathbf{d}| |\pm, \mathbf{d}\rangle, \quad (34)$$

where $|\pm, \mathbf{d}\rangle$ is the eigenstates of \hat{H} . So the Berry curvature

$$\mathbf{B}_+ = i \frac{\langle + | \boldsymbol{\sigma} | - \rangle \times \langle - | \boldsymbol{\sigma} | + \rangle}{2|\mathbf{d}|^2}. \quad (35)$$

If we choose \hat{e}_z as quantisation axis, i.e., $\mathbf{d} \parallel (0, 0, 1)$. Then the Berry curvature becomes

$$\begin{aligned} \mathbf{B}_+ &= i \frac{\langle + | \hat{\sigma}_1 | - \rangle (\mathbf{e}_1 \times \mathbf{e}_2) \langle - | \hat{\sigma}_2 | + \rangle}{(2d)^2} - (1 \leftrightarrow 2) \\ &= i \frac{\langle + | \hat{\sigma}_1 | - \rangle \langle - | \hat{\sigma}_2 | + \rangle - \langle + | \hat{\sigma}_2 | - \rangle \langle - | \hat{\sigma}_1 | + \rangle}{(2d)^2} \hat{e}_3 = -\frac{\mathbf{d}}{2|\mathbf{d}|^3}. \end{aligned} \quad (36)$$

Then we calculate the geometry phase. If we choose the hemisphere of radius d that the value of Barry curvature is a constant, then

$$\int_D \mathbf{B}_+ \cdot d\mathbf{S} = -\frac{1}{2d^2} 2\pi d^2 = -\pi. \quad (37)$$

We can add a phase 2π , i.e., $\gamma_{+, \text{geom}} = (-\pi) + 2\pi = \pi$ so that the geometry phase is single-values.

Recall that the energy levels are $\pm|\mathbf{d}|$. At $\mathbf{d} = 0$, there is no field and the two spin states are degenerate in energy. In other words, the origin is special because the system has a degeneracy there. In general, this degeneracy appears as a result of fine-tuning all three parameters instead of as a consequence of a symmetry. This is sometimes called an ‘‘accidental degeneracy’’. The **degenerate point** in parameter space is also called a diabolical point.

The geometric phase factor for a closed loop C in the parameter space of a two-level system is

$$\exp[i\gamma_{\pm, \text{geom}}(C)] = \exp\left[\mp \frac{i}{2} \Omega(C)\right] \quad (38)$$

where $\Omega(C)$ is the solid angle subtended by the loop C at the degeneracy point in parameter space.

2 Electron bands

In this chapter, we talk about the Bloch's theorem. Then we introduce two models about electrons in solid: nearly free electron model (electrons in a weak periodic potential) and tight binding model (electrons in a strong periodic potential).

2.1 Bloch's theorem

Consider an electron in the presence of a crystalline array of positive nuclei at the lattice sites \mathbf{R} . It experiences a periodic potential V . The Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}), \quad V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r}) \text{ for any lattice vector } \mathbf{R}. \quad (39)$$

Bloch's theorem tells us that the electron eigenstates $\psi(\mathbf{r})$ are also periodic, except for a plane-wave phase factor when we go from one lattice site to another:

$$\psi_{\alpha\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{\alpha\mathbf{k}}(\mathbf{r}) \text{ for any lattice vector } \mathbf{R} \quad (\mathbf{k} \in \text{1st Brillouin zone}). \quad (40)$$

Given Bloch's result, it is natural to factor out the plane-wave part from $\psi_{\alpha\mathbf{k}}$. An equivalent statement of the theorem is that the eigenstates in a periodic potential can be written as:

$$\psi_{\alpha\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\phi_{\alpha\mathbf{k}}(\mathbf{r}) \quad \text{with} \quad \phi_{\alpha\mathbf{k}}(\mathbf{r}) = \phi_{\alpha\mathbf{k}}(\mathbf{r} + \mathbf{R}) \quad (\mathbf{k} \in \text{1st Brillouin zone}). \quad (41)$$

2.2 *Nearly free electron model

The nearly free electron model (NFE model) describes the behavior of electrons in metals and other conductive materials. This model is an extension of the free electron gas model, with modifications to account for the influence of the periodic potential of the lattice on electron motion. In the free electron model, electrons are assumed to move freely without any external forces, whereas in the NFE model, electrons mostly behave like free electrons but are subjected to slight scattering due to the periodic potential of the crystal lattice.

2.3 Tight binding model

The tight binding model describes the behavior of electrons in crystals, particularly effective for insulators and semiconductors. Unlike the NFE model, the tight binding model focuses on the strong coupling between atoms in the crystal.

The atom at lattice site \mathbf{R} will have several bound states, labelled by α . We can denote the state as $|\mathbf{R}, \alpha\rangle$. Instead of N degenerate states at energy ϵ_α , we have N delocalized eigenstates with a spread of eigenenergies centered at ϵ_α , forming an **energy band**, labelled by α .

2.3.1 Tight binding Hamiltonian

These site-localized states $|\mathbf{R}, \alpha\rangle$ are often called Fock states. Since the bound state label does not change in the hopping, we can consider each energy band separately and drop the α label: $|\mathbf{R}, \alpha\rangle \rightarrow |\mathbf{R}\rangle$. In this basis, we can write the electron state as

$$|\psi\rangle = \sum_{\mathbf{R}} c_{\mathbf{R}} |\mathbf{R}\rangle, \quad (42)$$

where $c_{\mathbf{R}}$ is the probability amplitude for finding the electron at site \mathbf{R} . If we only consider the interaction between the nearest-neighbour pairs, the Hamiltonian for the tight binding model is

$$\hat{H} = \epsilon_{\alpha} \sum_{\mathbf{R}} |\mathbf{R}\rangle \langle \mathbf{R}| - t_{\alpha} \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} (|\mathbf{R}\rangle \langle \mathbf{R}'| + |\mathbf{R}'\rangle \langle \mathbf{R}|), \quad (43)$$

where the sign $\langle \dots \rangle$ means that we are summing over all nearest-neighbour pairs, \mathbf{R} and \mathbf{R}' , on the lattice. ϵ_{α} is the on-site energy, or the bound-state energy. t_{α} is the hopping integral.

2.3.2 Energy eigenstates

If we apply the tight binding Hamiltonian to the electron state

$$\begin{aligned} \hat{H} |\psi\rangle &= \epsilon_{\alpha} \sum_{\mathbf{R}, \mathbf{S}} c_{\mathbf{R}} |\mathbf{S}\rangle \langle \mathbf{S} | \mathbf{R} \rangle - t_{\alpha} \sum_{\mathbf{R}, \langle \mathbf{S}, \mathbf{S}' \rangle} c_{\mathbf{R}} (|\mathbf{S}\rangle \langle \mathbf{S}' | \mathbf{R} \rangle + |\mathbf{S}'\rangle \langle \mathbf{S} | \mathbf{R} \rangle) \\ &= \epsilon_{\alpha} \sum_{\mathbf{S}} c_{\mathbf{S}} |\mathbf{S}\rangle - t_{\alpha} \sum_{\langle \mathbf{S}, \mathbf{S}' \rangle} (c_{\mathbf{S}'} |\mathbf{S}\rangle + c_{\mathbf{S}} |\mathbf{S}'\rangle). \end{aligned} \quad (44)$$

To see what happens at site \mathbf{R} , we take overlap of both sides with $\langle \mathbf{R} |$

$$\langle \mathbf{R} | \hat{H} |\psi\rangle = \epsilon_{\alpha} c_{\mathbf{R}} - t_{\alpha} \sum_{\langle \mathbf{S}, \mathbf{S}' \rangle} (c_{\mathbf{S}'} \delta_{\mathbf{R}, \mathbf{S}} + c_{\mathbf{S}} \delta_{\mathbf{R}, \mathbf{S}'}) = \epsilon_{\alpha} c_{\mathbf{R}} - t_{\alpha} \sum_{\delta} c_{\mathbf{R}+\delta}, \quad (45)$$

where the set of vectors δ contains all the vectors joining \mathbf{R} to its nearest neighbours. For an eigenstate with energy E , we must have $\langle \mathbf{R} | \hat{H} |\psi\rangle = E_{\alpha} \langle \mathbf{R} | \psi\rangle$, which gives

$$\epsilon_{\alpha} c_{\mathbf{R}} - t_{\alpha} \sum_{\delta} c_{\mathbf{R}+\delta} = E_{\alpha} c_{\mathbf{R}} \quad \text{for all sites } \mathbf{R}, \quad (46)$$

where $c_{\mathbf{R}} = e^{i\mathbf{k} \cdot \mathbf{R}}$. So the eigenvectors and eigenvalues can be expressed in terms of \mathbf{k} :

$$|\mathbf{k}, \alpha\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} |\mathbf{R}, \alpha\rangle, \quad E_{\alpha \mathbf{k}} = \epsilon_{\alpha} - t_{\alpha} \sum_{\delta} e^{i\mathbf{k} \cdot \delta} \quad (\mathbf{k} \in \text{1st Brillouin zone}). \quad (47)$$

The factor $1/\sqrt{N}$ in $|\mathbf{k}, \alpha\rangle$ is the normalization factor for N sites. For a 2D square lattice model with lattice spacing a , the energy spectrum is

$$E_{\alpha \mathbf{k}} = \epsilon_{\alpha} - 2t_{\alpha} [\cos(k_x a) + \cos(k_y a)]. \quad (48)$$

3 Tight binding chains

In this chapter, we talk about the alternating tight binding chains.

3.1 Number and current on a lattice

Let us consider an infinite one-dimensional (spinless) chain where an electron at site n can hop to nearest neighbours at $n \pm 1$. The Hamiltonian is given by

$$\hat{H} = - \sum_n v_n (|n\rangle \langle n+1| + |n+1\rangle \langle n|) \quad (49)$$

where v_n is the hopping integral for the link between site n and $n+1$. The **number operator** at site m is

$$\hat{n}_m = |m\rangle \langle m|. \quad (50)$$

The number of the electrons in the left block denoted as $\hat{N}_L = \sum_{n \leq n_L} |n\rangle \langle n|$. In terms of \hat{N}_L , using Ehrenfest theorem

$$\frac{\partial \langle \hat{N}_L \rangle}{\partial t} = \frac{i}{\hbar} \langle [\hat{H}, \hat{N}_L] \rangle = - \langle \hat{J}_{n_L} \rangle \quad (51)$$

where \hat{J} is the current operator for tight binding chains. To calculate the commutator, we can divide the Hamiltonian into three parts: $\hat{H} = \hat{H}_L + \hat{H}_R + \hat{H}_{LR}$, where \hat{H}_R involves links inside the right block only, \hat{H}_L involves links inside the left block only, and \hat{H}_{LR} contains the link joining the left and right blocks together. First of all, we calculate $[\hat{H}_L, \hat{N}_L]$:

$$\begin{aligned} [\hat{H}_L, \hat{N}_L] &= \sum_{n < n_L} v_n [|n\rangle \langle n+1|, \hat{N}_L] \\ &= \sum_{n < n_L} \sum_{m \leq n_L} v_n [|n\rangle \langle n+1|, |m\rangle \langle m|] \\ &= \sum_{n < n_L} \sum_{m \leq n_L} v_n (|n\rangle \langle n+1|m\rangle \langle m| - |m\rangle \langle m|n\rangle \langle n+1|) \\ &= \sum_{n < n_L} v_n (|n\rangle \langle n+1| - |n\rangle \langle n+1|) = 0. \end{aligned} \quad (52)$$

Similarly, we find that $[\hat{H}_R, \hat{N}_L] = [\hat{H}_L, \hat{N}_L] = 0$. Now we calculate $[\hat{H}_{LR}, \hat{N}_L]$, where $\hat{H}_{LR} = -v_{n_L} (|n_L\rangle \langle n_L+1| + |n_L+1\rangle \langle n_L|)$.

$$\begin{aligned} [|n_L\rangle \langle n_L+1|, \hat{N}_L] &= \sum_{m \leq n_L} (|n_L\rangle \langle n_L+1|m\rangle \langle m| - |m\rangle \langle m|n_L\rangle \langle n_L+1|) \\ &= - |n_L\rangle \langle n_L+1|, \end{aligned} \quad (53)$$

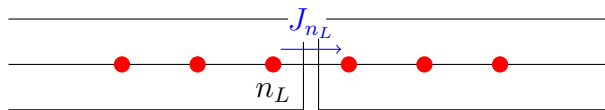


Figure 1: An infinite one-dimensional chain.

$$\begin{aligned}
[|n_L + 1\rangle \langle n_L|, \hat{N}_L] &= \sum_{m \leq n_L} (|n_L + 1\rangle \langle n_L| m\rangle \langle m| - |m\rangle \langle m| n_L + 1\rangle \langle n_L|) \\
&= |n_L + 1\rangle \langle n_L|.
\end{aligned} \tag{54}$$

So the commutator is

$$[\hat{H}, \hat{N}_L] = [\hat{H}_{LR}, \hat{N}_L] = -v_{n_L} (|n_L + 1\rangle \langle n_L| - |n_L\rangle \langle n_L + 1|), \tag{55}$$

and the current operator is given by

$$\hat{J}_n = \frac{i}{\hbar} v_n (|n + 1\rangle \langle n| - |n\rangle \langle n + 1|). \tag{56}$$

If we choose the Bloch state $|\psi_k\rangle = \frac{1}{\sqrt{N}} \sum_m e^{ikma} |m\rangle$, the current due to each Bloch state is

$$\begin{aligned}
\langle \psi_k | \hat{J}_n | \psi_k \rangle &= \frac{iv_n}{\hbar N} \sum_{m, m'} e^{ik(m-m')a} \langle m' | (|n + 1\rangle \langle n| - |n\rangle \langle n + 1|) | m \rangle \\
&= \frac{iv_n}{\hbar N} (e^{-ika} - e^{ika}) = \frac{2v_n}{\hbar N} \sin(ka) \\
&= \frac{1}{Na} \times \frac{2v_n a}{\hbar} \sin(ka).
\end{aligned} \tag{57}$$

number density
group velocity

We see that the group velocity here is consistent with the group velocity as defined from the dispersion relation: $v_g = \partial E_k / \partial(\hbar k)$ where $E_k = -2v_n \cos(ka)$ is the energy of the eigenstate $|\psi_k\rangle$.

3.2 Variations on a chain

3.2.1 Alternating chain

Now, let's discuss the tight binding chain with alternating hoppings v and w . The unit cell labelled by n , and there are two sites A and B per unit cell. The on-site electron states are denoted as $|n, A\rangle$ and $|n, B\rangle$. The Hamiltonian is given by

$$\hat{H}_{\text{alt}} = - \sum_n [v(|n, A\rangle \langle n, B| + \text{h.c.}) + w(|n, B\rangle \langle n + 1, A| + \text{h.c.})]. \tag{58}$$

The eigenstate is given by

$$|\psi_k\rangle = \sum_n (c_{n,A} |n, A\rangle + c_{n,B} |n, B\rangle), \tag{59}$$

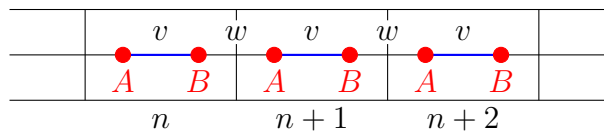


Figure 2: An one-dimensional alternating chain.

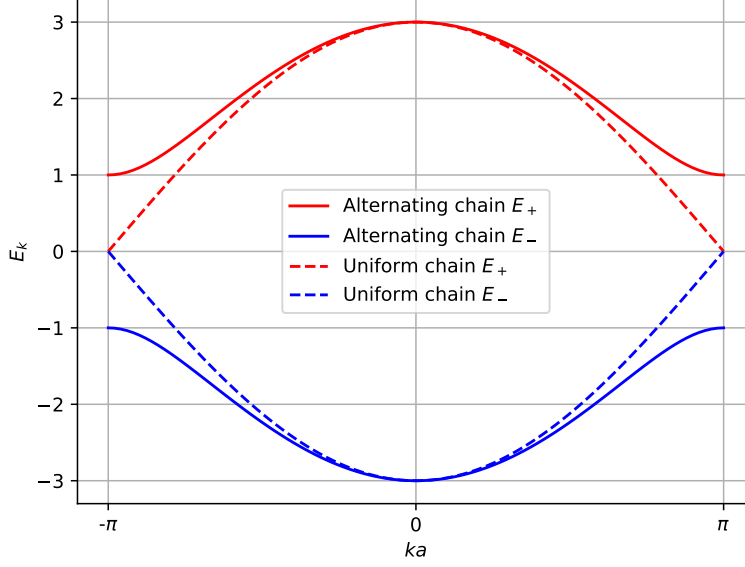


Figure 3: Energy spectrum for a tight binding chain. The dashed line corresponds to an uniform chain with hopping integral $t = 1.5$. The solid line corresponds to an alternating chain with hopping integrals $v = 1.0$ and $w = 2.0$. This has a band gap of $2|v - w| = 2.0$.

where $c_{n,A} = c_A e^{ikna}$ and $c_{n,B} = c_B e^{ikna}$ due to the Bloch theorem. The Schrödinger equation $\hat{H}_{\text{alt}} |\psi\rangle = E |\psi\rangle$ gives

$$E c_{n,A} = -w c_{n-1,B} - v c_{n,B}, \quad (60)$$

$$E c_{n,B} = -w c_{n+1,A} - v c_{n,A}, \quad (61)$$

which equivalent to

$$-\begin{pmatrix} 0 & v + w e^{-ika} \\ v + w e^{ika} & 0 \end{pmatrix} \begin{pmatrix} c_A \\ c_B \end{pmatrix} = h_k \begin{pmatrix} c_A \\ c_B \end{pmatrix} = E \begin{pmatrix} c_A \\ c_B \end{pmatrix}. \quad (62)$$

Then $\det(h_k - E\mathbb{1}) = 0$ gives the energy spectrum

$$E_k = \pm \sqrt{v^2 + w^2 + 2vw \cos ka} = \pm \sqrt{(v - w)^2 + 4vw \cos^2 \left(\frac{ka}{2} \right)}, \quad (63)$$

with k in the first Brillouin zone, i.e., $-\pi/a < k \leq \pi/a$. For an uniform chain, we have $v = w = t$, then the band energy

$$E_k = \pm 2t \cos(ka/2). \quad (64)$$

3.2.2 Sublattice symmetry

The dispersion relations of the two energy bands of the alternating chain are exactly symmetric under reflection on the $E = 0$ axis. This property is called **bipartite**.

The important ingredients are that the two sites have the same on-site energy (zero in this case) and that the Hamiltonian only connects sites of different sublattices. Let us call this the **sublattice symmetry**. A general Hamiltonian that possesses this property is

$$\hat{H}_{\text{sym}} = - \sum_{m,n} (t_{mn} |m, A\rangle \langle n, B| + t_{nm} |n, B\rangle \langle m, A|), \quad (65)$$

with $t_{nm} = t_{mn}^*$ for a Hermitian Hamiltonian. Let an eigenstate at energy E be

$$|\psi\rangle = \sum_n (c_{n,A} |n, A\rangle + c_{n,B} |n, B\rangle). \quad (66)$$

Substituting this into the Hamiltonian and solving for $\hat{H}_{\text{sym}} |\psi\rangle = E |\psi\rangle$ gives

$$- \sum_m t_{nm} c_{m,B} = E c_{n,A}, \quad - \sum_n t_{nm} c_{m,A} = E c_{n,B}. \quad (67)$$

If we change the sign on every other site, i.e., $\tilde{c}_{n,A} = c_{n,A}$ and $\tilde{c}_{n,B} = -c_{n,B}$, then the new state is

$$|\tilde{\psi}\rangle = \sum_n (\tilde{c}_{n,A} |n, A\rangle + \tilde{c}_{n,B} |n, B\rangle) = \sum_n (c_{n,A} |n, A\rangle - c_{n,B} |n, B\rangle) \quad (68)$$

is also an eigenstate with energy $-E$. This proves that the energy spectrum of \hat{H}_{sym} has reflection symmetry in $E = 0$ for a hopping Hamiltonian that only hops between sites in different sublattices.

More formally, we have performed a transformation $|\psi\rangle \rightarrow \hat{\Gamma} |\tilde{\psi}\rangle$. The symmetry operator $\hat{\Gamma}$ performs $\hat{\Gamma} |n, A\rangle = |n, A\rangle$ and $\hat{\Gamma} |n, B\rangle = -|n, B\rangle$. So the symmetry operator can be expressed as

$$\hat{\Gamma} = \sum_n (|n, A\rangle \langle n, A| - |n, B\rangle \langle n, B|), \quad (69)$$

and we also find

$$\hat{H}'_{\text{sym}} = \hat{\Gamma} \hat{H}_{\text{sym}} \hat{\Gamma} = -\hat{H}. \quad (70)$$

This property is named **chiral symmetry**.

3.3 Polyacetylene and Peierls instability

Consider the structure of polyacetylene in Fig. 4, the structural change to alternating bond lengths is called “**dimerization**” because each unit cell now contains a dimer of carbon atoms.

