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NOTES

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DEPARTMENT OF PHYSICS

Quantum Theory of Matter

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Contents

1 Geometry phase

In this chapter, we talk about the geometric and dynamical phases under adiabatic evolution.

1.1 Berry connection

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

$$\hat{H}(\boldsymbol{R})\left|\nu,\boldsymbol{R}\right\rangle = E_\nu(\boldsymbol{R})\left|\nu,\boldsymbol{R}\right\rangle. \tag{1}$$

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

Consider time evolution in the adiabatic regime

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}(\boldsymbol{R}(t))\left|\psi(t)\right\rangle. \tag{2}$$

We prepare the system in eigenstate

$$\left|\psi(t=0)\right\rangle = \left|\nu,\boldsymbol{R}(t=0)\right\rangle. \tag{3}$$

For a constant $\boldsymbol{R}$, we have $|\psi(t)\rangle = \exp\left(-\frac{i}{\hbar}E_\nu(\boldsymbol{R})t\right)|\nu,\boldsymbol{R}\rangle$. So we guess the evolution of $|\psi(t)\rangle$

$$\left|\psi(t)\right\rangle = \exp\left(-\frac{i}{\hbar}\int_0^t E_\nu(\boldsymbol{R}(t'))\mathrm{d}t'\right)\left|\nu,\boldsymbol{R}(t=0)\right\rangle. \tag{4}$$

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

$$\left|\psi(t)\right\rangle = \mathrm{e}^{i\gamma(t)}\left|\nu,\boldsymbol{R}(t)\right\rangle. \tag{5}$$

Let's consider the Schrodinger equation Eq.(2)

$$\text{LHS} = i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \mathrm{e}^{i\gamma}\left(-\hbar\dot{\gamma}+i\hbar\dot{\boldsymbol{R}}\cdot\boldsymbol{\nabla}_{\boldsymbol{R}}\right)\left|\nu,\boldsymbol{R}(t)\right\rangle, \tag{6}$$

$$\text{RHS} = \hat{H}(\boldsymbol{R}(t))\left|\psi(t)\right\rangle = \mathrm{e}^{i\gamma}E_\nu(\boldsymbol{R}(t))\left|\nu,\boldsymbol{R}(t)\right\rangle. \tag{7}$$

Then we have

$$E_\nu(\boldsymbol{R}(t))\left|\nu,\boldsymbol{R}(t)\right\rangle = \left(-\hbar\dot{\gamma}+i\hbar\dot{\boldsymbol{R}}\cdot\boldsymbol{\nabla}_{\boldsymbol{R}}\right)\left|\nu,\boldsymbol{R}(t)\right\rangle. \tag{8}$$

Take overlap with $\langle\nu,\boldsymbol{R}|$, we have

$$E_\nu(\boldsymbol{R}) = -\hbar\dot{\gamma}+i\hbar\dot{\boldsymbol{R}}\cdot\left\langle\nu,\boldsymbol{R}\right|\boldsymbol{\nabla}_{\boldsymbol{R}}\left|\nu,\boldsymbol{R}\right\rangle. \tag{9}$$

Rearranging this equation and then

$$\begin{aligned}\gamma(t) &= -\frac{1}{\hbar}\int_0^t E(\boldsymbol{R}(t'))\mathrm{d}t' + i\int_0^t\left\langle\nu,\boldsymbol{R}\right|\boldsymbol{\nabla}_{\boldsymbol{R}}\left|\nu,\boldsymbol{R}\right\rangle\cdot\frac{\mathrm{d}\boldsymbol{R}}{\mathrm{d}t'}\mathrm{d}t' \\ &= -\frac{1}{\hbar}\int_0^t E(\boldsymbol{R}(t'))\mathrm{d}t' + i\int_C\left\langle\nu,\boldsymbol{R}\right|\boldsymbol{\nabla}_{\boldsymbol{R}}\left|\nu,\boldsymbol{R}\right\rangle\cdot\mathrm{d}\boldsymbol{R}.\end{aligned} \tag{10}$$

Here, we get two phases. The first term is called the *dynamic phase*

$$\gamma_{\text{dyn}} = -\frac{1}{\hbar}\int_0^t E(\boldsymbol{R}(t'))\mathrm{d}t', \tag{11}$$

and the dynamic phase γ_{dyn} is explicitly real. The second term is called the *geometric phase*.