Recall the tight binding model, we expect the hopping integral between two sites at x and x' to decay exponentially with the distance between the sites: $t \propto e^{-|x-x'|/x_t}$ where x_t is a length scale determined by the microscopic atomic physics. If we move the sites towards / away from each other by a distance $u = \delta x_t$, the hopping should strengthen / weaken. We expect the strong (v) and weak (w) hopping integrals to be:

$$v(\delta) = te^{u/x_t} = te^\delta \simeq t(1 + \delta), \quad w(\delta) = te^{-u/x_t} = te^{-\delta} \simeq t(1 - \delta). \quad (71)$$

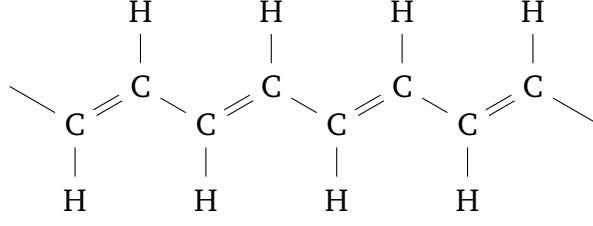


Figure 4: The structure of polyacetylen.

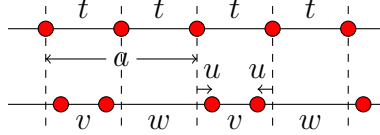


Figure 5: An alternating chain is created by displacing the A and B sites by distances u and $-u$ respectively from their positions in a uniform chain.

Then the energy spectrum

$$\begin{aligned}
 E_k(\delta) &= \pm \sqrt{v^2 + w^2 + 2vw \cos ka} \\
 &= \pm \sqrt{(v - w)^2 + 4vw \cos^2(ka/2)} \\
 &= \pm 2t \sqrt{\sinh^2 \delta + \cos^2(ka/2)}.
 \end{aligned} \tag{72}$$

Furthermore, we find that the missing ingredient is the elastic energy for the displacement of the atoms. The total Hamiltonian is given by

$$\hat{H}_{\text{SSH}} = \hat{H}_{\text{alt}} + \hat{H}_{\text{elastic}}, \tag{73}$$

$$\hat{H}_{\text{elastic}} = \frac{\kappa}{2} \sum_n [(u_{n,A} - u_{n,B})^2 + (u_{n,B} - u_{n+1,A})^2], \tag{74}$$

where κ is a bond stiffness determined by microscopic atomic physics. This model of electron band structure with elastic energy for polyacetylene is known as the **Su-Schrieffer-Heeger model**. Here, we have ignored the kinetic energy of the carbon atoms and assumed that they are stationary on the timescale of electronic motion (\hbar /hopping integral). This is known as the **Born-Oppenheimer approximation**.

For $u_{n,A} = -u_{n,B} = u$, the total energy of the system is $E_{\text{gnd}} = E_{\text{elastic}} + E_{\text{elec}}$, where

$$E_{\text{elastic}} = \frac{\kappa}{2} [(2u)^2 + (-2u)^2] N = 4\kappa x_t^2 N \delta^2, \tag{75}$$

$$E_{\text{elec}} = 2 \sum_{k \in \text{BZ}} E_{k,-} = -4tNa \int_{-\pi/a}^{\pi/a} \sqrt{\sinh^2 \delta + \cos^2(ka/2)} \frac{dk}{2\pi}. \tag{76}$$

For a small dimerization ($|\delta| \ll 1$)

$$\frac{E_{\text{gnd}}(\delta) - E_{\text{gnd}}(0)}{N} \simeq \left[4\kappa x_t^2 - \frac{8t}{\pi} \left(\ln 2 + \frac{1}{4} \right) \right] \delta^2 - \frac{4t}{\pi} \delta^2 \ln \frac{1}{|\delta|} < 0. \tag{77}$$

Even if the first term quadratic in δ is positive ($\kappa x_t^2 \gg t$), we see that the second term involving $\ln(1/\delta)$ makes this energy change negative for sufficiently small δ . So, it is always advantageous to dimerise, no matter how stiff the carbon backbone is! We come to the conclusion that the **dimerization occurs spontaneously** to lower the energy of the system. This phenomenon is known as a **Peierls instability**. The translational symmetry by one C-C bond is broken in dimerised state is called **spontaneous symmetry breaking**.

4 Edge states on chains

In this chapter, we explore further the tight-binding model with alternating hopping integrals as a model for the dimerized phase of the Su-Schrieffer-Heeger (SSH) model for polyacetylene. We will find that it has an interesting eigenstate localised at an edge. The Hamiltonian for the alternating chain is

$$\hat{H}_{\text{alt}} = - \sum_n [v(|n, A\rangle \langle n, B| + \text{h.c.}) + w(|n, B\rangle \langle n+1, A| + \text{h.c.})]. \quad (78)$$

For an infinite chain, these amplitudes obey the equation:

$$Ec_{n,A} = -wc_{n-1,B} - vc_{n,B}, \quad (79)$$

$$Ec_{n,B} = -wc_{n+1,A} - vc_{n,A}. \quad (80)$$

4.1 Semi-infinite SSH chains

For a semi-infinite SSH chain, it is clear that we have two possible terminations. The key point is whether first bond is weak or strong. For the convenience of calculation, we set the convention that B -site is always on the left and the first hopping integral is w .

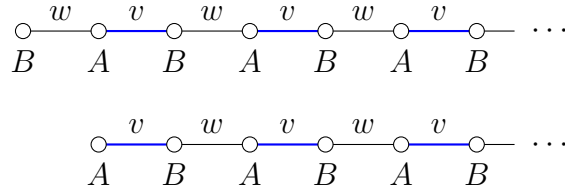


Figure 6: Two possible terminations of a semi-infinite alternating chain.

4.1.1 Fully dimerized limit

Consider the case $w = 0$, the dimer at site n is

$$\hat{H}_{\text{dimer}} = -v(|A\rangle \langle B| + |B\rangle \langle A|), \quad (81)$$

with two electron eigenstates and the eigenvalues:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|A\rangle \pm |B\rangle), \quad E = \mp v. \quad (82)$$

Alternatively, we can also take the limit of $v = 0$. Then, the system also consists of dimers and the electronic eigenstates on each dimer have energies $\pm w$.

We now truncate the infinite chain to produce a semi-infinite chain. In the limit $v \rightarrow 0$, the eigenstates of the system are the same as the one for the infinite chain. However, if we take the limit $w \rightarrow 0$, we are left with an isolated atom at the edge. This has energy $E = 0$ since we have constructed the Hamiltonian to have zero on-site energy.

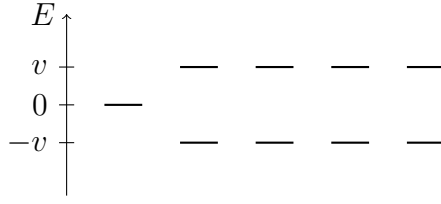


Figure 7: The energy spectrum when $w = 0$.

4.1.2 Away from isolated dimers

Now we consider $w \ll v$ as a perturbation and perform perturbation theory in w/v . Now we find even at non-zero w , **the energy of this localized state is exactly zero!** This is a consequence of the sublattice symmetry of the problem.

In summary, edge state exists inside the band gap for propagating states for $w < v$.

4.1.3 Exact solution for the edge state of a semi-infinite chain

Suppose the B -site is on left edge, and the first hopping integral is denoted as w . We can write the Hamiltonian for the semi-infinite SSH chain as

$$\hat{H} = - \sum_{n=1} [v (|n, A\rangle \langle n, B| + \text{h.c.}) + w (|n, A\rangle \langle n-1, B| + \text{h.c.})]. \quad (83)$$

The eigenstate at energy E is

$$|\psi\rangle = \sum_{n=0} (c_{n,A} |n, A\rangle + c_{n,B} |n, B\rangle), \quad (84)$$

with $c_{0,A} = 0$ as the hard-well boundary condition at $|0, A\rangle$. The eigenfunction gives

$$\begin{aligned} \hat{H} |\psi\rangle &= - \sum_{n=0} \sum_{m=1} [v (|m, A\rangle \langle m, B| + |m, B\rangle \langle m, A|) \\ &\quad + w (|m, A\rangle \langle m-1, B| + |m-1, B\rangle \langle m, A|)] (c_{n,A} |n, A\rangle + c_{n,B} |n, B\rangle) \\ &= - \sum_{n=1} (vc_{n,B} |n, A\rangle + vc_{n,A} |n, B\rangle + wc_{n,B} |n+1, A\rangle + wc_{n,A} |n-1, B\rangle) \\ &= - \sum_{n=1} (vc_{n,B} |n, A\rangle + vc_{n,A} |n, B\rangle + wc_{n-1,B} |n, A\rangle - wc_{n+1,A} |n, B\rangle) \\ &\quad + wc_{1,A} |0, B\rangle \\ &= E \sum_{n=0} (c_{n,A} |n, A\rangle + c_{n,B} |n, B\rangle). \end{aligned} \quad (85)$$

The amplitudes $c_{n,A}$ and $c_{n,B}$ obey the relations

$$-vc_{n,B} - wc_{n-1,B} = Ec_{n,A}, \quad -vc_{n,A} - wc_{n+1,A} = Ec_{n,B} \quad \text{for } n \geq 1, \quad (86)$$

$$-wc_{1,A} = Ec_{0,B}. \quad (87)$$

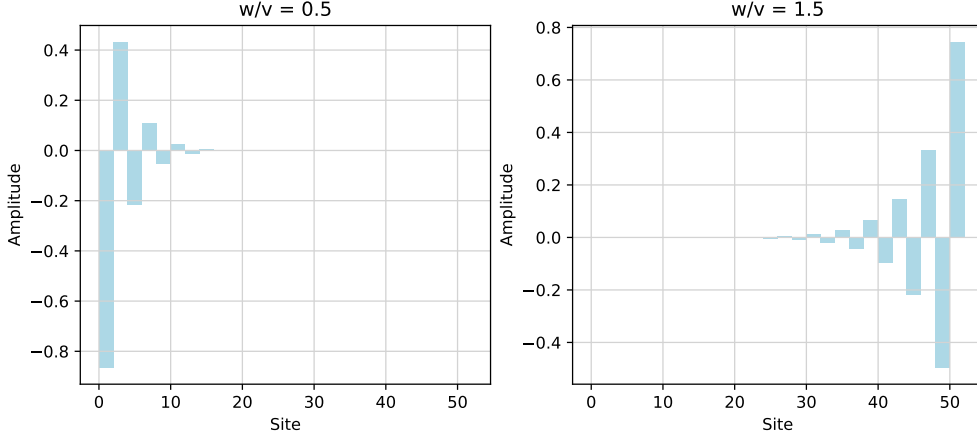


Figure 8: Zero-energy state localised towards end of chain.

Let's now derive the zero-energy state of this system. At zero-energy state, we have

$$-v c_{n,B} - w c_{n-1,B} = 0, \quad -v c_{n,A} - w c_{n+1,A} = 0, \quad c_{1,A} = 0. \quad (88)$$

These equations gives the following results

$$c_{n,A} = 0, \quad c_{n,B} = c_{0,B} \left(-\frac{w}{v} \right)^n = c_{0,B} (-1)^n e^{-n/\xi}, \quad (89)$$

where $\xi = 1/\ln(v/w)$ is named the **localisation length**. For $c_{n,A} = 0$, we find that the edge state has nodes at all the A -sites. The localisation length ξ is very short when $w \rightarrow 0$, corresponding to the electron completely localized on end site. As we approach a uniform chain ($w \rightarrow v$), it diverges as a power law: $\xi \sim (1 - w/v)^{-1}$.

In summary, we have found a transition between the presence and absence of an edge state in the alternating chain as a function of the ratio of hopping integrals w/v . For $w < v$, the edge state exists and is adiabatically connected to the simple isolated site at $w = 0$. **The sublattice symmetry of the system together with the existence of a band gap protects the mid-gap edge state.** The loss of the edge state coincides with the closure of the band gap at $w = v$.

4.1.4 Finite chains

The simulation of a 51-site chain with hopping w, v, w, v, \dots, w, v in python refers to github.com/chenx820.

4.2 Topological protection of the edge state

More generally, a translationally invariant Hamiltonian with the sublattice chiral cymmetry can be written as

$$\hat{H}_{\text{sym}} = - \sum_{m,n} (t_{m-n} |m, A\rangle \langle n, B| + t_{m-n}^* |n, B\rangle \langle m, A|). \quad (90)$$

From the Bloch theorem, we can write the eigenstates

$$|\psi_k\rangle = \sum_n (c_A e^{ikn} |n, A\rangle + c_B e^{ikn} |n, B\rangle), \quad (91)$$

with $-\pi < k \leq \pi$. To solve the eigenfunction $\hat{H}_{\text{sym}} |\psi_k\rangle = E |\psi_k\rangle$, we have

$$\begin{aligned} \hat{H}_{\text{sym}} |\psi_k\rangle &= - \sum_{m,n,p} (t_{m-n} c_B e^{ikp} |m, A\rangle \langle n, B|_p, B\rangle + t_{m-n}^* c_A e^{ikp} |n, B\rangle \langle m, A|_p, A\rangle), \\ &= - \sum_{m,n} (t_{m-n} c_B e^{ikn} |m, A\rangle + t_{m-n}^* c_A e^{ikm} |n, B\rangle), \\ &= - \sum_{m,n} (t_{n-m} c_B e^{ikm} |n, A\rangle + t_{m-n}^* c_A e^{ikm} |n, B\rangle), \\ &= E \sum_n (c_A e^{ikn} |n, A\rangle + c_B e^{ikn} |n, B\rangle). \end{aligned} \quad (92)$$

Comparing the coefficients, then we get

$$- \sum_m t_{n-m} e^{-ik(n-m)} c_B = E c_A, \quad - \sum_m t_{m-n}^* e^{ik(m-n)} c_A = E c_B, \quad (93)$$

which gives

$$- \begin{pmatrix} 0 & t(k) \\ t(k)^* & 0 \end{pmatrix} \begin{pmatrix} c_A \\ c_B \end{pmatrix} = E_k \begin{pmatrix} c_A \\ c_B \end{pmatrix}, \quad t(k) = \sum_m t_m e^{-ikm}. \quad (94)$$

The eigenstates have energies $E_k = \pm |t(k)|$. The chain \hat{H}_{sym} completely describe by $t(k)$ for $-\pi < k \leq \pi$. **The system is completely described geometrically by a loop in the complex t -plane.** For SSH chain, $t(k) = v + w e^{-ika}$ (Fig. 9).

All of the chiral chains can be divided into two classes. One class supports edge states and the other does not. This is decided by whether the loop $t(k)$ winds around the origin (degeneracy point) or not. This winding is a topological criterion: *The zero-energy edge state is **topologically protected** — changes to the Hamiltonian does not destroy the edge state, as long as the changes preserve the chiral sublattice symmetry and the system is adiabatically connected to the fully dimerized limit with such a state.*

Now we look at the two-level system, which we have talked about in Chapter 1. The Bloch Hamiltonian can be written as

$$h(k) = \begin{pmatrix} 0 & t(k) \\ t(k)^* & 0 \end{pmatrix} = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}. \quad (95)$$

The Berry phase for taking the eigenstates around the Brillouin zone will tell us about the **winding** of the loop C :

$$\gamma = i \int_{-\pi}^{\pi} \langle k, \pm | \partial_k | k, \pm \rangle dk. \quad (96)$$

In this context of a one-dimensional Brillouin zone, the Berry phase is called the **Zak phase** in the literature.

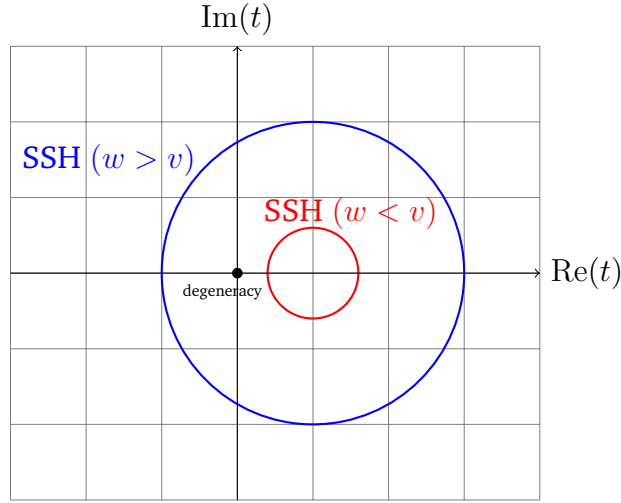


Figure 9: In SSH chain, the hopping $t(k) = w + ve^{-ika}$ forms a closed loop as k traverses the Brillouin zone. Red: $w < v$ has edge state, loop can be shrunk to a point (isolated end atom) without crossing the origin (degeneracy point). Blue: $w > v$ has no edge state, loop encloses origin and cannot be shrunk to a point without passing through degeneracy point.

5 Adiabatic transport

In this chapter, we will discuss how a charge can be transported by cycling the parameters of a system adiabatically.

5.1 Adiabatic cycle on a dimerized chain

5.1.1 Rice-Mele model

The Rice-Mele model is an extension of the Su-Schrieffer-Heeger lattice in the presence of a staggered potential such that there is an imbalance in the on-site energies at A and B sites. The Rice-Mele Hamiltonian is

$$\hat{H}_{\text{RM}} = \hat{H}_{\text{alt}} + u \sum_n (|n, A\rangle \langle n, A| - |n, B\rangle \langle n, B|), \quad (97)$$

$$\hat{H}_{\text{alt}} = - \sum_n [v(|n, A\rangle \langle n, B| + \text{h.c.}) + w(|n, B\rangle \langle n+1, A| + \text{h.c.})]. \quad (98)$$

A positive u raises the energy of the A sites and lowers the energy of the B sites. The eigenstate $|\psi_n\rangle = c_{n,A} |n, A\rangle + c_{n,B} |n, B\rangle$. The eigenfunction $\hat{H}_{\text{RM}} |\psi\rangle = E |\psi\rangle$ gives

$$\begin{pmatrix} u & -v - we^{-ika} \\ -v - we^{ika} & -u \end{pmatrix} \begin{pmatrix} c_A \\ c_B \end{pmatrix} = E \begin{pmatrix} c_A \\ c_B \end{pmatrix}. \quad (99)$$

We can solve the eigenfunction for \hat{H}_{RM} :

$$E_k = \pm \sqrt{v^2 + w^2 + u^2 + 2vw \cos(ka)}. \quad (100)$$

The two-level Hamiltonian at each wavevector k can be written as a spin model $\hat{H} = \mathbf{d} \cdot \hat{\boldsymbol{\sigma}}$ with

$$d_x = -v - w \cos(ka), \quad d_y = -w \sin(ka), \quad d_z = u, \quad (101)$$

$$\hat{\sigma}_x = |A, k\rangle \langle B, k| + |B, k\rangle \langle A, k|, \quad \hat{\sigma}_y = -i(|A, k\rangle \langle B, k| - |B, k\rangle \langle A, k|), \quad (102)$$

$$\hat{\sigma}_z = |A, k\rangle \langle B, k| - |B, k\rangle \langle A, k|. \quad (103)$$

5.1.2 Charge pump cycle

Based on the Rice-Mele model, let us consider the adiabatic protocol with period of T :

$$v(t) = v_0, \quad w(t) = v_0[1 + \cos(2\pi t/T)], \quad u(t) = -v_0 \sin(2\pi t/T), \quad (104)$$

$$\mathbf{d}(k, t) = (-v(t) - w(t) \cos(ka), -w(t) \sin(ka), u(t)). \quad (105)$$

This protocol has four stages between the times $t = 0, \frac{1}{4}T, \frac{1}{2}T, \frac{3}{4}T$ and T .

1. At the start, the chain has no edge states ($w > v$) and all the on-site energies the same. With the Fermi level in the band gap, all the states in the lower band are filled. The electron density is the same on every site (one per site).
2. At time $t = T/4$, the hopping w goes below v so that edge states appear at both ends. For a negative u , the right edge state (A sites) is below the Fermi level and is occupied. The left edge state (B sites) has an energy above the Fermi level and is unoccupied.
3. After $t = T/4$, we increase u and continue to decrease w so that $w = 0$ at $t = T/2$. At this point, we have a set of isolated dimers with the edge state localized completely on the end sites, still occupied on the right and unoccupied on the left.
4. After $t = T/2$, the staggered field u becomes positive. This raises the right edge state above the Fermi level and the left edge state goes below the Fermi level. Being an adiabatic process, we cannot abruptly empty the right edge state and fill up the left edge state because they are widely separated in space. So, *the right edge state remains occupied and the left edge state remains unoccupied.*
5. At $t = 3T/4$, the value of w rises above v . This means that the size of the edge states diverges and the states merge into the bulk spectrum. Since $u = +v_0$ at this point, the right edge state becomes the lowest state in the conduction band and the left edge state becomes the highest state in the valence band.
6. By the end of the cycle at $t = T$, we have switched off the staggered potential and we have returned to an SSH model. Although the edge states have gone and the spectrum has returned to its original form at $t = 0$, we see that the occupation of the eigenstates has changed. *There is an electron at the bottom of the conduction band and a hole at top of the valence band.* In other words, the protocol has done work on the system and excited (“pumped”) an electron across the band gap!

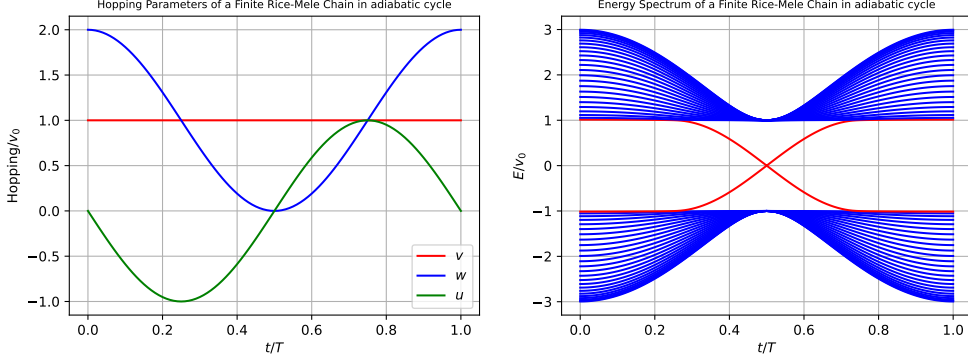


Figure 10: Left: Adiabatic cycle of the system parameters of a Rice-Mele chain. Right: Instantaneous energy spectrum of the chain with 50 sites.

5.2 Quasi-adiabatic regime

If we start the system in an eigenstate $|\psi(t=0)\rangle = |\nu, \mathbf{R}(t=0)\rangle$ and change the parameters \mathbf{R} infinitesimally slowly, the system will stay in this eigenstate and in terms of the form

$$|\psi(t)\rangle \simeq e^{i\gamma_{\nu, \text{dyn}}(t)} e^{i\gamma_{\nu, \text{geom}}(t)} |\nu, \mathbf{R}(t)\rangle, \quad (106)$$

where

$$\hbar\dot{\gamma}_{\nu, \text{dyn}}(t) = -E_{\nu}(\mathbf{R}(t)), \quad (107)$$

$$\dot{\gamma}_{\nu, \text{geom}}(t) = i \langle \nu, \mathbf{R} | \partial_t | \nu, \mathbf{R} \rangle = i \dot{\mathbf{R}} \cdot \langle \nu, \mathbf{R} | \nabla_{\mathbf{R}} | \nu, \mathbf{R} \rangle. \quad (108)$$

If we change gauge to absorb geometric phase, i.e.,

$$|\tilde{\nu}(t)\rangle = e^{i\gamma_{\nu, \text{geom}}(t)} |\nu, \mathbf{R}(t)\rangle. \quad (109)$$

This is called the **parallel transport gauge**. And we note that

$$\hat{H}(t) |\nu, \mathbf{R}(t)\rangle = E_{\nu}(t) |\nu, \mathbf{R}(t)\rangle, \quad (110)$$

$$|\partial_t \tilde{\nu}\rangle = e^{i\gamma_{\nu, \text{geom}}} [i(\partial_t \gamma_{\nu, \text{geom}}) |\nu\rangle + |\partial_t \nu\rangle] = e^{i\gamma_{\nu, \text{geom}}} [-\langle \nu | \partial_t \nu \rangle |\nu\rangle + |\partial_t \nu\rangle]. \quad (111)$$

Thus, we see that $\langle \tilde{\nu} | \partial_t | \tilde{\nu} \rangle = 0$ by design. The state $|\psi\rangle$ evolves according to the time-dependent Schrödinger equation

$$i\hbar\partial_t |\psi\rangle = \hat{H}(t) |\psi\rangle \quad \text{with} \quad \hat{H}(T) = \hat{H}(0), \quad |\psi(0)\rangle = |\tilde{\nu}(0)\rangle. \quad (112)$$

Let us write the state as

$$\begin{aligned} |\psi(t)\rangle &\simeq e^{i\gamma_{\nu, \text{dyn}}(t)} |\tilde{\nu}(t)\rangle + \sum_{\mu \neq \nu} c_{\mu}(t) e^{i\gamma_{\mu, \text{dyn}}(t)} |\tilde{\mu}(t)\rangle \\ &= e^{i\gamma_{\nu, \text{dyn}}(t)} \left[|\tilde{\nu}(t)\rangle + \sum_{\mu \neq \nu} c_{\mu}(t) e^{i\Delta\gamma_{\mu\nu}(t)} |\tilde{\mu}(t)\rangle \right]. \end{aligned} \quad (113)$$

where $\Delta\gamma_{\mu\nu}(t) = \gamma_{\mu,\text{dyn}}(t) - \gamma_{\nu,\text{dyn}}(t)$. When $\hbar/(T\Delta E) \ll 1$, we expect the coefficients c_μ to be small and of the order of $\hbar/T\Delta E$. So we have

$$|\psi(t)\rangle \simeq e^{-\frac{i}{\hbar} \int_0^t E_\nu(t') dt'} \left[|\tilde{\nu}(t)\rangle + i\hbar \sum_{\mu \neq \nu} |\tilde{\mu}(t)\rangle \frac{\langle \tilde{\mu} | \partial_t |\tilde{\nu}\rangle}{E_\mu - E_\nu} \right]. \quad (114)$$

This is sometimes called the **quasi-adiabatic regime** to distinguish it from the limit of infinitely slow variations.

5.3 Thouless adiabatic current

Now, let us work out the thouless adiabatic current. The current operator

$$\hat{J}(t) = \sum_{k \in \text{BZ}} \frac{1}{\hbar L} \frac{\partial \hat{H}_k}{\partial k} \quad \text{with} \quad \hat{H}_k = \sum_{\mu} E_{\mu,k} |\mu, k\rangle \langle \mu, k|. \quad (115)$$

So we have

$$J(t) = \frac{1}{\hbar L} \sum_{k \in \text{BZ}} \langle \psi_k(t) | (\partial_k \hat{H}_k) | \psi_k(t) \rangle, \quad (116)$$

where $-\pi/a < k \leq \pi/a$. Then we calculate

$$\partial_k \hat{H}_k = \sum_{\mu} [(\partial_k E_{\mu,k}) |\mu, k\rangle \langle \mu, k| + E_{\mu,k} (|\partial_k \mu\rangle \langle \mu, k| + |\mu, k\rangle \langle \partial_k \mu|)], \quad (117)$$

where $|\partial_k \mu\rangle$ is shorthand for $\partial_k |\mu, k\rangle$. From last section we know, in the adiabatic limit

$$|\psi_k(t)\rangle \simeq e^{-\frac{i}{\hbar} \int_0^t E_\nu(t') dt'} \left[|\tilde{\nu}(t), k\rangle + i\hbar \sum_{\mu \neq \nu} |\tilde{\mu}(t), k\rangle \frac{\langle \tilde{\mu}, k | \partial_t |\tilde{\nu}, k\rangle}{E_\mu - E_\nu} \right]. \quad (118)$$

So the current in the zeroth order and the first order

$$J^{(0)} = \frac{1}{\hbar L} \sum_{k \in \text{BZ}} \langle \tilde{\nu}, k | (\partial_k \hat{H}_k) | \tilde{\nu}, k \rangle = \frac{1}{\hbar L} \sum_{k \in \text{BZ}} \partial_k E_{\nu,k} = 0, \quad (119)$$

$$J_{\nu,k}^{(1)} = \frac{1}{L} \sum_{\mu \neq \nu} \left[i \langle \tilde{\nu}, k | (\partial_k \hat{H}_k) | \tilde{\mu}(t), k \rangle \frac{\langle \tilde{\mu}, k | \partial_t |\tilde{\nu}, k\rangle}{E_{\mu,k} - E_{\nu,k}} + \text{c.c.} \right] \quad (120)$$

From Eq.(117)

$$\langle \tilde{\nu} | (\partial_k \hat{H}_k) | \tilde{\mu} \rangle = E_{\mu,k} \langle \tilde{\nu} | \partial_k \tilde{\mu} \rangle + E_{\nu,k} \langle \partial_k \tilde{\nu} | \tilde{\mu} \rangle = (E_{\nu,k} - E_{\mu,k}) \langle \partial_k \tilde{\nu} | \tilde{\mu} \rangle. \quad (121)$$

Substituting into the equation for the current correction gives

$$\begin{aligned} J_{\nu,k}^{(1)} &= \frac{1}{L} \sum_{\mu \neq \nu} (-i \langle \partial_k \tilde{\nu} | \tilde{\mu} \rangle \langle \tilde{\mu} | \partial_t \tilde{\nu} \rangle + i \langle \partial_t \tilde{\nu} | \tilde{\mu} \rangle \langle \tilde{\mu} | \partial_k \tilde{\nu} \rangle) \\ &= -\frac{i}{L} (\langle \partial_k \tilde{\nu} | \partial_t \tilde{\nu} \rangle - \langle \partial_t \tilde{\nu} | \partial_k \tilde{\nu} \rangle) \\ &= -\frac{i}{L} (\langle \partial_k \nu | \partial_t \nu \rangle - \langle \partial_t \nu | \partial_k \nu \rangle). \end{aligned} \quad (122)$$

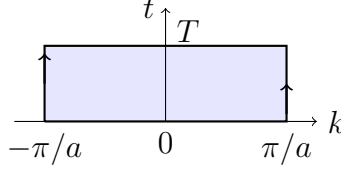


Figure 11: Line integral around the perimeter of an unwrapped torus.

The expression for current is gauge-invariant, valid for any gauge choice. The current can be expressed in the form of integral:

$$J(t) = \frac{1}{\hbar L} \sum_{k \in \text{BZ}} \langle \psi_k(t) | (\partial_k \hat{H}) | \psi_k(t) \rangle = \frac{1}{2\pi i} \oint_{\text{BZ}} (\langle \partial_k \nu | \partial_t \nu \rangle - \langle \partial_t \nu | \partial_k \nu \rangle) dk. \quad (123)$$

Link to the Berry phase, the Berry curvature and Berry connection is

$$B(k, t) = i(\langle \partial_k \nu | \partial_t \nu \rangle - \langle \partial_t \nu | \partial_k \nu \rangle), \quad A_{k,t} = i \langle \nu | \partial_{k,t} | \nu \rangle. \quad (124)$$

5.4 First Chern number

If the system completes an adiabatic cycle of the parameters in time T , then the total number of particles Q transferred across a link is the integral of the current at the link.

$$Q = \int_0^T J(t) dt = \frac{1}{2\pi i} \int_0^T dt \oint_{\text{BZ}} dk (\langle \partial_k \nu | \partial_t \nu \rangle - \langle \partial_t \nu | \partial_k \nu \rangle). \quad (125)$$

The quantity Q is called the **first Chern number**. We will now show that the Chern number for the torus is an integer:

$$\begin{aligned} 2\pi Q &= -i \int_0^T dt \oint_{\text{BZ}} dk (\langle \partial_k \nu | \partial_t \nu \rangle - \langle \partial_t \nu | \partial_k \nu \rangle) \\ &= - \int_{-\pi/a}^{\pi/a} dk [A_k(k, 0) - A_k(k, T)] - \int_0^T dt [A_t(\pi/a, t) - A_t(-\pi/a, t)] \\ &= - \int_{-\pi/a}^{\pi/a} dk \partial_k \chi_k + \int_0^T dt \partial_t \chi_t \\ &= -\chi_k(\pi/a) + \chi_k(-\pi/a) + \chi_t(T) - \chi_t(0), \end{aligned} \quad (126)$$

where

$$A_k = i \langle \nu, k, t | \partial_k | \nu, k, t \rangle, \quad A_t = i \langle \nu, k, t | \partial_t | \nu, k, t \rangle, \quad (127)$$

$$|\nu, k, T\rangle = e^{i\chi_k(k)} |\nu, k, 0\rangle, \quad |\nu, \pi/a, t\rangle = e^{i\chi_t(t)} |\nu, -\pi/a, t\rangle. \quad (128)$$

The number transported is quantised

$$Q = \frac{1}{2\pi} [-\chi_k(\pi/a) + \chi_k(-\pi/a) + \chi_t(T) - \chi_t(0)] = \text{integer}. \quad (129)$$

In summary, we have shown that **the number of particles transported in one adiabatic cycle of the parameters must be an integer**.

6 Electrons in a vector potential

In this chapter, we explore the interaction of quantum particles with electromagnetic fields, focusing on three key concepts crucial for advanced physics students. First, we discuss how charged particles are influenced by vector potentials, introducing the foundational ideas linking quantum mechanics to electromagnetism. Next, we delve into local gauge invariance, illustrating its role in maintaining the consistency of physical laws across different reference frames. Finally, we examine the Aharonov-Bohm effect, demonstrating the observable consequences of electromagnetic potentials on quantum systems.

6.1 Gauge choice in electromagnetic

We consider a non-relativistic particle with charge q with a vector potential \mathbf{A} and the scalar potential ϕ

$$\hat{H} = \frac{1}{2m}(-i\hbar\nabla - q\mathbf{A})^2 + q\phi, \quad (130)$$

where $\mathbf{B} = \nabla \times \mathbf{A}$ is the magnetic field and $\mathbf{E} = -\nabla\phi - \frac{\partial\mathbf{A}}{\partial t}$ is the electric field.

There is a degree of freedom in the choice of the vector and scalar potentials, which is called a **choice of gauge**. The key point is that *physics should be the same no matter what gauge we use* and this is the principle of **gauge invariance**. In classical mechanics, we need to ensure that the force on a charged particle (which depends only \mathbf{B} and \mathbf{E}) remains the same when we change the gauge. The magnetic field does not change if we add a gradient of a scalar function φ to the vector potential. \mathbf{B} and \mathbf{E} is invariant under the transformation

$$\mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \nabla\varphi, \quad \phi \rightarrow \phi' = \phi - \frac{\partial\varphi}{\partial t}. \quad (131)$$

And the Hamiltonian also transforms

$$\hat{H} \rightarrow \hat{H}' = \frac{1}{2m}(-i\hbar\nabla - q\mathbf{A} - q\nabla\varphi)^2 + q\phi - q\frac{\partial\varphi}{\partial t}. \quad (132)$$

With the new Hamiltonian, the wavefunctions also need to transform under

$$\psi \rightarrow \psi' = e^{iq\varphi/\hbar}\psi. \quad (133)$$

Now we examine the Schrödinger equation $i\hbar\partial\psi'/\partial t = \hat{H}'\psi'$. To begin with, we calculate the right handside of the equation. First, we calculate the relation

$$\begin{aligned} (-i\hbar\nabla - q\mathbf{A} - q\nabla\varphi)\psi' &= (-i\hbar\nabla - q\mathbf{A} - q\nabla\varphi)e^{iq\varphi/\hbar}\psi \\ &= q(\nabla\varphi)e^{iq\varphi/\hbar}\psi - i\hbar(\nabla\psi)e^{iq\varphi/\hbar} - q\mathbf{A}e^{iq\varphi/\hbar}\psi - q(\nabla\varphi)e^{iq\varphi/\hbar}\psi \\ &= -i\hbar(\nabla\psi)e^{iq\varphi/\hbar} - q\mathbf{A}e^{iq\varphi/\hbar}\psi \\ &= e^{iq\varphi/\hbar}(-i\hbar\nabla - q\mathbf{A})\psi. \end{aligned} \quad (134)$$

Then we apply the operator $(-i\hbar\nabla - q\mathbf{A} - q\nabla\varphi)$ on ψ' twice:

$$(-i\hbar\nabla - q\mathbf{A} - q\nabla\varphi)^2\psi' = e^{iq\varphi/\hbar}(-i\hbar\nabla - q\mathbf{A})^2\psi. \quad (135)$$

So the right handside of the Schrödinger equation is

$$\text{RHS} = \hat{H}'\psi' = e^{iq\varphi/\hbar} \left[\frac{1}{2m}(-i\hbar\nabla - q\mathbf{A})^2\psi + q\phi - q\frac{\partial\varphi}{\partial t} \right] \psi = e^{iq\varphi/\hbar} H\psi. \quad (136)$$

The left handside of the equation is

$$\text{LHS} = i\hbar\frac{\partial\psi'}{\partial t} = e^{iq\varphi/\hbar} i\hbar\frac{\partial\psi}{\partial t}. \quad (137)$$

with the Schrödinger equation of the original Hamiltonian $i\hbar\partial\psi/\partial t = \hat{H}\psi$, the Schrödinger equation under gauge transformation are verified.

6.2 Current in a vector potential

The current density in the absence of a vector potential is

$$\mathbf{J} = \frac{1}{2m}[\psi^*(-i\hbar\nabla)\psi + \psi(i\hbar\nabla)\psi^*]. \quad (138)$$

To obtain the current in the presence of a vector potential, we make the replacement $-i\hbar\nabla \rightarrow -i\hbar\nabla - q\mathbf{A}$ so that

$$\begin{aligned} \mathbf{J} &= \frac{1}{2m}[\psi^*(-i\hbar\nabla - q\mathbf{A})\psi + \psi(i\hbar\nabla - q\mathbf{A})\psi^*] \\ &= -\frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{q\mathbf{A}}{2m}|\psi|^2. \end{aligned} \quad (139)$$

The current is gauge invariance and we can examine this:

$$\begin{aligned} \mathbf{J}' &= -\frac{i\hbar}{2m}[(\psi')^*\nabla\psi' - \psi'\nabla(\psi')^*] - \frac{q\mathbf{A}'}{2m}|\psi'|^2 \\ &= \frac{1}{2m}[\psi^*(-i\hbar\nabla + q\nabla\varphi)\psi + \psi(i\hbar\nabla + q\nabla\varphi)\psi^*] - \frac{q}{2m}(\mathbf{A} + \nabla\varphi)|\psi|^2 \\ &= -\frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{q\mathbf{A}}{2m}|\psi|^2 = \mathbf{J}. \end{aligned} \quad (140)$$

6.3 Aharonov-Bohm effect

6.3.1 Adiabatic derivation

Consider a long strait solenoid parallel to the z -axis with magnetic flux Φ . Classically, there is no effect on the classical dynamics due to the solenoid (the magnetic

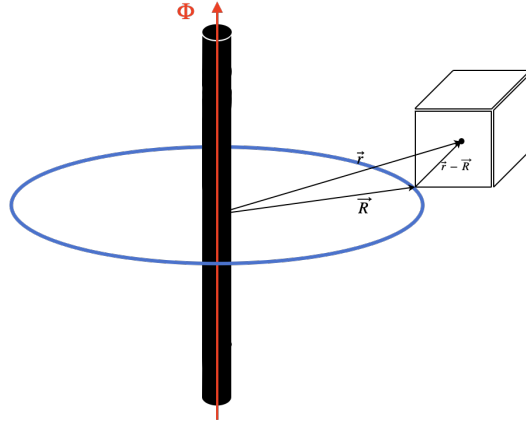


Figure 12: A particle is confined to a ox at position $R(t)$ which is moved adiabatically along path C around an infinite solenoid carrying flux Φ . The box does not move through any region with non-zero magnetic field.

field outside the solenoid is zero). With the relation

$$\oint_C \mathbf{A} \cdot d\mathbf{r} = \int_S \mathbf{B} \cdot d\mathbf{S} = \Phi, \quad (141)$$

the vector potential outside the solenoid is $A_\phi = \Phi/2\pi r$, where r is the distance of a point outside the solenoid and the center of solenoid.