$$\gamma_{\text{geom}} = i\int_C \langle \nu, \boldsymbol{R}|\, \nabla_{\boldsymbol{R}}\, |\nu, \boldsymbol{R}\rangle \cdot \mathrm{d}\boldsymbol{R} = \int_C \boldsymbol{A}(\boldsymbol{R})\cdot \mathrm{d}\boldsymbol{R}. \tag{12}$$

We know that $\mathrm{e}^{i\gamma}$ is a phase factor of modulus unity at all times. This means $\langle\nu|\boldsymbol{\nabla}_{\boldsymbol{R}}\nu\rangle$ should be purely imaginary. Now we prove this:

$$\boldsymbol{\nabla}_{\boldsymbol{R}}(\langle\nu,\boldsymbol{R}|\nu,\boldsymbol{R}\rangle) = \langle\boldsymbol{\nabla}_{\boldsymbol{R}}\nu|\nu\rangle + \langle\nu|\boldsymbol{\nabla}_{\boldsymbol{R}}\nu\rangle = \langle\nu|\boldsymbol{\nabla}_{\boldsymbol{R}}\nu\rangle^* + \langle\nu|\boldsymbol{\nabla}_{\boldsymbol{R}}\nu\rangle = 0. \tag{13}$$

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

$$\boldsymbol{A}_\nu(\boldsymbol{R}) = i\,\langle\nu,\boldsymbol{R}|\,\nabla_{\boldsymbol{R}}\,|\nu,\boldsymbol{R}\rangle = -\operatorname{Im}\langle\nu,\boldsymbol{R}|\,\nabla_{\boldsymbol{R}}\,|\nu,\boldsymbol{R}\rangle\,. \tag{14}$$

1.1.1 Example: spin-half electron in a magnetic field (I)

Let's consider a magnetic field $\boldsymbol{d} = (d_x, d_y, 0) = d(\cos\phi, \sin\phi, 0)$. Then the Zeeman Hamiltonian can be expressed as

$$\hat{H} = \boldsymbol{d}(t)\cdot\hat{\boldsymbol{\sigma}} = d_x\hat{\sigma}_x + d_y\hat{\sigma}_y = \sum_{s,s'=\uparrow,\downarrow} h_{ss'}\,|s\rangle\,\langle s'|\,, \tag{15}$$

where the $h_{ss'}$ is the element of the matrix

$$\boldsymbol{h} = \begin{pmatrix} 0 & d_x - id_y \\ d_x + id_y & 0 \end{pmatrix} = d\begin{pmatrix} 0 & \mathrm{e}^{-i\phi} \\ \mathrm{e}^{i\phi} & 0 \end{pmatrix}. \tag{16}$$

The eigenvalues are $\pm d$ and the corresponding eigenvectors are denoted as $|\pm,\phi\rangle$. Suppose the magnetic field rotates by 2π and $\phi(t) = 2\pi t/T$. And d is a constant when the system evolves from $t = 0$ to $t = T$. The instantaneous eigenstates at given ϕ

$$E_+ = +d, \qquad |+,\phi\rangle = \frac{1}{\sqrt{2}}(+\mathrm{e}^{-i\phi}\,|\uparrow\rangle + |\downarrow\rangle), \tag{17}$$

$$E_- = -d, \qquad |-,\phi\rangle = \frac{1}{\sqrt{2}}(-\mathrm{e}^{-i\phi}\,|\uparrow\rangle + |\downarrow\rangle). \tag{18}$$

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

$$\gamma_{\text{dyn}} = -\frac{1}{\hbar}\int_0^T E_+\mathrm{d}t = -\frac{d}{\hbar}T, \tag{19}$$

$$\gamma_{\text{geom}} = i\int_0^{2\pi}\langle+,\phi|\,\partial_\phi\,|+,\phi\rangle\,\mathrm{d}\phi = i\int_0^{2\pi}\langle\uparrow|\,\frac{\mathrm{e}^{i\phi}}{\sqrt{2}}(-i)\frac{\mathrm{e}^{-i\phi}}{\sqrt{2}}\,|\uparrow\rangle\,\mathrm{d}\phi = \pi. \tag{20}$$