Consider a charged partical confined by a tight potential well $V(\mathbf{r} - \mathbf{R})$ centred at \mathbf{R} far away from the solenoid. The Hamiltonian of the particle is

$$\hat{H} = \frac{1}{2m}(-i\hbar\nabla_{\mathbf{r}} - q\mathbf{A}(\mathbf{r}))^2 + V(\mathbf{r} - \mathbf{R}). \quad (142)$$

Suppose that we prepare the charged particle in its ground state in the potential well at time $t = 0$, and then adiabatically move the potential well along a path C encircling the solenoid. The Schrödinger equation is

$$i\hbar\frac{\partial\psi}{\partial t} = \left[\frac{1}{2m}(-i\hbar\nabla_{\mathbf{r}} - q\mathbf{A}(\mathbf{r}))^2 + V(\mathbf{r} - \mathbf{R}(t)) \right] \psi. \quad (143)$$

Suppose that the eigenstate of the particle in the potential well at \mathbf{R} without the vector potential has energy E and wave function $u(\mathbf{r} - \mathbf{R})$ centred at \mathbf{R} , that is, $\left[-\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 + V(\mathbf{r}) \right] u(\mathbf{r}) = Eu(\mathbf{r})$. It can be seen that a choice for the instantaneous eigenstate $\psi_{\mathbf{R}}(\mathbf{r})$ in the presence of the vector potential $\mathbf{A} \neq 0$ with the well at position \mathbf{R} is

$$\psi_{\mathbf{R}}(\mathbf{r}) = e^{i\chi_{\mathbf{R}}(\mathbf{r})}u(\mathbf{r} - \mathbf{R}), \quad \chi_{\mathbf{R}}(\mathbf{r}) = \frac{q}{\hbar} \int_{\mathbf{R}}^{\mathbf{r}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}'. \quad (144)$$

Now we examine the solutions given in Eq.(144). Let's begin with the relation

$$(-i\hbar\nabla_{\mathbf{r}} - q\mathbf{A})e^{i\chi(\mathbf{r})}u(\mathbf{r} - \mathbf{R}) = e^{i\chi(\mathbf{r})}(-i\hbar\nabla_{\mathbf{r}} + \hbar\nabla\chi - q\mathbf{A})u(\mathbf{r} - \mathbf{R}). \quad (145)$$

If we set $\hbar\nabla\chi - q\mathbf{A} = 0$ and $\mathbf{B} = \nabla \times \mathbf{A} = \frac{\hbar}{q}\nabla \times (\nabla\chi) = 0$, which gives $\chi_{\mathbf{R}}(\mathbf{r}) = \frac{q}{\hbar} \int_{\mathbf{R}}^{\mathbf{r}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}'$, then the relation above becomes

$$(-i\hbar\nabla_{\mathbf{r}} - q\mathbf{A})e^{i\chi(\mathbf{r})}u(\mathbf{r} - \mathbf{R}) = e^{i\chi(\mathbf{r})}(-i\hbar\nabla_{\mathbf{r}})u(\mathbf{r} - \mathbf{R}), \quad (146)$$

$$(-i\hbar\nabla_{\mathbf{r}} - q\mathbf{A})^2 e^{i\chi(\mathbf{r})}u(\mathbf{r} - \mathbf{R}) = e^{i\chi(\mathbf{r})}(-i\hbar\nabla_{\mathbf{r}})^2 u(\mathbf{r} - \mathbf{R}). \quad (147)$$

So we have

$$\left[-\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 + V(\mathbf{r} - \mathbf{R}) \right] u(\mathbf{r} - \mathbf{R}) = Eu(\mathbf{r} - \mathbf{R}). \quad (148)$$

Take the box at \mathbf{R} move around the solenoid slowly, then the geometry phase / Berry phase is

$$\gamma_{\text{geom}} = \oint_C \mathbf{a}(\mathbf{R}) \cdot d\mathbf{R}, \quad (149)$$

where the Berry connection is

$$\mathbf{a}(\mathbf{R}) = i \langle \psi_{\mathbf{R}} | \nabla_{\mathbf{R}} | \psi_{\mathbf{R}} \rangle = -\nabla_{\mathbf{R}}\chi_{\mathbf{R}}(\mathbf{r}) + i \langle u_{\mathbf{R}} | \nabla_{\mathbf{R}} | u_{\mathbf{R}} \rangle = \frac{q}{\hbar}\mathbf{A}(\mathbf{R}). \quad (150)$$

So the Berry phase is

$$\gamma_{\text{geom}} = \frac{q}{\hbar} \oint_C \mathbf{A}(\mathbf{R}) \cdot d\mathbf{R} = \frac{q}{\hbar}\Phi. \quad (151)$$

6.3.2 Aharonov-Bohm interferometry

We can measure the Aharonov-Bohm effect by Young slits. Consider two beams start from \mathbf{r}_0 and focus together at \mathbf{r}_1 , the paths are denoted as C_R and C_L . Then the phase difference will cause interference between the two beams. Their phase difference is

$$\Delta(\text{phase}) = \frac{q}{\hbar} \int_{C_L} \mathbf{A}(\mathbf{R}) \cdot d\mathbf{R} - \frac{q}{\hbar} \int_{C_R} \mathbf{A}(\mathbf{R}) \cdot d\mathbf{R} = \frac{q\Phi}{\hbar}. \quad (152)$$

In experiments, the "flux lines" due to an Aharonov-Bohm phase difference $(2n+1)\pi$ where n is a integer. So the flux

$$\Phi = \frac{\hbar}{e}(2n+1)\pi = \frac{h}{e} \left(n + \frac{1}{2} \right), \quad (153)$$

where $h = 2\pi\hbar$. A phase of π was observed and thus shows that the flux through the solenoid is quantized in units of h/e .

7 Electrons in a magnetic field

7.1 Electrons in a uniform magnetic field

Consider electrons in xy -plane with a uniform magnetic field \mathbf{B} parallels to the z -direction, i.e., $\mathbf{B} = (0, 0, B)$. For circular motion, Newton's law

$$\frac{mv^2}{r} = eBv, \quad (154)$$

gives the **cyclotron frequency**

$$\omega_c = \frac{v}{r} = \frac{eB}{m}. \quad (155)$$

The Hamiltonian of the electron

$$\begin{aligned} \hat{H} &= \frac{1}{2m}(-i\hbar\nabla + e\mathbf{A})^2 + V(z) \\ &= \frac{1}{2m}(-\hbar^2\nabla^2 - 2ie\hbar\mathbf{A} \cdot \nabla + e^2\mathbf{A}^2) + V(z), \end{aligned} \quad (156)$$

with $\mathbf{A} = \nabla \times \mathbf{B}$. To proceed further, we have to choose a specific gauge for the vector potential. For example, there are **Landau gauge** $\mathbf{A} = (-By, 0, 0)$ and **symmetric gauge** $\mathbf{A} = \frac{B}{2}(-y, x, 0)$. Now we choose the Landau gauge. The Hamiltonian becomes

$$\begin{aligned} \hat{H} &= \frac{1}{2m} \left[-\hbar^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - 2ie\hbar(-By) \frac{\partial}{\partial x} + e^2 B^2 y^2 \right] + V(z) \\ &= \frac{1}{2m} \left[-\hbar^2 \frac{\partial^2}{\partial y^2} + \left(-i\hbar \frac{\partial}{\partial x} - eBy \right)^2 \right] - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + V(z) \\ &= \hat{H}_{xy} + \hat{H}_z, \end{aligned} \quad (157)$$

where

$$\hat{H}_{xy} = \frac{1}{2m} \left[-\hbar^2 \frac{\partial^2}{\partial y^2} + \left(-i\hbar \frac{\partial}{\partial x} - eBy \right)^2 \right], \quad \hat{H}_z = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + V(z). \quad (158)$$

The eigenstates of the Hamiltonian \hat{H} can be written as $\Psi(x, y, z) = \psi(x, y)u(z)$ where

$$\hat{H}_{xy}\psi(x, y) = E_{xy}\psi(x, y), \quad \hat{H}_z u(z) = E_z u(z), \quad E = E_{xy} + E_z. \quad (159)$$

Now we focus on the xy -plane. In Landau gauge, this Hamiltonian has translational symmetry in the x -direction but not in the y -direction. This means that eigenstates should be plane waves in the x -direction: $\psi(x, y) = e^{ik_x x} v_{k_x}(y)$. Then

$$\hat{H}_{xy} e^{ik_x x} v_{k_x}(y) = \frac{\hbar^2}{2m} \left[-\partial_y^2 + \left(k_x - \frac{y}{l_B^2} \right)^2 \right] e^{ik_x x} v_{k_x}(y) = E_{xy} e^{ik_x x} v_{k_x}(y), \quad (160)$$

or

$$\hat{H}_{k_x} v_{k_x}(y) = \frac{\hbar^2}{2m} \left[-\partial_y^2 + \left(k_x - \frac{y}{l_B^2} \right)^2 \right] v_{k_x}(y) = E_{xy} v_{k_x}(y), \quad (161)$$

where $l_B = \sqrt{\frac{\hbar}{eB}}$ is called the **magnetic length** and is the natural quantum length scale for this system.

Recall the simple harmonic oscillator (SHO) with natural frequency ω_0 centered at $y_{k_x} = k_x l_B^2$ with energies $E_n = (n + \frac{1}{2})\hbar\omega_0$. The Hamiltonian of SHO is

$$\hat{H}_{\text{SHO}} = -\frac{\hbar^2}{2m} \frac{d^2}{dy^2} + \frac{1}{2} m \omega_0^2 (y - y_k)^2 = \frac{\hbar^2}{2m} \left[-\frac{d^2}{dy^2} + \frac{m^2 \omega_0^2}{\hbar^2} (y - y_k)^2 \right]. \quad (162)$$

Compare the terms with \hat{H}_{k_x} :

$$\hat{H}_{k_x} = \frac{\hbar^2}{2m} \left[-\frac{d^2}{dy^2} + \frac{e^2 B^2}{\hbar^2} (y - l_B^2 k_x)^2 \right], \quad (163)$$

the natural frequency for our problem is $\omega_0 = eB/m = \omega_c$. So the eigenvalues of \hat{H}_{xy} are

$$E_{xy}(k_x) = \left(n + \frac{1}{2} \right) \hbar \omega_c, \quad (164)$$

which is independent of k_x .

We can denote the quantum states in $|k_x, n\rangle$, which is labelled by k_x and the harmonic scillator number $n = 0, 1, 2, \dots$. How many degenerate states at each n ?

Applying periodic boundary condition on x -direction (length L_x) which requires $e^{ik_x L_x} = 1$. The wavevector k are quantised in steps of $\delta k_x = 2\pi/L_x$. So the $|k_x, n\rangle$ states separated in y by

$$\delta y_{k_x} = l_B^2 \delta k_x = \frac{2\pi l_B^2}{L_x}. \quad (165)$$

For region with area $A = L_x L_y$, the number of states is

$$g = \frac{L_y}{\delta y_{k_x}} = \frac{L_x L_y}{2\pi l_B^2} = \frac{e}{h} B A = \frac{\Phi}{\Phi_0}, \quad (166)$$

and this is called **macroscopic degeneracy**, where Φ is the total flux through area A , $\Phi_0 = h/e$ is known as the **flux quantum**.

7.2 Classical Hall effect

Consider an electron moving parallel to the xy -plane in a magnetic field \mathbf{B} in the z -direction and an electric field \mathcal{E} in the y -direction. The equation of motion for the electron is

$$m\ddot{x} = -eB\dot{y}, \quad m\ddot{y} = eB\dot{x} - e\mathcal{E}_y. \quad (167)$$

It is convenient to think of this as motion in the complex plane with $z = x + iy$ as the complex number. Then the equation of motion can be written as

$$m\ddot{z} - ieB\dot{z} = -ie\mathcal{E}_y. \quad (168)$$

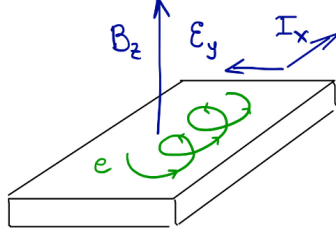


Figure 13: Classical free electrons in crossed magnetic and electric fields.

This is an inhomogeneous first-order differential equation in \dot{z} and the solution is

$$\dot{z} = Ae^{i\omega_c t} + \frac{\mathcal{E}_y}{B}, \quad z = z_0 e^{i\omega_c t} + \frac{\mathcal{E}_y t}{B} + z_1, \quad (169)$$

where $\omega_c = eB/m$ is the cyclotron frequency with electric field $\mathcal{E} = 0$, $z_0 = A/i\omega_c$ and z_1 is a constant dependent with the initial conditions. From the expression, we see the electric field along the y -direction causes the cyclotron orbits to drift in the x -direction with speed $v_x = \mathcal{E}_y/B$.

Consider now a thin metallic plate (in the xy -plane) with an electron areal density n . Applying the same field above, then we find the current density

$$J_x = -nev_x = -(ne/B)\mathcal{E}_y. \quad (170)$$

For a sample of width L_y , the current is $I_x = J_x L_y = -ne\mathcal{E}_y L_y/B$ and the voltage $V_y = -\mathcal{E}_y L_y$. Therefore, the Hall resistance is

$$R_H = \frac{V_y}{I_x} = \frac{B}{ne}. \quad (171)$$

More general, we can write the current density \mathbf{J} of the system as a linear response to applied electric fields \mathcal{E} in the x - and y -directions along the plate

$$\begin{pmatrix} J_x \\ J_y \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{pmatrix} \begin{pmatrix} \mathcal{E}_x \\ \mathcal{E}_y \end{pmatrix}, \quad (172)$$

where the matrix σ is the **conductivity tensor**. Note that this is an anti-symmetric tensor. Conversely, we can define a resistivity tensor

$$\begin{pmatrix} \mathcal{E}_x \\ \mathcal{E}_y \end{pmatrix} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ -\rho_{xy} & \rho_{xx} \end{pmatrix} \begin{pmatrix} J_x \\ J_y \end{pmatrix}, \quad (173)$$

with

$$\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}, \quad \rho_{xy} = -\frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2}. \quad (174)$$

In this way, the Hall effect can be written as

$$\sigma_{xy} = -\frac{ne}{B}, \quad \rho_{xy} = \frac{B}{en}, \quad \sigma_{xx} = 0, \quad \rho_{xx} = 0. \quad (175)$$

Therefore, the Hall effect can be used to measure the charge carrier in metals.

7.3 Interger quantum Hall effect

7.3.1 Landau levels in an electric field

Let's consider the 2D electron gas in a strong perpendicular magnetic field B and an electric field \mathcal{E} in the y -direction. In the Landau gauge $\mathbf{A} = (-By, 0, 0)$, the Hamiltonian is given by

$$\hat{H} = \frac{1}{2m} \left[-\hbar^2 \frac{\partial^2}{\partial y^2} + \left(-i\hbar \frac{\partial}{\partial x} - eBy \right)^2 \right] + e\mathcal{E}y. \quad (176)$$

This can be solved with a separable solution: $\psi(x, y) = e^{ik_x x} v_{k_x}(y)$, for a system of length L_x in the x -direction with periodic boundary conditions. The motion in the y -directions obeys

$$\hat{H}_{k_x} v_{k_x}(y) = \frac{\hbar^2}{2m} \left[-\frac{d^2}{dy^2} + \left(k_x - \frac{y}{l_B^2} \right)^2 + \frac{2me\mathcal{E}y}{\hbar^2} \right] v_{k_x}(y) = E(k_x) v_{k_x}(y). \quad (177)$$

It is a simple harmonic oscillator:

$$\hat{H}_{k_x} = \frac{\hbar\omega_c}{2} \left[-l_B^2 \frac{d^2}{dy^2} + \frac{1}{l_B^2} (y - y_{k_x} + y_\mathcal{E})^2 \right] + e\mathcal{E} \left(y_{k_x} - \frac{y_\mathcal{E}}{2} \right), \quad y_\mathcal{E} = \frac{m\mathcal{E}}{eB^2}, \quad (178)$$

where $y_{k_x} = k_x l_B^2$ is the center of the harmonic potential in the absence of an electric field. Now the centre has shifted to $y_{k_x} - y_\mathcal{E}$. The eigenenergies are

$$\begin{aligned} E_n(k_x) &= \left(n + \frac{1}{2} \right) \hbar\omega_c + e\mathcal{E} \left(y_{k_x} - \frac{y_\mathcal{E}}{2} \right) \\ &= \left(n + \frac{1}{2} \right) \hbar\omega_c + e\mathcal{E} (y_{k_x} - y_\mathcal{E}) + \frac{1}{2} m \left(\frac{\mathcal{E}}{B} \right)^2. \end{aligned} \quad (179)$$

The group velocity is

$$v_g(k_x) = \frac{1}{\hbar} \frac{\partial E_n(k_x)}{\partial k_x} = \frac{e\mathcal{E}}{\hbar} \frac{\partial y_{k_x}}{\partial k_x} = \frac{\mathcal{E}}{B}. \quad (180)$$

Recall the degeneracy of the Landau level. The number of electron states in a strip of width L_y is $g = \Phi/\Phi_0 = L_x L_y eB/h$ (per Landau level). For M filled Landau levels, the density of electrons $n = MeB/h$. The current density is

$$J_x = -nev_g = -M \frac{e^2}{h} \mathcal{E}_y. \quad (181)$$

So the conductivities are

$$\sigma_{xy} = -M \frac{e^2}{h}, \quad \sigma_{xx} = 0. \quad (182)$$

One can easily check the cyclotron drift current is independent of Landau level index. So, if there are M occupied Landau levels, then the contributions add up and $\sigma_{xy} = -Me^2/h$.

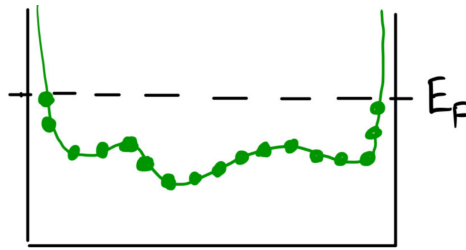


Figure 14: The energy of an edge state arising from that Landau level can still cross the Fermi level.

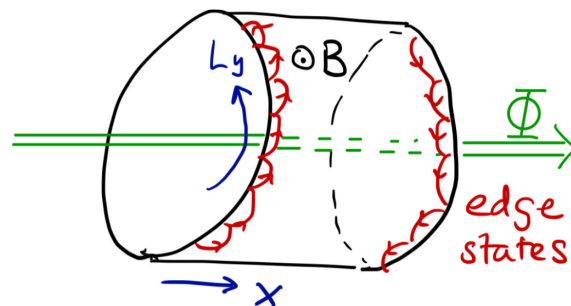


Figure 15: Take the two-dimensional electron gas and wrap the sheet in the y -direction so that it is now a cylinder of circumference L_y with the axis of symmetry in the x -direction.

7.3.2 Edge states

If the Fermi level lies between two Landau levels, then the system should be an insulator. So where does the current come from in the quantum Hall regime? It turns out that there is always an edge state at the Fermi level. In other words, this two-dimensional insulator has a metallic perimeter!

If we have filled Landau levels in the bulk, the Fermi level E_F is above the bulk Landau level energy $(n + 1/2)\hbar\omega_c$. However, the energy of an edge state arising from that Landau level can still cross the Fermi level, as depicted in Fig. 14. This means that there is a one-dimensional conduction channel at the edge of this insulating system! This is the first example **topological insulator**.

7.3.3 Laughlin's gauge argument: adiabatic transport

Laughlin provided an important insight⁸ into the physics of the quantum Hall effect. This makes use of the **Aharonov-Bohm effect**, **adiabatic continuity** and **Thouless pumping**.

Laughlin proposed the following thought experiment. Take the two-dimensional electron gas and wrap the sheet in the y -direction so that it is now a cylinder of circumference L_y with the axis of symmetry in the x -direction (see Fig. 15).

According to Faraday's law $\dot{\Phi} = -\oint_{L_y} \mathcal{E}_y dy$, electromotive force (emf) can be produced by the change in magnetic flux, i.e., $\mathcal{E}_y = -\dot{\Phi}/L_y$. Suppose the rate of flux introduction is such that the flux Φ changes by a flux quantum $\Phi_0 = h/e$ in time T ,

then

$$V_y = -\mathcal{E}_y L_y = \frac{\Phi_0}{T} = \frac{h}{eT}. \quad (183)$$

In the adiabatic process, electrons cannot be excited to higher Landau levels, and only the edge states near Fermi level can be affected. Suppose there are M electrons transported from one edge to another edge, then the current density

$$J_x = -M \frac{e^2}{h} \mathcal{E}_y = -\frac{eM}{TL_y}. \quad (184)$$

The conductivity is

$$\sigma_{xy} = \frac{J_x}{\mathcal{E}_y} = -M \frac{e^2}{h}. \quad (185)$$

This general argument is also applicable to disordered systems.

7.4 Kubo formula

7.4.1 Linear response theory

Now we derive the response of system \hat{H}_0 perturbation \hat{H}_1 switched on at $t = 0$. Then the Hamiltonian of the system is $\hat{H} = \hat{H}_0 + \hat{H}_1$ and the Schrödinger equation:

$$\hat{H} |\psi(t)\rangle = i\hbar \partial_t |\psi(t)\rangle. \quad (186)$$

We can take the eigenstates $|\mu\rangle$ of \hat{H}_0 as basis: $\hat{H}_0 |\mu\rangle = E_\mu |\mu\rangle$. The evolution under \hat{H}_0

$$|\mu(t)\rangle = e^{-iE_\mu t/\hbar} |\mu(0)\rangle, \quad (187)$$

$$|\psi_0(t)\rangle = \hat{U}_0(t) |\psi(0)\rangle = e^{-i\hat{H}_0 t/\hbar} |\psi(0)\rangle. \quad (188)$$

The evolution under \hat{H} is $|\psi(t)\rangle = \hat{U}(t, 0) |\psi(0)\rangle$. The evolution operator $\hat{U}(t, 0)$ can be divided into small time steps δt :

$$\begin{aligned} \hat{U}(t, 0) &= \exp \left[-\frac{i}{\hbar} \int_0^t \hat{H}(t') dt' \right] \\ &\simeq \exp \left[-\frac{i}{\hbar} \delta t (\hat{H}_0 + \hat{H}_1) \right]_t \dots \exp \left[-\frac{i}{\hbar} \delta t (\hat{H}_0 + \hat{H}_1) \right]_0 \\ &= \left[e^{-i\delta t \hat{H}_0/\hbar} \left(1 - \frac{i}{\hbar} \delta t \hat{H}_1 \right) \right]_t \dots \left[e^{-i\delta t \hat{H}_0/\hbar} \left(1 - \frac{i}{\hbar} \delta t \hat{H}_1 \right) \right]_0 \\ &= \hat{U}_0(t) + \sum_{i=0}^{t/\delta t} \hat{U}_0(t - t_i) \left(-\frac{i}{\hbar} \delta t \hat{H}_1(t_i) \right) \hat{U}_0(t_i) + \dots \\ &= \hat{U}_0(t) - \frac{i}{\hbar} \int_0^t dt' \hat{U}_0(t - t') \hat{H}_1(t') \hat{U}_0(t') + \dots \end{aligned} \quad (189)$$

If we measure the operator \hat{O} at time t , the expectation value is

$$O(t) = \langle \psi(t) | \hat{O} | \psi(t) \rangle = \langle \psi(0) | \hat{U}^\dagger(t, 0) \hat{O} \hat{U}(t, 0) | \psi(0) \rangle = \langle \psi(0) | \hat{O}(t) | \psi(0) \rangle, \quad (190)$$

where

$$\begin{aligned}
\hat{O}(t) &= \hat{U}^\dagger(t, 0) \hat{O} \hat{U}(t, 0) = \hat{U}(0, t) \hat{O} \hat{U}(t, 0) \\
&\simeq \hat{U}_0(-t) \hat{O} \hat{U}_0(t) - \frac{i}{\hbar} \hat{U}_0(-t) \hat{O} \int_0^t dt' \hat{U}_0(t-t') \hat{H}_1(t') \hat{U}_0(t') \\
&\quad + \frac{i}{\hbar} \hat{U}_0(-t) \hat{O} \int_0^t dt' \hat{H}_1(t') \hat{U}_0(t-t') \hat{O} \hat{U}_0(t).
\end{aligned} \tag{191}$$

The first term corresponds to the unperturbed expectation value; the second and third terms correspond to the response to first order in perturbation \hat{H}_1 .

7.4.2 Conductivity as linear response

We introduce a small change to the vector potential: $\mathbf{A} \rightarrow \mathbf{A} + \mathbf{a} \cos(\omega t)$, then the electric field $\mathcal{E}_y = -\partial_t a_y(t)$. Now we can write the Hamiltonians of the system:

$$\hat{H}_0 = \frac{1}{2m} (-i\hbar\nabla + e\mathbf{A})^2 + V(\mathbf{r}), \tag{192}$$

$$\hat{H}_1 = ea_y \cos(\omega t) \hat{v}_y + \mathcal{O}(a^2), \tag{193}$$

where $\hat{v} = (-i\hbar\nabla + e\mathbf{A})/m$. Then measure the current $\hat{O} = -e\hat{v}_x$. According to the linear response theory, we use Hall conductivity as the linear response function:

$$\sigma_{xy} = -\frac{ie^2\hbar}{L_x L_y} \sum_{E_\nu < E_F < E_\mu} \frac{\langle \nu | \hat{v}_x | \mu \rangle \langle \mu | \hat{v}_y | \nu \rangle - \langle \nu | \hat{v}_y | \mu \rangle \langle \mu | \hat{v}_x | \nu \rangle}{(E_\mu - E_\nu)^2}, \tag{194}$$

where $|\mu\rangle$ and $|\nu\rangle$ are eigenstates in the absence of \mathcal{E}_y . This is also called the **Kubo formula**. The Hall conductivity can also be expressed as

$$\sigma_{xy} = \frac{e^2}{h} \sum_{E_n < E_F} C_n, \quad C_n = \int_{\text{BZ}} \frac{d^2\mathbf{k}}{2\pi i} [\langle \partial_{k_x} n | \partial_{k_y} n \rangle - \langle \partial_{k_y} n | \partial_{k_x} n \rangle] = \text{integer} \tag{195}$$

The Chern number for each band n is called the **TKNN** (Thouless-Kohmoto-Nightingale-Nijs) invariant for the band. We see that the quantisation of the Hall conductivity for a system with filled Landau bands is intimately connected with a topological invariant of the electron bands.

8 Carbon and carbon allotropes

8.1 The carbon atom

The ground state configuration of carbon atom electrons is $1s^2 2s^2 2p^2$. The **core electrons**, which are located in $1s^2$, stay close to the carbon atom. They do not participate directly in bond formation. The **valence electrons**, located in $2s^2 2p^2$, participate in binding and conduction.

For the $2s$ and $2p$ states, the angular solutions for the wave functions are

$$Y_{0,0}(\theta, \phi) = \frac{1}{\sqrt{4\pi}}, \quad Y_{1,\pm 1}(\theta, \phi) = \mp \sqrt{\frac{3}{8\pi}} e^{\pm i\phi} \sin \theta, \quad Y_{1,0}(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta, \quad (196)$$

which are normalized to unity over the unit sphere. Alternative forms as angular solutions are obtained by a unitary transformation to real functions, which, in Dirac notation, are

$$|s\rangle = \frac{1}{\sqrt{4\pi}}, \quad (197)$$

$$|p_x\rangle = \sqrt{\frac{3}{4\pi}} \cos \phi \sin \theta, \quad |p_y\rangle = \sqrt{\frac{3}{4\pi}} \sin \phi \sin \theta, \quad |p_z\rangle = \sqrt{\frac{3}{4\pi}} \cos \theta. \quad (198)$$

8.2 Hybridization and the structure of carbon allotropes

The superposition of the $|2s\rangle$ with $n|2p_\alpha\rangle$ ($\alpha = x, y, z$) states is known as sp^n hybridization.

1. The hybridization sp^1 is found in one-dimensional atomic chains known as carbynes. For sp^1 hybridization, the unitary transformation from the atomic basis ($|s\rangle, |p_x\rangle$) to the basis ($|\varphi_1\rangle, |\varphi_2\rangle$) is

$$|\varphi_1\rangle = \frac{1}{\sqrt{2}}(|s\rangle + |p_x\rangle), \quad |\varphi_2\rangle = \frac{1}{\sqrt{2}}(|s\rangle - |p_x\rangle). \quad (199)$$

2. Hybridization sp^2 is found in 2D structures such as graphite, graphene, fullerenes, and nanotubes. The corresponding hybridization is given by the transformation from the atomic ($|s\rangle, |p_x\rangle, |p_y\rangle$) basis to the basis ($|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle$), where

$$|\varphi_1\rangle = \frac{1}{\sqrt{3}} \left(|s\rangle + \sqrt{\frac{3}{2}} |p_x\rangle + \frac{1}{\sqrt{2}} |p_y\rangle \right), \quad (200)$$

$$|\varphi_2\rangle = \frac{1}{\sqrt{3}} \left(|s\rangle - \sqrt{\frac{3}{2}} |p_x\rangle + \frac{1}{\sqrt{2}} |p_y\rangle \right), \quad (201)$$

$$|\varphi_3\rangle = \frac{1}{\sqrt{3}} \left(|s\rangle - \sqrt{2} |p_y\rangle \right). \quad (202)$$

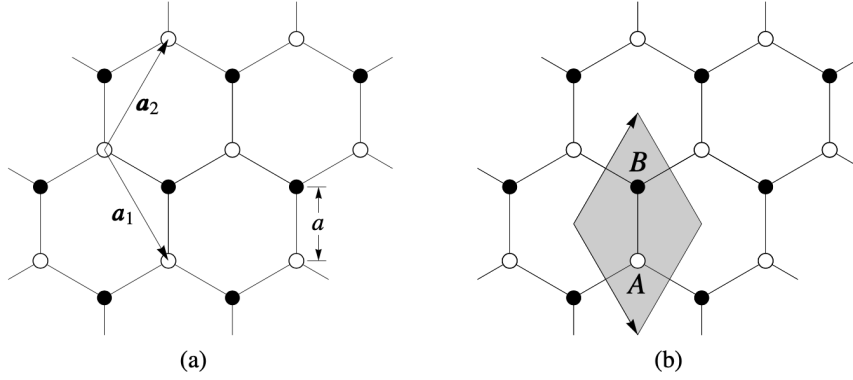


Figure 16: (a) The honeycomb lattice of graphene showing the two different types of atoms, indicated by filled and unfilled circles. As these atoms have different environments, the honeycomb lattice is not a Bravais lattice. The lattice spacing a and the primitive unit vectors \mathbf{a}_1 and \mathbf{a}_2 are indicated. (b) The graphene lattice with the unit cell (shown shaded) and the primitive unit vectors in (a), which define the edges of the unit cell. The unit cell contains one of each type of atom in the lattice.

3. Hybridization sp^3 is found in the diamond structure. The corresponding hybridization is given by the transformation from the atomic ($|s\rangle, |p_x\rangle, |p_y\rangle, |p_z\rangle$) basis to the basis ($|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle, |\varphi_4\rangle$), where

$$|\varphi_1\rangle = \frac{1}{2} (|s\rangle + |p_x\rangle + |p_y\rangle + |p_z\rangle), \quad (203)$$

$$|\varphi_2\rangle = \frac{1}{2} (|s\rangle - |p_x\rangle - |p_y\rangle + |p_z\rangle), \quad (204)$$

$$|\varphi_3\rangle = \frac{1}{2} (|s\rangle - |p_x\rangle + |p_y\rangle - |p_z\rangle), \quad (205)$$

$$|\varphi_4\rangle = \frac{1}{2} (|s\rangle + |p_x\rangle - |p_y\rangle - |p_z\rangle), \quad (206)$$

$$(207)$$

8.3 Crystallography of Graphene

The honeycomb lattice of graphene is not a Bravais lattice because not all atoms have the same environment. There are two distinct atoms A and B , and the primitive lattice vectors of the graphene lattice are

$$\mathbf{a}_1 = \frac{a\sqrt{3}}{2}(\mathbf{i} - \sqrt{3}\mathbf{j}), \quad \mathbf{a}_2 = \frac{a\sqrt{3}}{2}(\mathbf{i} + \sqrt{3}\mathbf{j}). \quad (208)$$

The primitive vectors \mathbf{b}_1 and \mathbf{b}_2 of the reciprocal lattice for graphene are

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{k}}{|\mathbf{a}_1 \times \mathbf{a}_2|} = \frac{2\pi}{a\sqrt{3}} \left(\mathbf{i} - \frac{\mathbf{j}}{\sqrt{3}} \right), \quad (209)$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{k} \times \mathbf{a}_1}{|\mathbf{a}_1 \times \mathbf{a}_2|} = \frac{2\pi}{a\sqrt{3}} \left(\mathbf{i} + \frac{\mathbf{j}}{\sqrt{3}} \right). \quad (210)$$

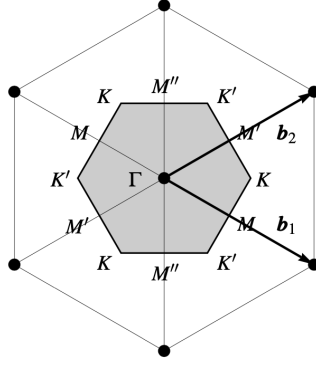


Figure 17: Reciprocal lattice with the first Brillouin zone (shaded) and points on its boundary.

9 Electronic states in graphene

9.1 The tight-binding method

The tight-binding method is a semi-empirical method that is used to calculate the energy bands and Bloch states of a material. The specific assumptions of the tight-binding method are:

1. Near each atomic site, the Hamiltonian of the crystal is a good approximation to the full Hamiltonian for the atom.
2. The atomic states are localized around the atomic sites, with a small overlap with the states on neighbouring sites.
3. The Bloch sum is a good approximation to the Bloch functions.

We begin with the assumption that an electron bound to a particular atom at lattice position \mathbf{R}_i . Based on these assumptions, we can write the trial wave function $\psi_{\mathbf{k}}(\mathbf{r})$ of the system in the form of a **Bloch sum**:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_i} e^{i\mathbf{k} \cdot \mathbf{R}_i} \phi(\mathbf{r} - \mathbf{R}_i), \quad (211)$$

where N is the number of unit cells in the crystal, and $\mathbf{k} = (k_x, k_y)$ is the two-dimensional wave vector. We now show this wave function satisfies Bloch's theorem.

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_i} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{r})} \phi(\mathbf{r} - \mathbf{R}_i) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{\mathbf{k}}(\mathbf{r}), \quad (212)$$

where

$$u_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_i} e^{-i\mathbf{k} \cdot (\mathbf{r} - \mathbf{R}_i)} \phi(\mathbf{r} - \mathbf{R}_i). \quad (213)$$

So we have

$$\begin{aligned}
u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}_j) &= \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_i} e^{-i\mathbf{k}\cdot(\mathbf{r}+\mathbf{R}_j-\mathbf{R}_i)} \phi(\mathbf{r} + \mathbf{R}_j - \mathbf{R}_i) \\
&= \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_k} e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_k)} \phi(\mathbf{r} - \mathbf{R}_k) = u_{\mathbf{k}}(\mathbf{r}),
\end{aligned} \tag{214}$$

where $\mathbf{R}_k = \mathbf{R}_i - \mathbf{R}_j$. Thus, $u_{\mathbf{k}}(\mathbf{r})$ has the periodicity of the lattice and $\psi_{\mathbf{k}}(\mathbf{r})$ is a Bloch function:

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}), \quad u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}_i) = u_{\mathbf{k}}(\mathbf{r}). \tag{215}$$

Then we can calculate the energy dispersion $E(\mathbf{k})$:

$$\begin{aligned}
E(\mathbf{k}) &= \langle \psi_{\mathbf{k}}(\mathbf{r}) | \hat{H} | \psi_{\mathbf{k}}(\mathbf{r}) \rangle \\
&= \frac{1}{N} \sum_{\mathbf{R}_i} \sum_{\mathbf{R}_j} e^{i\mathbf{k}\cdot(\mathbf{R}_j-\mathbf{R}_i)} \langle \phi(\mathbf{r} - \mathbf{R}_i) | \hat{H} | \phi(\mathbf{r} - \mathbf{R}_j) \rangle \\
&= \frac{1}{N} \sum_{\mathbf{R}_i} \sum_{\mathbf{R}_j} e^{i\mathbf{k}\cdot(\mathbf{R}_j-\mathbf{R}_i)} \langle \phi(\mathbf{r}') | \hat{H} | \phi(\mathbf{r}' - (\mathbf{R}_j - \mathbf{R}_i)) \rangle \\
&= \sum_{\mathbf{R}_k} e^{i\mathbf{k}\cdot\mathbf{R}_k} \langle \phi(\mathbf{r}') | \hat{H} | \phi(\mathbf{r}' - \mathbf{R}_k) \rangle,
\end{aligned} \tag{216}$$

where $\mathbf{r}' = \mathbf{r} - \mathbf{R}_i$ and $\mathbf{R}_k = \mathbf{R}_j - \mathbf{R}_i$. Consider the case $\mathbf{R}_k = 0$, then the integral $\langle \phi(\mathbf{r}') | \hat{H} | \phi(\mathbf{r}' - \mathbf{R}_k) \rangle$ reduces to

$$\langle \phi(\mathbf{r}') | \hat{H} | \phi(\mathbf{r}') \rangle = E_0 \langle \phi(\mathbf{r}') | \phi(\mathbf{r}') \rangle = E_0, \tag{217}$$

where E_0 is the energy of the atomic state ϕ . If the k th nearest neighbours are located at the positions $\mathbf{R}_k = \boldsymbol{\tau}_k$, then

$$E(\mathbf{k}) = E_0 + \sum_{\boldsymbol{\tau}_k} e^{i\mathbf{k}\cdot\boldsymbol{\tau}_k} \langle \phi(\mathbf{r}') | \hat{H} | \phi(\mathbf{r}' - \boldsymbol{\tau}_k) \rangle = E_0 + \sum_{\boldsymbol{\tau}_k} e^{i\mathbf{k}\cdot\boldsymbol{\tau}_k} t(|\boldsymbol{\tau}_k|), \tag{218}$$

where $t(|\boldsymbol{\tau}_k|) = \langle \phi(\mathbf{r}') | \hat{H} | \phi(\mathbf{r}' - \boldsymbol{\tau}_k) \rangle$ is a **hopping integral** that describes the coupling between an orbital at the origin to one at the k th neighbour shell.

9.2 Tight-binding formulation for graphene

Graphene has two atoms A and B per unit cell, with each atom contributing 4 electrons to the bonding: 3 to the σ -bonds between adjacent atoms for binding, and 1 π -orbital which is perpendicular to the graphene for conduction. We will consider only the π electrons. The Bloch sums for the two atomic types A and B are

$$\psi_{\mathbf{k}}^{(\alpha)}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_\alpha} e^{i\mathbf{k}\cdot\mathbf{R}_\alpha} \phi_\alpha(\mathbf{r} - \mathbf{R}_\alpha), \quad \alpha = A, B. \tag{219}$$

The trial wave function for graphene is a Bloch sum:

$$\psi_{\mathbf{k}}(\mathbf{r}) = a_{\mathbf{k}} \psi_{\mathbf{k}}^{(A)}(\mathbf{r}) + b_{\mathbf{k}} \psi_{\mathbf{k}}^{(B)}(\mathbf{r}) \tag{220}$$

where the coefficients $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ are to be determined. This wave function is a solution of the Schrödinger equation $\hat{H}\psi_{\mathbf{k}} = E_{\mathbf{k}}\psi_{\mathbf{k}}$, i.e.,

$$\hat{H} \left[a_{\mathbf{k}}\psi_{\mathbf{k}}^{(A)}(\mathbf{r}) + b_{\mathbf{k}}\psi_{\mathbf{k}}^{(B)}(\mathbf{r}) \right] = E_{\mathbf{k}} \left[a_{\mathbf{k}}\psi_{\mathbf{k}}^{(A)}(\mathbf{r}) + b_{\mathbf{k}}\psi_{\mathbf{k}}^{(B)}(\mathbf{r}) \right]. \quad (221)$$

Multiply in turn by $\psi_{\mathbf{k}}^{(A)*}(\mathbf{r})$ and $\psi_{\mathbf{k}}^{(B)*}(\mathbf{r})$, and integrating over the unit cell. Using Dirac notation, we obtain

$$a_{\mathbf{k}} \langle A, \mathbf{k} | \hat{H} | A, \mathbf{k} \rangle + b_{\mathbf{k}} \langle A, \mathbf{k} | \hat{H} | B, \mathbf{k} \rangle = a_{\mathbf{k}} E_{\mathbf{k}} \langle A, \mathbf{k} | A, \mathbf{k} \rangle + b_{\mathbf{k}} E_{\mathbf{k}} \langle A, \mathbf{k} | B, \mathbf{k} \rangle, \quad (222)$$

$$a_{\mathbf{k}} \langle B, \mathbf{k} | \hat{H} | A, \mathbf{k} \rangle + b_{\mathbf{k}} \langle B, \mathbf{k} | \hat{H} | B, \mathbf{k} \rangle = a_{\mathbf{k}} E_{\mathbf{k}} \langle B, \mathbf{k} | A, \mathbf{k} \rangle + b_{\mathbf{k}} E_{\mathbf{k}} \langle B, \mathbf{k} | B, \mathbf{k} \rangle. \quad (223)$$

By using the abbreviated notation $(H_{\mathbf{k}})_{\alpha\beta} = \langle \alpha, \mathbf{k} | \hat{H} | \beta, \mathbf{k} \rangle$ and $(S_{\mathbf{k}})_{\alpha\beta} = \langle \alpha, \mathbf{k} | \beta, \mathbf{k} \rangle$, the equations simplify to

$$(H_{\mathbf{k}})_{AA}a_{\mathbf{k}} + (H_{\mathbf{k}})_{AB}b_{\mathbf{k}} = E_{\mathbf{k}}(S_{\mathbf{k}})_{AA}a_{\mathbf{k}} + E_{\mathbf{k}}(S_{\mathbf{k}})_{AB}b_{\mathbf{k}}, \quad (224)$$

$$(H_{\mathbf{k}})_{BA}a_{\mathbf{k}} + (H_{\mathbf{k}})_{BB}b_{\mathbf{k}} = E_{\mathbf{k}}(S_{\mathbf{k}})_{BA}a_{\mathbf{k}} + E_{\mathbf{k}}(S_{\mathbf{k}})_{BB}b_{\mathbf{k}}, \quad (225)$$

which can be expressed in matrix form:

$$\begin{pmatrix} (H_{\mathbf{k}})_{AA} - E_{\mathbf{k}}(S_{\mathbf{k}})_{AA} & (H_{\mathbf{k}})_{AB} - E_{\mathbf{k}}(S_{\mathbf{k}})_{AB} \\ (H_{\mathbf{k}})_{BA} - E_{\mathbf{k}}(S_{\mathbf{k}})_{BA} & (H_{\mathbf{k}})_{BB} - E_{\mathbf{k}}(S_{\mathbf{k}})_{BB} \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ b_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (226)$$

The eigenvalues $E_{\mathbf{k}}$ obtained from solutions of the secular equation

$$\det(H_{\mathbf{k}} - E_{\mathbf{k}}S_{\mathbf{k}}) = 0. \quad (227)$$

9.2.1 Nearest-neighbour approximation

We first consider the diagonal elements $(H_{\mathbf{k}})_{\alpha\alpha}$ and $(S_{\mathbf{k}})_{\alpha\alpha}$. For $\alpha = A$, we have

$$\begin{aligned} (H_{\mathbf{k}})_{AA} &= \frac{1}{N} \sum_{\mathbf{R}_A} \sum_{\mathbf{R}'_A} e^{i\mathbf{k} \cdot (\mathbf{R}'_A - \mathbf{R}_A)} \langle \phi_A(\mathbf{r} - \mathbf{R}_A) | \hat{H} | \phi_A(\mathbf{r} - \mathbf{R}'_A) \rangle \\ &= \sum_{\mathbf{R}_A} e^{i\mathbf{k} \cdot \mathbf{R}_A} \langle \phi_A(\mathbf{r}) | \hat{H} | \phi_A(\mathbf{r} - \mathbf{R}_A) \rangle, \end{aligned} \quad (228)$$

$$\begin{aligned} (S_{\mathbf{k}})_{AA} &= \frac{1}{N} \sum_{\mathbf{R}_A} \sum_{\mathbf{R}'_A} e^{i\mathbf{k} \cdot (\mathbf{R}'_A - \mathbf{R}_A)} \langle \phi_A(\mathbf{r} - \mathbf{R}_A) | \phi_A(\mathbf{r} - \mathbf{R}'_A) \rangle \\ &= \sum_{\mathbf{R}_A} e^{i\mathbf{k} \cdot \mathbf{R}_A} \langle \phi_A(\mathbf{r}) | \phi_A(\mathbf{r} - \mathbf{R}_A) \rangle. \end{aligned} \quad (229)$$

Since there is only one A -atom in the unit cell, $\mathbf{R}_A = 0$, then

$$(H_{\mathbf{k}})_{AA} \approx \langle \phi_A(\mathbf{r}) | \hat{H} | \phi_A(\mathbf{r}) \rangle \approx E_0, \quad (230)$$

$$(S_{\mathbf{k}})_{AA} \approx \langle \phi_A(\mathbf{r}) | \phi_A(\mathbf{r}) \rangle = 1, \quad (231)$$

where E_0 is the energy of the atomic $2p$ level. Similarly,

$$(H_{\mathbf{k}})_{BB} = (H_{\mathbf{k}})_{AA} \approx E_0, \quad (S_{\mathbf{k}})_{BB} = (S_{\mathbf{k}})_{AA} \approx 1. \quad (232)$$

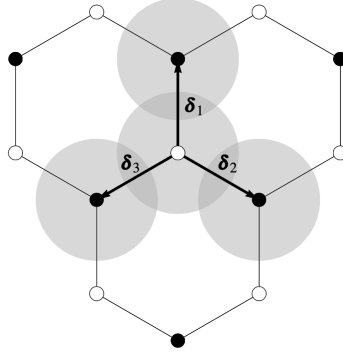


Figure 18: An A -atom (open circle) and nearest-neighbor B -atoms (filled circles) at positions δ_1 , δ_2 , and δ_3 with respect to that A -atom. The shaded circles indicate the circular symmetry of the p_z orbitals with respect to each atomic centre.