1.2 Berry curvature

The instantaneous eigenstates chosen to be single-valued and differentiable. If we change instantaneous eigenstates by a single-valued, differentiable phase factor $\mathrm{e}^{i\chi(\boldsymbol{R})}$

$$|\nu, \boldsymbol{R}\rangle \to \mathrm{e}^{i\chi(\boldsymbol{R})} |\nu, \boldsymbol{R}\rangle . \tag{21}$$

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

$$\boldsymbol{A}_\nu(\boldsymbol{R}) \to \boldsymbol{A}_\nu(\boldsymbol{R}) - \boldsymbol{\nabla}_{\boldsymbol{R}}\chi(\boldsymbol{R}). \tag{22}$$

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

$$\gamma_{\text{geom}} = \oint_C \boldsymbol{A}_\nu(\boldsymbol{R}) \cdot \mathrm{d}\boldsymbol{R} \to \oint_C \boldsymbol{A}_\nu(\boldsymbol{R}) \cdot \mathrm{d}\boldsymbol{R} - \underbrace{[\chi(\boldsymbol{R}(T)) - \chi(\boldsymbol{R}(0))]}_{\Delta\chi = 2\pi n} . \tag{23}$$

Hence, geometric phase γ_{geom} changes, but $\mathrm{e}^{i\gamma_{\text{geom}}}$ is invariant.

We can define Berry curvature $\boldsymbol{B}_\nu$ as a gauge invariant:

$$\boldsymbol{B}_\nu = \boldsymbol{\nabla}_{\boldsymbol{R}} \times \boldsymbol{A}_\nu(\boldsymbol{R}) \tag{24}$$

By using the Einstein summation convention

$$(\boldsymbol{B}_\nu)_i = i\varepsilon_{ijk}\partial_j \langle \nu|\partial_k\nu\rangle = i\varepsilon_{ijk} \left(\langle \partial_j v|\partial_k\nu\rangle + \langle \nu|\partial_j\partial_k\nu\rangle\right) = i\varepsilon_{ijk} \langle \partial_j v|\partial_k\nu\rangle , \tag{25}$$

the Berry curvature can be expressed as

$$\boldsymbol{B}_\nu = i \langle \boldsymbol{\nabla}_{\boldsymbol{R}}\nu| \times |\boldsymbol{\nabla}_{\boldsymbol{R}}\nu\rangle . \tag{26}$$

Now we use perturbation theory to find out $|\boldsymbol{\nabla}_{\boldsymbol{R}}\nu\rangle$. Consider a small variation $\delta\boldsymbol{R}$

$$\begin{aligned} |\nu, \boldsymbol{R} + \delta\boldsymbol{R}\rangle &\simeq |\nu.\boldsymbol{R}\rangle + \delta\boldsymbol{R} \cdot \sum_{\mu\neq\nu} |\mu, \boldsymbol{R}\rangle \frac{\langle \mu, \boldsymbol{R}| \left(\boldsymbol{\nabla}_{\boldsymbol{R}}\hat{H}\right) |\nu, \boldsymbol{R}\rangle}{E_\nu(\boldsymbol{R}) - E_\mu(\boldsymbol{R})} \\ &= |\nu.\boldsymbol{R}\rangle + \delta\boldsymbol{R} \cdot \boldsymbol{\nabla}_{\boldsymbol{R}} |\nu, \boldsymbol{R}\rangle . \end{aligned} \tag{27}$$

So we have

$$|\boldsymbol{\nabla}_{\boldsymbol{R}}\nu\rangle = \sum_{\mu\neq\nu} |\mu, \boldsymbol{R}\rangle \frac{\langle \mu, \boldsymbol{R}| \left(\boldsymbol{\nabla}_{\boldsymbol{R}}\hat{H}\right) |\nu, \boldsymbol{R}\rangle}{E_\nu(\boldsymbol{R}) - E_\mu(\boldsymbol{R})}. \tag{28}$$

Hence the Berry curvature

$$\boldsymbol{B}_\nu = i \sum_{\mu\neq\nu} \frac{\langle \nu| \left(\boldsymbol{\nabla}_{\boldsymbol{R}}\hat{H}\right) |\mu\rangle \times \langle \mu| \left(\boldsymbol{\nabla}_{\boldsymbol{R}}\hat{H}\right) |\nu\rangle}{(E_\nu(\boldsymbol{R}) - E_\mu(\boldsymbol{R}))^2}. \tag{29}$$