We now turn our attention to the off-diagonal matrix elements

$$(H_{\mathbf{k}})_{AB} = \frac{1}{N} \sum_{\mathbf{R}_A} \sum_{\mathbf{R}_B} e^{i\mathbf{k} \cdot (\mathbf{R}_A - \mathbf{R}_B)} \langle \phi_A(\mathbf{r} - \mathbf{R}_A) | \hat{H} | \phi_B(\mathbf{r} - \mathbf{R}_B) \rangle. \quad (233)$$

Taking an A -atom as a reference, the three nearest-neighbor B -atoms are located at positions δ_1 , δ_2 , and δ_3 with respect to that A -atom

$$\delta_1 = a\mathbf{j}, \quad \delta_2 = \frac{a\sqrt{3}}{2}\mathbf{i} - \frac{a}{2}\mathbf{j}, \quad \delta_3 = -\frac{a\sqrt{3}}{2}\mathbf{i} - \frac{a}{2}\mathbf{j}. \quad (234)$$

the positions of B atoms are $\mathbf{R}_B - \mathbf{R}_A = \delta_i$, for $i = 1, 2, 3$. Thus, the nearest-neighbor approximation to the matrix element

$$\begin{aligned} (H_{\mathbf{k}})_{AB} = \frac{1}{N} \sum_{\mathbf{R}_A} [& e^{i\mathbf{k} \cdot \delta_1} \langle \phi_A(\mathbf{r} - \mathbf{R}_A) | \hat{H} | \phi_B(\mathbf{r} - (\mathbf{R}_A + \delta_1)) \rangle \\ & + e^{i\mathbf{k} \cdot \delta_2} \langle \phi_A(\mathbf{r} - \mathbf{R}_A) | \hat{H} | \phi_B(\mathbf{r} - (\mathbf{R}_A + \delta_2)) \rangle \\ & + e^{i\mathbf{k} \cdot \delta_3} \langle \phi_A(\mathbf{r} - \mathbf{R}_A) | \hat{H} | \phi_B(\mathbf{r} - (\mathbf{R}_A + \delta_3)) \rangle]. \end{aligned} \quad (235)$$

The circular symmetry of the p_z orbitals about each site means that each of the three integrals on the right-hand side has the same value. We can define

$$t = \langle \phi_A(\mathbf{r} - \mathbf{R}_A) | \hat{H} | \phi_B(\mathbf{r} - (\mathbf{R}_A + \delta_i)) \rangle, \quad i = 1, 2, 3. \quad (236)$$

So the matrix element

$$\begin{aligned} (H_{\mathbf{k}})_{AB} &= t (e^{i\mathbf{k} \cdot \delta_1} + e^{i\mathbf{k} \cdot \delta_2} + e^{i\mathbf{k} \cdot \delta_3}) \\ &= t \left[e^{ik_y a} + \exp\left(\frac{ik_x a \sqrt{3}}{2} - \frac{ik_y a}{2}\right) + \exp\left(-\frac{ik_x a \sqrt{3}}{2} - \frac{ik_y a}{2}\right) \right] \\ &= t \left[e^{ik_y a} + 2 \exp\left(-\frac{ik_y a}{2}\right) \cos\left(\frac{k_x a \sqrt{3}}{2}\right) \right] = t f(\mathbf{k}). \end{aligned} \quad (237)$$

And similarly,

$$(H_{\mathbf{k}})_{BA} = (H_{\mathbf{k}})_{AB}^* = tf^*(\mathbf{k}), \quad (S_{\mathbf{k}})_{AB} = (S_{\mathbf{k}})_{BA}^* = sf(\mathbf{k}), \quad (238)$$

where

$$s = \langle \phi_A(\mathbf{r} - \mathbf{R}_A) | \phi_B(\mathbf{r} - (\mathbf{R}_A + \boldsymbol{\delta}_i)) \rangle, \quad i = 1, 2, 3. \quad (239)$$

9.2.2 Energy bands of graphene

From the results of the previous section, the matrix elements of the Hamiltonian and the overlap matrix are

$$H_{\mathbf{k}} = \begin{pmatrix} E_0 & tf(\mathbf{k}) \\ tf^*(\mathbf{k}) & E_0 \end{pmatrix}, \quad S_{\mathbf{k}} = \begin{pmatrix} 1 & sf(\mathbf{k}) \\ sf^*(\mathbf{k}) & 1 \end{pmatrix}, \quad (240)$$

then

$$\det(H_{\mathbf{k}} - E_{\mathbf{k}}S_{\mathbf{k}}) = (E_0 - E_{\mathbf{k}})^2 - (t - sE_{\mathbf{k}})^2|f(\mathbf{k})|^2 = 0. \quad (241)$$

This yields

$$E_{\pm}(\mathbf{k}) = \frac{E_0 \pm t|f(\mathbf{k})|}{1 \pm s|f(\mathbf{k})|}, \quad (242)$$

where

$$\begin{aligned} |f(\mathbf{k})| &= \sqrt{f(\mathbf{k})f^*(\mathbf{k})} \\ &= \sqrt{1 + 4 \cos\left(\frac{3k_y a}{2}\right) \cos\left(\frac{k_x a \sqrt{3}}{2}\right) + 4 \cos^2\left(\frac{k_x a \sqrt{3}}{2}\right)}. \end{aligned} \quad (243)$$

There are three fitting parameters in the energy dispersion: E_0 (atomic energy level), t (hopping parameter), and s (overlap parameter). These parameters can be determined from first principles calculations or estimated from experiments. We use

$$E_0 = 0, \quad t = -3.033 \text{ eV}, \quad s = 0.129. \quad (244)$$

The two bands $E_{\pm}(\mathbf{k})$ meet at the **Dirac points** \mathbf{K} and \mathbf{K}' . The dispersion of the energy bands near the cusp at the \mathbf{K} points is *linear* in \mathbf{k} . The typical dispersion of an energy band near an extremum is quadratic in \mathbf{k} , as is seen near the Γ point (the origin of \mathbf{k}).

9.3 Low-energy dispersion and the Dirac equation

The \mathbf{K} points in the graphene satisfy $f(\mathbf{K}_{\xi}) = 0$. This gives

$$\mathbf{K}_{\xi} = \xi \left(\frac{4\pi}{3a\sqrt{3}} \right) \mathbf{i}, \quad (245)$$

where $\xi = \pm 1$ ($\xi = 1$ refers to \mathbf{K} and $\xi = -1$ refers to \mathbf{K}'). Defining $\mathbf{k} = \mathbf{K}_{\xi} + \mathbf{p}$, so we have

$$k_x = \frac{4\pi\xi}{3a\sqrt{3}} + p_x, \quad k_y = p_y. \quad (246)$$

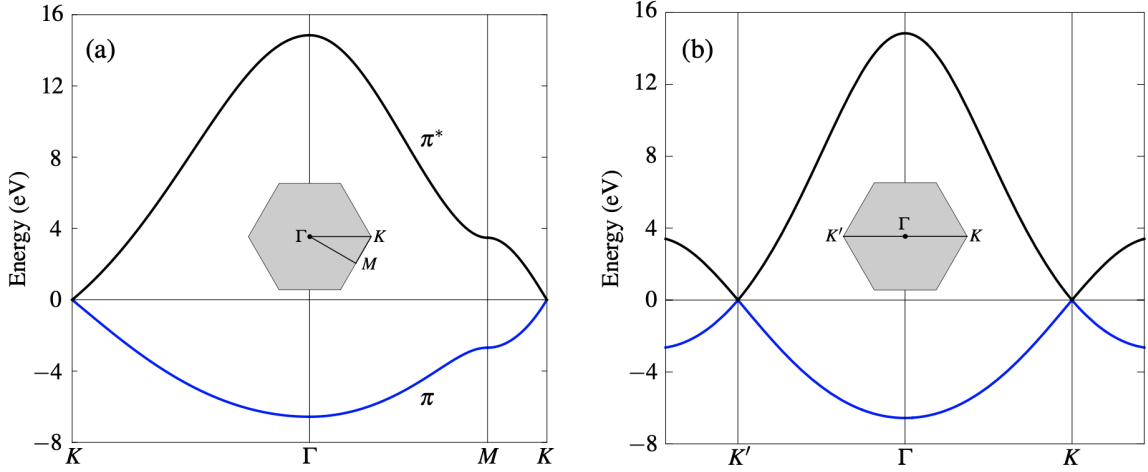


Figure 19: The energy bands for graphene.

Thus

$$f(\mathbf{K}_\xi + \mathbf{p}) = -\frac{3a}{2}(p_x\xi - ip_y) + \dots, \quad (247)$$

$$|f(\mathbf{K}_\xi + \mathbf{p})| = \frac{3a}{2}\sqrt{p_x^2 + p_y^2} = \frac{3a|\mathbf{p}|}{2}. \quad (248)$$

The dispersion near the \mathbf{K} points are

$$E_\pm(\mathbf{p}) = \pm \frac{t|f(\mathbf{k})|}{1 \pm s|f(\mathbf{k})|} \approx \pm \frac{3at|\mathbf{p}|}{2} = \pm \hbar v|\mathbf{p}|, \quad (249)$$

where v is the speed of the electrons in the linear regime of the dispersion relation:

$$v = \frac{3a|t|}{2\hbar} \simeq \frac{c}{300}. \quad (250)$$

Recall the Hamiltonian. We have set $E_0 = 0$, so the linearized form of the Hamiltonian is

$$\hat{H}(\mathbf{p}) = -\frac{3ta}{2} \begin{pmatrix} 0 & \xi p_x - ip_y \\ \xi p_x + ip_y & 0 \end{pmatrix} = \hbar v(\xi p_x \hat{\sigma}_x + p_y \hat{\sigma}_y). \quad (251)$$

9.4 Pseudospin and chirality

Using the identifications

$$p_x = -i\hbar\partial_x, \quad p_y = -i\hbar\partial_y, \quad (252)$$

we write the effective Hamiltonian as

$$\hat{H} = -i\hbar v \begin{pmatrix} 0 & \xi\partial_x - i\partial_y \\ \xi\partial_x + i\partial_y & 0 \end{pmatrix}. \quad (253)$$

Solve the eigenfunction $\hat{H}\psi = E\psi$, in which ψ is a two-component spinor

$$\psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}, \quad (254)$$

where α and β are to be determined, and $\mathbf{r} = (x, y)$. Then

$$-i\hbar \frac{\partial \psi}{\partial x} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} p_x, \quad -i\hbar \frac{\partial \psi}{\partial y} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} p_y. \quad (255)$$

The eigenfunction becomes

$$\begin{pmatrix} -E & v(\xi p_x - i p_y) \\ v(\xi p_x + i p_y) & -E \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (256)$$

This yields the eigenvalues $E_{\pm} = \pm v \sqrt{p_x^2 + p_y^2} = \pm v p$. This relation gives

$$v(\xi p_x + i p_y)\alpha + v p \beta = 0 \quad \Rightarrow \quad \frac{\xi p_x + i p_y}{p} = -\frac{\beta}{\alpha} = \xi e^{i\xi\varphi}, \quad (257)$$

where

$$p_x = p \cos \varphi, \quad p_y = p \sin \varphi. \quad (258)$$

The corresponding eigenvectors

$$\psi_{\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm \xi e^{i\xi\varphi} \end{pmatrix} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}. \quad (259)$$

To simplify the calculation, we use the notation $\psi_{\pm} = |\pm\rangle$. The lower sign(-) refers to the lower (valence) band and the upper sign (+) to the upper (conduction) band, $\xi = 1$ to the K -point in the Brillouin zone and $\xi = -1$ to the K' point. The two eigenfunctions are orthogonal and normalized:

$$\langle \pm | \pm \rangle = 1, \quad \langle \pm | \mp \rangle = 0. \quad (260)$$

The electron density localised on the A sites corresponds to a pseudo-spin ‘‘up’’ state, and the electron density localized on the B sites corresponds to a pseudo-spin ‘‘down’’ state:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\uparrow\rangle, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\downarrow\rangle. \quad (261)$$

So the eigenvectors

$$\psi_{\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm \xi e^{i\xi\varphi} \end{pmatrix} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} = \frac{1}{\sqrt{2}} (|\uparrow\rangle \pm \xi e^{i\xi\varphi} |\downarrow\rangle) e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}. \quad (262)$$

In addition to the pseudospin degree of freedom, the electrons are chiral, meaning that the orientation of the pseudospin is related to the direction of momentum. The spinor part of the Hamiltonian

$$\hat{H}(\mathbf{p}) = \hbar v (\xi p_x \hat{\sigma}_x + p_y \hat{\sigma}_y) = \hbar p v (\xi \hat{\sigma}_x \cos \varphi + \hat{\sigma}_y \sin \varphi). \quad (263)$$

By defining the pseudospin vector $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y)$ and the unit vector $\mathbf{n} = (\xi \cos \varphi, \sin \varphi)$, the Hamiltonian can be written as

$$\hat{H}(\mathbf{p}) = \hbar v p \hat{\boldsymbol{\sigma}} \cdot \mathbf{n}. \quad (264)$$

The chiral operator $\hat{\sigma} \cdot \mathbf{n}$ projects the pseudospin onto the direction of quantization. And we can see

$$(\hat{\sigma} \cdot \mathbf{n})\psi_{\pm} = \pm\psi_{\pm}. \quad (265)$$

Another way to determine the relationship between the pseudospin and the momentum is to calculate the expectation $\langle \hat{\sigma} \rangle_{\pm} = (\langle \hat{\sigma}_x \rangle_{\pm}, \langle \hat{\sigma}_y \rangle_{\pm})$ of the pseudospin operator in the state ψ_{\pm} .

$$\langle \hat{\sigma}_x \rangle_{\pm} = \langle \pm | \hat{\sigma}_x | \pm \rangle = \pm \xi \cos \varphi, \quad (266)$$

$$\langle \hat{\sigma}_y \rangle_{\pm} = \langle \pm | \hat{\sigma}_y | \pm \rangle = \pm \sin \varphi. \quad (267)$$

The probability $p(\varphi)$ to scatter in a direction φ , where $\alpha = 0$ is the forward direction, and

$$p(\varphi) = |\psi_{\pm}^*(\varphi)\psi_{\pm}(0)|^2 = \cos^2(\varphi/2). \quad (268)$$

This probability is anisotropic and displays an absence of backscattering, that is, $p(\pi) = 0$. Scattering into a state with opposite momentum is prohibited because it requires a reversal of the pseudospin.

10 Symmetries of electronic states

10.1 Symmetry in quantum mechanics

10.1.1 Unitary transformations

Unitary matrices \hat{U} are defined by the property that

$$\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \mathbb{1}. \quad (269)$$

This definition implies that

$$\det(\hat{U}\hat{U}^\dagger) = \det(\hat{U})\det(\hat{U}^\dagger) = \det(\hat{U})[\det(\hat{U})]^* = |\det(\hat{U})|^2, \quad (270)$$

so $|\det(\hat{U})| = 1$. In special case, we have $\det(\hat{U}) = 1$. Such matrices, which have a direct connection to rotations in Euclidean space, arise in many applications, including two-level systems, such as spin and isospin.

In d -dimensional complex space, the vectors connected by a unitary matrix \hat{U} are defined as $\mathbf{a}' = \hat{U}\mathbf{a}$ and $\mathbf{b}' = \hat{U}\mathbf{b}$. The transformation of inner product

$$\mathbf{a}'^\dagger\mathbf{b}' = (\hat{U}\mathbf{a})^\dagger(\hat{U}\mathbf{b}) = \mathbf{a}^\dagger\hat{U}^\dagger\hat{U}\mathbf{b} = \mathbf{a}^\dagger\mathbf{b}, \quad (271)$$

is invariant under unitary transformations.

In quantum mechanics, we have $\phi' = \hat{U}\phi$ and $\psi' = \hat{U}\psi$. Then the transformation of the inner product

$$\langle\phi'|\psi'\rangle = \langle\hat{U}\phi|\hat{U}\psi\rangle = \langle\phi|\hat{U}^\dagger\hat{U}\psi\rangle = \langle\phi|\psi\rangle. \quad (272)$$

So the unitary transformations conserve probability amplitudes.

10.1.2 Symmetries of Hamiltonians

Consider the time-independent Schrodinger equation

$$\hat{H}\psi = E\psi. \quad (273)$$

The unitary transformation of the equation

$$\hat{U}(\hat{H}\psi) = E(\hat{U}\psi) = E\psi'. \quad (274)$$

We now insert the unitary operator $\mathbb{1} = \hat{U}^\dagger\hat{U}$ then obtain

$$(\hat{U}\hat{H})\psi = \hat{U}\hat{H}\hat{U}^\dagger\hat{U}\psi = (\hat{U}\hat{H}\hat{U}^\dagger)(\hat{U}\psi) = \hat{H}'\psi' = E\psi', \quad (275)$$

where $\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger$. The transformation of \hat{H} is called a **similarity transformation**.

Suppose the transformed and the original Hamiltonian are the same: $\hat{H}' = \hat{H}$, i.e., $\hat{U}\hat{H}\hat{U}^\dagger$, then we obtain

$$\hat{H}\hat{U} - \hat{U}\hat{H}\hat{U}^\dagger\hat{U} = \hat{H}\hat{U} - \hat{U}\hat{H} = [\hat{H}, \hat{U}] = 0, \quad (276)$$

so that \hat{U} commutes with the Hamiltonian. A unitary operator that commutes with the Hamiltonian is said to be a **symmetry** of that Hamiltonian.

10.2 Parity in quantum mechanics

10.2.1 Coordinate and momentum eigenstates

The **inversion operator** / **parity operator** is defined on the Hilbert space. In the coordinate representation

$$\hat{P} |\mathbf{r}\rangle = |-\mathbf{r}\rangle. \quad (277)$$

Applying the inversion operator again

$$\hat{P}^2 |\mathbf{r}\rangle = \hat{P} |-\mathbf{r}\rangle = |\mathbf{r}\rangle, \quad (278)$$

so we have $\hat{P}^2 = \mathbb{1}$. We also have

$$\langle \mathbf{r}' | \hat{P}^\dagger \hat{P} | \mathbf{r} \rangle = \langle -\mathbf{r}' | -\mathbf{r} \rangle = \langle \mathbf{r}' | \mathbf{r} \rangle, \quad (279)$$

so $\hat{P}^\dagger \hat{P} = \mathbb{1}$. So we find

$$\hat{P}^\dagger = \hat{P}, \quad \hat{P}^\dagger \hat{P} = \hat{P} \hat{P}^\dagger = \mathbb{1}, \quad (280)$$

which shows that \hat{P} is both **Hermitian** and **unitary**.

Now we look the momentum eigenstates

$$\hat{P} |p\rangle = \int \hat{P} |\mathbf{r}\rangle \langle \mathbf{r} | p \rangle d\mathbf{r} = \int |-\mathbf{r}\rangle \langle \mathbf{r} | p \rangle d\mathbf{r} = \int |\mathbf{r}\rangle \langle -\mathbf{r} | p \rangle d\mathbf{r}, \quad (281)$$

with the relationship

$$\langle \mathbf{r} | p \rangle = \frac{1}{\sqrt{2\pi}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}. \quad (282)$$

Therefore we have

$$\hat{P} |p\rangle = | -p \rangle. \quad (283)$$

Thus, the momentum operator changes sign under inversion.

10.2.2 Operators under parity

For the position operator \hat{r} , we begin with the action of $\hat{P}^\dagger \hat{r} \hat{P}$ on an arbitrary state vector $|\psi\rangle$

$$\begin{aligned} \hat{P}^\dagger \hat{r} \hat{P} |\psi\rangle &= \int \hat{P}^\dagger \hat{r} \hat{P} |\mathbf{r}'\rangle \langle \mathbf{r}' | \psi \rangle d\mathbf{r}' = \int \hat{P}^\dagger \hat{r} |-\mathbf{r}'\rangle \langle \mathbf{r}' | \psi \rangle d\mathbf{r}' \\ &= \int (-\mathbf{r}') \hat{P}^\dagger |-\mathbf{r}'\rangle \langle \mathbf{r}' | \psi \rangle d\mathbf{r}' = \int (-\mathbf{r}') |\mathbf{r}'\rangle \langle \mathbf{r}' | \psi \rangle d\mathbf{r}' \\ &= \int (-\hat{r}) |\mathbf{r}'\rangle \langle \mathbf{r}' | \psi \rangle d\mathbf{r}' = -\hat{r} |\psi\rangle. \end{aligned} \quad (284)$$

Since $|\psi\rangle$ is an arbitrary state vector, we conclude that

$$\hat{P}^\dagger \hat{r} \hat{P} = -\hat{r}, \quad (285)$$

then we have

$$\hat{P} \hat{P}^\dagger \hat{r} \hat{P} + \hat{P} \hat{r} = \hat{r} \hat{P} + \hat{P} \hat{r} = \underbrace{\{\hat{P}, \hat{r}\}}_{\text{anti-commute}} = 0. \quad (286)$$

Similarly, for $\hat{\mathbf{p}}$, we obtain $\hat{P}^\dagger \hat{\mathbf{p}} \hat{P} = -\hat{\mathbf{p}}$ and $\{\hat{P}, \hat{\mathbf{p}}\} = 0$.

The transformation of the angular momentum under inversion then follows

$$\hat{P}^\dagger \hat{\mathbf{L}} \hat{P} = \hat{P}^\dagger (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \hat{P} = (\hat{P}^\dagger \hat{\mathbf{r}} \hat{P}) \times (\hat{P}^\dagger \hat{\mathbf{p}} \hat{P}) = (-\hat{\mathbf{r}}) \times (-\hat{\mathbf{p}}) = \hat{\mathbf{L}}. \quad (287)$$

In this case

$$[\hat{P}, \hat{\mathbf{L}}] = \hat{P} \hat{\mathbf{L}} - \hat{\mathbf{L}} \hat{P} = 0. \quad (288)$$

The spin operator $\hat{\mathbf{S}}$, being a (non-classical) form of angular momentum, also commutes with the inversion operator

$$[\hat{P}, \hat{\mathbf{S}}] = \hat{P} \hat{\mathbf{S}} - \hat{\mathbf{S}} \hat{P} = 0, \quad (289)$$

and the total angular momentum $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$.

10.2.3 Commutation with a Hamiltonian

Suppose we have a Hamiltonian

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}}). \quad (290)$$

The transformation of this Hamiltonian takes the form

$$\hat{P}^\dagger \hat{H} \hat{P} = \frac{1}{2m} \hat{P}^\dagger \hat{\mathbf{p}}^2 \hat{P} + \hat{P}^\dagger V(\hat{\mathbf{r}}) \hat{P} = \frac{\hat{\mathbf{p}}^2}{2m} + \hat{P}^\dagger V(\hat{\mathbf{r}}) \hat{P}. \quad (291)$$

As for $\hat{P}^\dagger V(\hat{\mathbf{r}}) \hat{P}$, we find that $[\hat{P}, \hat{\mathbf{r}}^2] = 0$. Hence, for every even power $\hat{\mathbf{r}}^{2k}$, $k = 0, 1, 2, \dots$, $\hat{\mathbf{r}}^{2k}$ is invariant under the transformation. So with even potential, the inversion operator commutes with the Hamiltonian

$$\{\hat{H}, \hat{P}\} = 0, \quad (292)$$

in which case parity is a symmetry of the Hamiltonian.

10.3 Time-reversal

10.3.1 Time-reversal in classical mechanics

Consider Hamilton's equations of motion in classical mechanics

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad i = 1, 2, \dots, N. \quad (293)$$

The Hamiltonian has the general form

$$H = \sum_{i=1}^n \frac{\mathbf{p}_i^2}{2m_i} + V(q_1, q_2, \dots, q_N). \quad (294)$$

Now we consider **time-reversal** ($t \rightarrow -t$). The coordinates \mathbf{q}_i are invariant, but time-derivatives $\dot{\mathbf{q}}_i$ are changed:

$$\hat{T}\mathbf{q}_i(t) = \mathbf{q}_i(-t), \quad \hat{T}\dot{\mathbf{q}}_i(t) = -\dot{\mathbf{q}}_i(-t). \quad (295)$$

Similarly, since $\mathbf{p}_i = m\frac{d\mathbf{q}_i(t)}{dt}$,

$$\hat{T}\mathbf{p}_i(t) = -\mathbf{p}_i(-t), \quad \hat{T}\dot{\mathbf{p}}_i(t) = \dot{\mathbf{p}}_i(-t). \quad (296)$$

Thus, Hamilton's equations become

$$\dot{\mathbf{q}}(-t) = \frac{\partial H}{\partial \mathbf{p}_i(-t)}, \quad \dot{\mathbf{p}}(-t) = -\frac{\partial H}{\partial \mathbf{q}_i(-t)}. \quad (297)$$

So Hamilton's equations of motion are invariant under time reversal.

For Newton's second law

$$m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F}, \quad (298)$$

and a time-independent force \mathbf{F}

$$\hat{T}\mathbf{F} = \hat{T}\left(m\frac{d^2\mathbf{r}}{dt^2}\right) = m\frac{d^2\mathbf{r}}{d(-t)^2} = m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F}, \quad (299)$$

which shows that Newton's second law is time-reversal invariant provided the force is time-reversal invariant.

A different story emerges for the Lorentz force of a charged particle moving in a constant magnetic field

$$m\frac{d^2\mathbf{r}}{dt^2} = q(\mathbf{v} \times \mathbf{B}) = q\left(\frac{d\mathbf{r}}{dt} \times \mathbf{B}\right). \quad (300)$$

Motion in a static electric field is time-reversal invariant, but apparently not in a magnetic field.

The magnetic field is produced by the curl of a vector potential $\mathbf{B} = \nabla \times \mathbf{A}$, where

$$\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int \frac{\mathbf{J}(\mathbf{r}')d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}. \quad (301)$$

The current density is determined by charges moving with velocities $v(t)$, that is $\mathbf{J} = q\mathbf{v}$. Under time reversal symmetry the velocities of all particles change sign, $v(-t) = -v(t)$, so $\mathbf{J} \rightarrow -\mathbf{J}$, which leads to $\mathbf{A} \rightarrow -\mathbf{A}$ and therefore to $\mathbf{B} \rightarrow -\mathbf{B}$. Thus, if we expand "the system" to include the charges that produce these fields, time-reversal invariance is restored.

10.3.2 Time-reversal in quantum mechanics

The time-dependent Schrödinger equation for a charged particle in a static electric field $\mathbf{E} = -\nabla\Phi$ is

$$i\hbar\frac{\partial\Psi(\mathbf{r}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + q\Phi\right)\Psi(\mathbf{r}, t). \quad (302)$$

Firstly, we transfer $t \rightarrow -t$:

$$-i\hbar \frac{\partial \Psi(\mathbf{r}, -t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + q\Phi \right) \Psi(\mathbf{r}, -t), \quad (303)$$

and take the complex conjugate of the Schrödinger equation:

$$i\hbar \frac{\partial \Psi^*(\mathbf{r}, -t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + q\Phi \right) \Psi^*(\mathbf{r}, -t). \quad (304)$$

So we find $\Psi(\mathbf{r}, t)$ and $\Psi^*(\mathbf{r}, -t)$ satisfy the same Schrödinger equation.

Next, we look at the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, the Schrödinger equation becomes

$$\begin{aligned} i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} &= \frac{1}{2m} (-i\hbar \nabla - q\mathbf{A})^2 \Psi(\mathbf{r}, t) \\ &= \frac{1}{2m} [-\hbar^2 \nabla^2 + i\hbar q(\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla) + q^2 \mathbf{A}^2] \Psi(\mathbf{r}, t). \end{aligned} \quad (305)$$

In this case, if $\Psi(\mathbf{r}, t)$ is a solution, we cannot immediately conclude that $\Psi^*(\mathbf{r}, -t)$ is also a solution, because of the terms linear in \mathbf{A} :

$$i\hbar \frac{\partial \Psi^*(\mathbf{r}, -t)}{\partial t} = \frac{1}{2m} [-\hbar^2 \nabla^2 - i\hbar q(\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla) + q^2 \mathbf{A}^2] \Psi^*(\mathbf{r}, -t). \quad (306)$$

If we get the magnetic field by replace $\mathbf{A} \rightarrow -\mathbf{A}$, then the Schrödinger equation is invariant under time-reversal.

10.3.3 More general

To explore time reversibility in greater generality, we define the **time-reversal operator** \hat{T} . The time-dependent Schrödinger equation is

$$i\hbar \frac{\partial}{\partial t} \psi = \hat{H} \psi. \quad (307)$$

We first operator the equation from the left by the time-reversal operator \hat{T} :

$$\hat{T} \left(i\hbar \frac{\partial}{\partial t} \psi \right) = \hat{T} \left(\hat{H} \psi \right). \quad (308)$$

Then we insert the identity $\mathbb{1} = \hat{T}^{-1} \hat{T}$

$$\left(\hat{T} i\hbar \hat{T}^{-1} \right) \left(\hat{T} \frac{\partial}{\partial t} \hat{T}^{-1} \right) \left(\hat{T} \psi \right) = \left(\hat{T} \hat{H} \hat{T}^{-1} \right) \left(\hat{T} \psi \right). \quad (309)$$

For the time-independent Hamiltonian

$$\hat{T} \hat{H} \hat{T}^{-1} = \hat{H}, \quad (310)$$

and the transformation of the time-derivative is

$$\hat{T} \frac{\partial}{\partial t} \hat{T}^{-1} = \frac{\partial}{\partial(-t)} = -\frac{\partial}{\partial t}. \quad (311)$$

So the transformations becomes

$$-\left(\hat{T}i\hbar\hat{T}^{-1}\right) \frac{\partial(\hat{T}\psi)}{\partial t} = \hat{H}(\hat{T}\psi). \quad (312)$$

Now we want to find the transformation of i . We note that $[\hat{x}, \hat{p}] = i\hbar$, and this yields

$$\begin{aligned} \hat{T}i\hbar\hat{T}^{-1} &= \hat{T}[\hat{x}, \hat{p}]\hat{T}^{-1} = \hat{T}(\hat{x}\hat{p} - \hat{p}\hat{x})\hat{T}^{-1} \\ &= (\hat{T}\hat{x}\hat{T}^{-1})(\hat{T}\hat{p}\hat{T}^{-1}) - (\hat{T}\hat{p}\hat{T}^{-1})(\hat{T}\hat{x}\hat{T}^{-1}) \\ &= \hat{x}(-\hat{p}) - (-\hat{p})\hat{x} = -[\hat{x}, \hat{p}] = -i\hbar. \end{aligned} \quad (313)$$

Thus, we have

$$\hat{T}i\hbar\hat{T}^{-1}\hat{T} + i\hbar\hat{T} = \hat{T}i\hbar + i\hbar\hat{T} = \{\hat{T}, i\hbar\} = 0. \quad (314)$$

So, the transformed time-reversed Schrödinger equation with a time-independent Hamiltonian read

$$i\hbar \frac{\partial(\hat{T}\psi)}{\partial t} = \hat{H}(\hat{T}\psi), \quad (315)$$

where

$$\hat{T}\psi(\mathbf{r}, t) = \psi^*(\mathbf{r}, -t). \quad (316)$$

$\psi(\mathbf{r}, t)$ and $\psi^*(\mathbf{r}, -t)$ are both satisfy the same Schrodinger equation.

10.3.4 Anti-unitary operator

Eq. (313) shows that \hat{T} must include complex conjugate \hat{K} . For any complex number $z = a + ib$, where a and b are real numbers,

$$\hat{K}z\hat{K}^{-1} = \hat{K}(a + ib)\hat{K}^{-1} = a - ib = z^*, \quad (317)$$

implies that $\hat{K}^2 = \mathbb{1}$. The time-reversal operator can be expressed as

$$\hat{T} = \hat{U}\hat{K}, \quad (318)$$

where \hat{U} is a unitary operator. Such operators \hat{T} are called **anti-unitary**.

To see the effect of \hat{T} on inner products, we choose the two states

$$|\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle, \quad |\phi\rangle = \sum_m \langle m|\phi\rangle |m\rangle. \quad (319)$$

Applying \hat{T} to $|\psi\rangle$ yields

$$|\psi'\rangle = \hat{T}|\psi\rangle = \hat{U}\hat{K}|\psi\rangle = \sum_n \left(\hat{K}\langle n|\psi\rangle\right) \left(\hat{U}|n\rangle\right) = \sum_n \langle\psi|n\rangle \hat{U}|n\rangle. \quad (320)$$

Similarly, we have

$$|\phi'\rangle = \sum_m \langle\phi|m\rangle \hat{U} |m\rangle. \quad (321)$$

So the inner product of the transformed states is

$$\begin{aligned} \langle\psi'|\phi'\rangle &= \sum_{m,n} \langle n|\psi\rangle \langle n|\hat{U}^\dagger \langle\phi|m\rangle \hat{U} |m\rangle = \sum_{m,n} \langle\phi|m\rangle \langle n|\hat{U}^\dagger \hat{U} |m\rangle \langle n|\psi\rangle \\ &= \sum_{m,n} \langle\phi|m\rangle \langle n|m\rangle \langle n|\psi\rangle = \sum_n \langle\phi|n\rangle \langle n|\psi\rangle = \langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*. \end{aligned} \quad (322)$$

Although this result shows that the two states are reversed in the inner product, leading to the complex conjugate of the *amplitude*, the *magnitude* of the inner product is unaffected

$$|\langle\psi'|\phi'\rangle| = |\langle\psi|\phi\rangle^*| = |\langle\psi|\phi\rangle|. \quad (323)$$

This is the essence of **Wigner's theorem**: Suppose there is a mapping of a ket space onto itself, say, $|\phi\rangle$ and $|\psi\rangle$ into $|\phi'\rangle$ and $|\psi'\rangle$, respectively, such that absolute values of the scalar products are preserved, that is,

$$|\langle\psi'|\phi'\rangle| = |\langle\psi|\phi\rangle|, \quad (324)$$

for all $|\phi\rangle$ and $|\psi\rangle$. Then, to within inessential phase factors, the mapping must be either a linear unitary operator or an anti-unitary operator:

$$\langle\psi'|\phi'\rangle = \begin{cases} \langle\psi|\phi\rangle, & \text{unitary,} \\ \langle\phi|\psi\rangle, & \text{anti-unitary.} \end{cases} \quad (325)$$

10.3.5 Transformations of operators

1. The transformation of the position operator and the momentum operator:

$$\hat{T} \hat{\mathbf{r}} \hat{T}^{-1} = \hat{\mathbf{r}}, \quad \hat{T} \hat{\mathbf{p}} \hat{T}^{-1} = -\hat{\mathbf{p}}. \quad (326)$$

2. The transformation of the angular momentum operator:

$$\hat{T} \hat{\mathbf{L}} \hat{T}^{-1} = \hat{T} (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \hat{T}^{-1} = -\hat{\mathbf{L}}. \quad (327)$$

3. our conclusion can be extended to all angular momenta with $[\hat{J}_i, \hat{J}_j] = i\hbar \varepsilon_{ijk} \hat{J}_k$: orbital, spin, and combinations of the two:

$$\hat{T} \hat{\mathbf{J}} \hat{T}^{-1} = -\hat{\mathbf{J}}. \quad (328)$$

10.3.6 Time-reversed with spin: Kramers' degeneracy

The spin angular momentum $\hat{\mathbf{S}}$ is odd under time-reversal

$$\hat{T} \hat{\mathbf{S}} \hat{T}^{-1} = -\hat{\mathbf{S}}. \quad (329)$$

For spin-1/2 particles, $\hat{S} = \frac{1}{2}\hat{\sigma}$, where $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ are the Pauli matrices. Hence

$$\hat{T}\hat{\sigma}\hat{T}^{-1} = -\hat{\sigma}. \quad (330)$$

The standard choice of \hat{T} is

$$\hat{T} = -i\hat{\sigma}_y\hat{K}, \quad (331)$$

where \hat{K} is the complex conjugation operator and we have

$$\hat{T}^2 = (-i\hat{\sigma}_y\hat{K})^2 = (-i\hat{\sigma}_y)^2 = -\mathbb{1}. \quad (332)$$

This should be compared by

$$\hat{T}^2\Psi(\mathbf{r}, t) = \hat{T}[\hat{T}\Psi(\mathbf{r}, t)] = \hat{T}\Psi^*(\mathbf{r}, -t) = \Psi(\mathbf{r}, t), \quad (333)$$

so $\hat{T}^2 = \mathbb{1}$. In general, for **integer spins** $\hat{T}^2 = \mathbb{1}$, and for **half integer spins**, $\hat{T}^2 = -\mathbb{1}$.

An important consequence of the time reversal of a spin-1/2 particle is **Kramer's theorem** for the degeneracy of states governed by a time-reversal-invariant Hamiltonian. We start from $\hat{H}\Psi = \lambda\Psi$. This Hamiltonian is taken to be time-reversal-invariant:

$$[\hat{H}, \hat{T}] = 0. \quad (334)$$

Applying the time-reversal operator to generate $\Psi' = \hat{T}\Psi$, then

$$\hat{H}\Psi' = \hat{H}\hat{T}\Psi = \hat{T}\hat{H}\Psi = \lambda\hat{T}\Psi = \lambda\Psi', \quad (335)$$

so Ψ and Ψ' have the same eigenvalue. There are two possibilities:

1. Ψ and Ψ' are the same;
2. Ψ and Ψ' are different.

We calculate the overlap

$$\langle\Psi|\Psi'\rangle = \langle\Psi|\hat{T}\Psi\rangle = \langle\hat{T}\Psi|\hat{T}^2\Psi\rangle^* = -\langle\hat{T}\Psi|\Psi\rangle^* = -\langle\Psi|\hat{T}\Psi\rangle = -\langle\Psi|\Psi'\rangle. \quad (336)$$

Hence $\langle\Psi|\Psi'\rangle = 0$, so the two states are orthogonal, which means they are distinct and degenerate. This is the **Kramer's theorem**: The states of a spin-1/2 particle governed by a time-reversal-invariant Hamiltonian are (at least) doubly degenerate.

10.4 Symmetries of Hamiltonians

The most general Hamiltonian in a two-dimensional Hilbert space is

$$\hat{H}(\mathbf{k}) = h_0(\mathbf{k})\mathbb{1} + \mathbf{h}(\mathbf{k}) \cdot \hat{\sigma} = \begin{pmatrix} h_0(\mathbf{k}) + h_3(\mathbf{k}) & h_1(\mathbf{k}) - ih_2(\mathbf{k}) \\ h_1(\mathbf{k}) + ih_2(\mathbf{k}) & h_0(\mathbf{k}) - h_3(\mathbf{k}) \end{pmatrix}. \quad (337)$$

The eigenvalues E_{\pm} of \hat{H} are

$$E_{\pm}(\mathbf{k}) = h_0(\mathbf{k}) \pm \sqrt{h_1^2(\mathbf{k}) + h_2^2(\mathbf{k}) + h_3^2(\mathbf{k})}. \quad (338)$$

Set $h_0 = 0$, then

$$\hat{H} = \begin{pmatrix} h_3(\mathbf{k}) & h_1(\mathbf{k}) - ih_2(\mathbf{k}) \\ h_1(\mathbf{k}) + ih_2(\mathbf{k}) & -h_3(\mathbf{k}) \end{pmatrix}. \quad (339)$$

10.4.1 Parity and time-reversal symmetry

The parity operator has two effects: (i) the reversal of wave vectors, $\mathbf{k} \rightarrow -\mathbf{k}$, and (ii) the exchange of A and B sites, $AA \leftrightarrow BB$ and $AB \leftrightarrow BA$. These are operated by \hat{P} and $\hat{\sigma}_x$:

$$\hat{P}f(\mathbf{k}) = f(-\mathbf{k}), \quad \hat{\sigma}_x \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} B \\ A \end{pmatrix}. \quad (340)$$

As \hat{P} and $\hat{\sigma}_x$ operate on different spaces, they commute, $\hat{P}\hat{\sigma}_x = \hat{\sigma}_x\hat{P}$, and $\hat{P}^2 = \hat{\sigma}_x^2 = \mathbb{1}$. We have

$$\begin{aligned} (\hat{\sigma}_x\hat{P})\hat{H}(\hat{\sigma}_x\hat{P})^{-1} &= \hat{\sigma}_x\hat{P}\hat{H}\hat{P}^{-1}\hat{\sigma}_x^{-1} = \hat{\sigma}_x\hat{H}(-\mathbf{k})\hat{\sigma}_x^{-1} \\ &= \begin{pmatrix} -h_3(-\mathbf{k}) & h_1(-\mathbf{k}) + ih_2(-\mathbf{k}) \\ h_1(-\mathbf{k}) - ih_2(-\mathbf{k}) & h_3(-\mathbf{k}) \end{pmatrix}. \end{aligned} \quad (341)$$

Compared to Eq.(339), $\mathbf{h}(\mathbf{k})$ must satisfy:

$$h_1(-\mathbf{k}) = h_1(\mathbf{k}), \quad h_2(-\mathbf{k}) = -h_2(\mathbf{k}), \quad h_3(-\mathbf{k}) = -h_3(\mathbf{k}). \quad (342)$$

Now we consider the time-reversal operator:

$$\hat{T}\hat{H}(\mathbf{k})\hat{T}^{-1} = \hat{H}(-\mathbf{k}) = \begin{pmatrix} h_3(-\mathbf{k}) & h_1(-\mathbf{k}) + ih_2(-\mathbf{k}) \\ h_1(-\mathbf{k}) - ih_2(-\mathbf{k}) & -h_3(-\mathbf{k}) \end{pmatrix}. \quad (343)$$

This requires

$$h_1(-\mathbf{k}) = h_1(\mathbf{k}), \quad h_2(-\mathbf{k}) = -h_2(\mathbf{k}), \quad h_3(-\mathbf{k}) = h_3(\mathbf{k}). \quad (344)$$

By comparing the two requirements, we that the restrictions on h_1 and h_2 are compatible and require that h_1 is an even function and h_2 is an odd function. The conditions on h_3 :

$$h_3(-\mathbf{k}) = h_3(\mathbf{k}) = -h_3(\mathbf{k}) = 0. \quad (345)$$

Hence, the general form of the Hamiltonian that is invariant under time-reversal and parity is

$$\hat{H}(\mathbf{k}) = \begin{pmatrix} 0 & h_1(\mathbf{k}) - ih_2(\mathbf{k}) \\ h_1(\mathbf{k}) + ih_2(\mathbf{k}) & 0 \end{pmatrix} = h_1(\mathbf{k})\hat{\sigma}_x + h_2(\mathbf{k})\hat{\sigma}_y. \quad (346)$$

The eigenvalues are

$$E_{\pm}(\mathbf{k}) = \pm \sqrt{h_1^2(\mathbf{k}) + h_2^2(\mathbf{k})}. \quad (347)$$

We have $E(\mathbf{D}) = 0$ at the Dirac points \mathbf{D} , so

$$h_1(-\mathbf{D}) = h_1(\mathbf{D}) = 0, \quad h_2(-\mathbf{D}) = -h_2(\mathbf{D}) = 0. \quad (348)$$

Near the Dirac points, we expand $h_1(\mathbf{D} + \mathbf{q})$ and $h_2(\mathbf{D} + \mathbf{q})$ in \mathbf{q} :

$$h_1(\mathbf{D} + \mathbf{q}) \approx \mathbf{v}_1 \cdot \mathbf{q}, \quad (349)$$

$$h_1(-\mathbf{D} + \mathbf{q}) \approx -\mathbf{v}_1 \cdot \mathbf{q}, \quad (350)$$

$$h_2(\mathbf{D} + \mathbf{q}) \approx \mathbf{v}_2 \cdot \mathbf{q}, \quad (351)$$

$$h_2(-\mathbf{D} + \mathbf{q}) \approx \mathbf{v}_2 \cdot \mathbf{q}, \quad (352)$$

where the coefficient $v_{i,x}$ and $v_{i,y}$ are

$$\pm v_{1,x} = \left. \frac{\partial h_1}{\partial q_x} \right|_{\pm D}, \quad \pm v_{1,y} = \left. \frac{\partial h_1}{\partial q_y} \right|_{\pm D}, \quad v_{2,x} = \left. \frac{\partial h_2}{\partial q_x} \right|_{\pm D}, \quad v_{2,y} = \left. \frac{\partial h_2}{\partial q_y} \right|_{\pm D}. \quad (353)$$

Recall the notation $\pm \mathbf{D} = \xi \mathbf{D}$, the low-energy Hamiltonian

$$\hat{H}(\mathbf{q}) = \xi v_{1x} q_x \hat{\sigma}_x + v_{2y} q_y \hat{\sigma}_y. \quad (354)$$

10.4.2 Lattice symmetry

The existence of Dirac cones at the edge of the hexagonal Brillouin zone originates with the honeycomb lattice. The band structure of graphene near the K and K' points of the Brillouin zone is determined by the function $tf(\mathbf{k})$ defined in

$$tf(\mathbf{k}) = te^{i\mathbf{k} \cdot \delta_1} + te^{i\mathbf{k} \cdot \delta_2} + te^{i\mathbf{k} \cdot \delta_3}. \quad (355)$$

10.4.3 Symmetry breaking

The symmetries in graphene contain (i) parity symmetry, (ii) time-reversal symmetry and (iii) lattice symmetry.

1. Parity symmetry is broken by hexagonal BN (h-BN), which has the same lattice as graphene, but with one atomic type (say, B) occupying the A -sites and the other (N) occupying the B -sites.
2. Time-reversal symmetry can be broken by adding to the basic Hamiltonian a complex second-neighbor hopping with the following characteristics: (i) the hoppings are purely imaginary and have the same chirality, in that their orientation follows the right-hand rule, and (ii) the same sublattices are coupled, i.e. A with A and B with B . These hoppings break time-reversal and sublattice symmetry.
3. The symmetry of the graphene lattice can be broken by applying strain to the lattice.

11 Topological materials

11.1 Topology and topological invariant

Topology is the mathematical study of properties that remain unchanged under continuous deformations, such as stretching, bending, and compression. It focuses on identifying objects that can be continuously deformed into one another and determining quantities associated with these objects that remain invariant during the deformation process. These quantities are called **topological invariants**. Topology does not allow operations like tearing, puncturing, or joining, as these are discontinuous changes.

11.1.1 The Gauss-Bonnet theorem

The basic theorem from plane geometry that the sum of the angles of a triangle is 180° has a generalisation to a triangle on any surface (such as a sphere, resulting in a spherical triangle). This generalization is the **Gauss–Bonnet theorem**:

$$\xi = \frac{1}{2\pi} \int_S K dA = 2 - 2g, \quad (356)$$

where ξ is known as the Euler characteristic, S is the (closed) surface in question, K is the Gaussian curvature, and g is the genus of the surface.

Take the sphere as an example. The Gaussian curvature of a sphere is a constant, $K = 1/R^2$, where R is the radius of the sphere. Then

$$\xi = \frac{R^2}{2\pi R^2} \int_0^{2\pi} \int_0^\pi \sin \theta d\theta d\phi = 2, \quad (357)$$

which implies $g = 0$ for the sphere. For the torus, $g = 1$, again as expected from the central hole.

The **genus** is a topological classification, meaning that two topologically equivalent surfaces have the same genus.

11.2 Topological band theory

In topological band theory, continuous deformations of an object are replaced by adiabatic evolutions of the band structure. Two insulators are considered **topologically equivalent** if they can be transformed into one another by slowly changing their Hamiltonians, ensuring that the systems always remain in their ground state.

Such a process is feasible if there is an energy gap, which dictates the time scale for how slowly the adiabatic process must occur. If the gap closes, the adiabatic process is no longer possible.

The two main goals of topological band theory are:

1. To identify new topological materials, including both two- and three-dimensional materials.

-
2. To classify distinct Hamiltonians, particularly to distinguish between ordinary and topological insulators, as well as between different types of topological insulators.

11.2.1 Two-level systems

Consider the Hamiltonian of a generic two-level system:

$$H = \mathbf{h} \cdot \hat{\boldsymbol{\sigma}} = \begin{pmatrix} h_3 & h_1 - ih_2 \\ h_1 + ih_2 & -h_3 \end{pmatrix}. \quad (358)$$

By parametrizing \mathbf{h} in terms of a polar angle θ and azimuthal angle ϕ

$$\mathbf{h} = h(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta), \quad (359)$$

the Hamiltonian becomes

$$H = h \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix}, \quad (360)$$

with eigenvalues $E_{\pm} = \pm h$ and the corresponding eigenstates

$$|u_{-}\rangle = \begin{pmatrix} \sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2) \end{pmatrix}, \quad |u_{+}\rangle = \begin{pmatrix} \cos(\theta/2)e^{-i\phi} \\ \sin(\theta/2) \end{pmatrix}, \quad (361)$$

where $(-)$ means occupied states and $(+)$ means unoccupied.

Consider the wave function corresponding to the lower energy level. The components of the Berry connection:

$$A_{\theta} = i \langle u_{-} | \partial_{\theta} | u_{-} \rangle = 0, \quad (362)$$

$$A_{\phi} = i \langle u_{-} | \partial_{\phi} | u_{-} \rangle = \sin^2(\theta/2). \quad (363)$$

So the Berry curvature

$$F_{\theta\phi} = \partial_{\theta} A_{\phi} - \partial_{\phi} A_{\theta} = \sin(\theta/2) \cos(\theta/2) = \frac{1}{2} \sin \theta. \quad (364)$$

In Cartesian coordinates $\mathbf{h} = (x, y, z)$, the Berry curvature

$$\mathbf{F} = \frac{1}{2} \frac{\mathbf{h}}{h^3} \quad (365)$$

is the field generated by a monopole at the origin $\mathbf{h} = 0$. By integrating the Berry curvature over a sphere containing the monopole, we find

$$\frac{1}{2\pi} \iint_S F_{\theta\phi} d\theta d\phi = 1. \quad (366)$$

In general, when integrated over a closed manifold, the Berry curvature is quantised in the units of 2π and is equal to the net number of monopoles enclosed by the manifold. This is called the **Chern number**.

The Berry phase can be computed only if the Hamiltonian has an energy gap. For a Hamiltonian $H(\mathbf{k})$ with many bands $E_n(\mathbf{k})$, where n is again a band index, this means that we can compute the Chern number only for an isolated band that does not touch any other band. If there is a band touching, the Berry phase is undefined. In terms of our analogy between the Berry phase and electromagnetism, we cannot compute the electric or magnetic flux through a surface if there are electric or magnetic charges located on the surface because the electric or magnetic fields are not defined at the points where their sources are. This analogy suggests that the sources for Berry flux in momentum space are points where two bands touch, such as the Dirac points at the K and K' points of the Brillouin zone in graphene.

11.3 Spin-orbit interaction

This coupling of the spin of the electron to its orbital motion is known as spin-orbit coupling. The Hamiltonian for spin-orbit coupling is

$$\hat{H}_{\text{SO}} = f(r)\mathbf{L} \cdot \mathbf{S}. \quad (367)$$

The Hamiltonian is *invariant* under parity and time-reversal.

11.4 The Kane-Mele Model

In the Kane-Mele model, a spin-orbit term

$$\hat{H}_{\text{SO}} = \lambda_{\text{SO}}\hat{\sigma}_z\tau_zs_z, \quad (368)$$

is added to the Hamiltonian near the K and K' points. Here, τ_z is the valleys (K and K' points) and s_z is the electron spin (\uparrow or \downarrow). For $s_z = 1$, the Hamiltonian reads

$$\hat{H}(\mathbf{k}) = v(k_x\tau_z\hat{\sigma}_x + k_y\hat{\sigma}_y) + \lambda_{\text{SO}}\hat{\sigma}_z\tau_z. \quad (369)$$

For each valleys (Dirac points at K and K') separately

$$\hat{H}_+(\mathbf{k}) = v(k_x\hat{\sigma}_x + k_y\hat{\sigma}_y) + \lambda_{\text{SO}}\hat{\sigma}_z, \quad (370)$$

$$\hat{H}_-(\mathbf{k}) = v(-k_x\hat{\sigma}_x + k_y\hat{\sigma}_y) - \lambda_{\text{SO}}\hat{\sigma}_z, \quad (371)$$

where \hat{H}_+ is the Hamiltonian near K and \hat{H}_- is the Hamiltonian near K' .

We now introduce a mass term $m > 0$, which applies to sublattice pseudospin, but not to valley pseudospin:

$$\hat{H}_+(\mathbf{k}) = v(k_x\hat{\sigma}_x + k_y\hat{\sigma}_y) + (m + \lambda_{\text{SO}})\hat{\sigma}_z, \quad (372)$$

$$\hat{H}_-(\mathbf{k}) = v(-k_x\hat{\sigma}_x + k_y\hat{\sigma}_y) + (m - \lambda_{\text{SO}})\hat{\sigma}_z. \quad (373)$$

There are two distinct possibilities (i) $m \gg \lambda_{\text{SO}}$ and (ii) $m \sim \lambda_{\text{SO}}$.

11.5 Edge states

11.5.1 States at zero energy

In this section, we show that the spin current is carried by edge states, using the \hat{H}_- block with $s_z = 1$ as an example. We suppose that our two-dimensional current-carrying material has an edge at $y = 0$, with the material occupying the region $y < 0$, and vacuum (or a trivial insulator) for $y > 0$. There is a translational symmetry along the x -direction. We consider the state at $k_x = 0$, with

$$p_y = \hbar k_y = -i\hbar \frac{\partial}{\partial y}, \quad (374)$$

the Hamiltonian reads

$$\hat{H}_-(y) = -i\hbar v \hat{\sigma}_y \frac{d}{dy} + (m - \lambda_{\text{so}}) \hat{\sigma}_z = -i\hbar v \hat{\sigma}_y \frac{d}{dy} + \tilde{m}(y) \hat{\sigma}_z, \quad (375)$$

where $\tilde{m} = m - \lambda_{\text{so}}$ changes sign at the edge $y = 0$. Now we consider the Schrödinger equation $\hat{H}_-(y)\psi_0(y) = 0$, and for $\psi_0(y)$, make the ansatz

$$\psi_0(y) = i\hat{\sigma}_y e^{f(y)} \phi. \quad (376)$$

Substituting this trial solution into the Schrödinger equation,

$$\hat{H}_-(y)\psi_0(y) = \hbar v \hat{\sigma}_y^2 e^f \frac{df}{dy} \phi + \tilde{m} e^f \hat{\sigma}_z (i\hat{\sigma}_y) \phi = e^{f(y)} \left[\hbar v \frac{df}{dy} \mathbb{1} + \tilde{m}(y) \hat{\sigma}_x \right] \phi = 0. \quad (377)$$

Choose

$$\phi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad (378)$$

then the equation becomes

$$\hbar v \frac{df}{dy} + \tilde{m}(y) = 0, \quad (379)$$

whose solution is

$$f(y) = -\frac{1}{\hbar v} \int_0^y \tilde{m}(y') dy'. \quad (380)$$

Finally we find

$$\psi_0(y) = \exp\left[-\frac{1}{\hbar v} \int_0^y \tilde{m}(y') dy'\right] i\hat{\sigma}_y \phi = \frac{1}{\sqrt{2}} \exp\left[-\frac{1}{\hbar v} \int_0^y \tilde{m}(y') dy'\right] \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \quad (381)$$

Note the following properties of the solution:

1. The spinor part of the wave function indicates that this state mixes the two sublattices by hopping along the boundary.
2. The same procedure applied to $s_z = -1$ would yield an edge state whose velocity is in the opposite direction.
3. We chose the Hamiltonian \hat{H}_- for one Dirac point. The same analysis applied to \hat{H}_+ again yields two edge states, one for each spin.

11.5.2 States at non-zero energy

We now consider edge states at non-zero energy. For $s_z = 1$, the Schrödinger equation reads

$$\hat{H}_-\psi = \left(i\hbar v \hat{\sigma}_x \frac{\partial}{\partial x} - i\hbar v \hat{\sigma}_y \frac{\partial}{\partial y} + \tilde{m}(y) \hat{\sigma}_z \right) \psi = E\psi. \quad (382)$$

We make the following ansatz for the eigenfunction:

$$\psi(x, y) = e^{ik_x x} \psi_0(y). \quad (383)$$

Substitution into the Hamiltonian yields

$$\begin{aligned} \hat{H}_-\psi &= \left(i\hbar v \hat{\sigma}_x \frac{\partial}{\partial x} - i\hbar v \hat{\sigma}_y \frac{\partial}{\partial y} + \tilde{m}(y) \hat{\sigma}_z \right) e^{ik_x x} \psi_0(y) \\ &= \left[-v\hbar k_x \psi_0(y) - i\hbar v \hat{\sigma}_y \frac{\partial \psi_0(y)}{\partial y} + \tilde{m} \hat{\sigma}_z \psi_0(y) \right] e^{ik_x x} \\ &= -v\hbar k_x \psi_0(y) e^{ik_x x} = -v\hbar k_x \psi = E(k_x) \psi, \end{aligned} \quad (384)$$

where $E(k_x) = -v\hbar k_x$.

11.6 Topological character of Kane-Mele model

We take $s_z = 1$ and consider $\hat{H}_\pm(\mathbf{k})$:

$$\hat{H}_+(\mathbf{k}) = v(k_x \hat{\sigma}_x + k_y \hat{\sigma}_y) + (m + \lambda_{\text{SO}}) \hat{\sigma}_z, \quad (385)$$

$$\hat{H}_-(\mathbf{k}) = v(-k_x \hat{\sigma}_x + k_y \hat{\sigma}_y) + (m - \lambda_{\text{SO}}) \hat{\sigma}_z. \quad (386)$$

These Hamiltonians can be written more concisely as $\hat{H}_\pm(\mathbf{k}) = \mathbf{h}_\pm(\mathbf{k}) \cdot \hat{\boldsymbol{\sigma}}$, where

$$\mathbf{h}_\pm(\mathbf{k}) = (\pm v k_x, v k_y, m \pm \lambda_{\text{SO}}). \quad (387)$$

Then, the unit vectors $\hat{\mathbf{h}}_\pm = \mathbf{h}_\pm / |\mathbf{h}_\pm|$ maps the 2D momentum space (k_x, k_y) to a unit space. The Chern number can be expressed as

$$\begin{aligned} Q &= \frac{1}{4\pi} \int_{\text{BZ}} \frac{\mathbf{h}_\pm}{h_\pm^3} \cdot \left(\frac{\partial \mathbf{h}_\pm}{\partial k_x} \times \frac{\partial \mathbf{h}_\pm}{\partial k_y} \right) dk_x dk_y \\ &= \frac{1}{4\pi} \int_{\text{BZ}} \frac{\mathbf{h}_\pm}{h_\pm^3} \cdot \left[\left(\frac{\partial \mathbf{h}_\pm}{\partial k_x} dk_x \right) \times \left(\frac{\partial \mathbf{h}_\pm}{\partial k_y} dk_y \right) \right] \\ &= \frac{1}{4\pi} \int_{\text{BZ}} d\Omega, \end{aligned} \quad (388)$$

where $h_\pm = |\mathbf{h}_\pm|$. For $m > \lambda_{\text{SO}}$, the h_z -component of \mathbf{h}_+ is always positive and is, therefore, confined to the upper hemisphere of the \mathbf{h} -surface. Thus

$$Q_+ = \frac{2\pi}{4\pi} = \frac{1}{2}. \quad (389)$$

The h_z -component of \mathbf{h}_- is also positive, but the minus sign in the h_x -component relative to that of \mathbf{h}_+ changes the sign of the integral, so

$$Q_- = -\frac{2\pi}{4\pi} = -\frac{1}{2}. \quad (390)$$

Hence $Q = Q_+ + Q_- = 0$. this is the topological index associated with a **trivial insulator**.

Now consider the case when $m < \lambda_{\text{SO}}$. h_+ is positive

$$Q_+ = \frac{2\pi}{4\pi} = \frac{1}{2}, \quad Q_- = \frac{2\pi}{4\pi} = \frac{1}{2}. \quad (391)$$

Therefore, $Q = Q_+ + Q_- = 1$. As this case corresponds to a **topological insulator**.