It is noteworthy that

$$\boldsymbol{B}_\nu = \boldsymbol{\nabla}_{\boldsymbol{R}} \times \boldsymbol{A}_\nu \quad \leftrightarrow \quad \oint_C \boldsymbol{A}_\nu \cdot \mathrm{d}\boldsymbol{R} = \iint_D \boldsymbol{B}_\nu \cdot \mathrm{d}^2\boldsymbol{R}, \tag{30}$$

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

$$\gamma = \oint_C \boldsymbol{A}_\nu \cdot \mathrm{d}\boldsymbol{R} = \iint_D \boldsymbol{B}_\nu \cdot \mathrm{d}^2\boldsymbol{R}. \tag{31}$$

1.2.1 Example: spin-half electron in a magnetic field (II)

Suppose a spin-half electron in a magnetic field $\boldsymbol{d}$, the Zeeman Hamiltonian

$$\hat{H} = \boldsymbol{d} \cdot \hat{\boldsymbol{\sigma}}, \tag{32}$$

and the eigenfunctions

$$\hat{H} \left|\pm, \boldsymbol{d}\right\rangle = \pm|\boldsymbol{d}| \left|\pm, \boldsymbol{d}\right\rangle, \tag{33}$$

where $|\pm, \boldsymbol{d}\rangle$ is the eigenstates of $\hat{H}$. We focus on the instantaneous eigenstate $|+, \boldsymbol{d}\rangle$, the Berry curvature

$$\boldsymbol{B}_+ = i \frac{\langle +, \boldsymbol{d}| \hat{\boldsymbol{\sigma}} |-, \boldsymbol{d}\rangle \times \langle -, \boldsymbol{d}| \hat{\boldsymbol{\sigma}} |+, \boldsymbol{d}\rangle}{(2d)^2}. \tag{34}$$

If we choose $\hat{\boldsymbol{e}}_z$ as quantisation axis, i.e., $\hat{\boldsymbol{e}}_3 = \boldsymbol{d}/\|\boldsymbol{d}\|$. So we have

$$\boldsymbol{B}_+ = i \frac{\langle +| \hat{\sigma}_1 |-\rangle \langle -| \hat{\sigma}_2 |+\rangle - \langle +| \hat{\sigma}_2 |-\rangle \langle -| \hat{\sigma}_1 |+\rangle}{(2d)^2} \hat{\boldsymbol{e}}_3 = -\frac{\boldsymbol{d}}{2|\boldsymbol{d}|^3}. \tag{35}$$

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

$$\iint_D \boldsymbol{B}_+ \cdot \mathrm{d}\boldsymbol{S} = -\frac{1}{2d^2} 2\pi d^2 = -\pi. \tag{36}$$

We can add a phase 2π so that the geometry phase is single-values

$$\gamma_{\text{geom}} = (-\pi) + 2\pi = \pi. \tag{37}$$

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 and tight binding model.

2.1 Bloch's theorem

When analyzing a periodic potential, $V(\boldsymbol{r})$, which satisfies $V(\boldsymbol{r}+\boldsymbol{R}) = V(\boldsymbol{r})$ for any lattice vector $\boldsymbol{R}$, we delve into the properties of the eigenstates of the Schrödinger equation. These eigenstates are denoted as $\psi_{\boldsymbol{k}}(\boldsymbol{r})$, where the vector $\boldsymbol{k}$ resides within the confines of the first Brillouin zone.

The behavior of these eigenstates upon translation by any lattice vector $\boldsymbol{R}$ is captured by the equation:

$$\psi_{\alpha\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{R}) = \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}}\psi_{\alpha\boldsymbol{k}}(\boldsymbol{r}), \tag{38}$$

an expression that embodies the essence of **Bloch's theorem**.

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.

2.3.1 Tight binding Hamiltonian

The electron at lattice site $\boldsymbol{R}$ are denoted as $|\boldsymbol{R}\rangle$, then the electron state can be written as

$$|\psi\rangle = \sum_{\boldsymbol{R}} c_{\boldsymbol{R}} |\boldsymbol{R}\rangle , \tag{39}$$

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

$$\hat{H} = \epsilon \sum_{\boldsymbol{R}} |\boldsymbol{R}\rangle \langle \boldsymbol{R}| - t \sum_{\langle \boldsymbol{R},\boldsymbol{R}'\rangle} \left(|\boldsymbol{R}\rangle \langle \boldsymbol{R}'| + |\boldsymbol{R}'\rangle \langle \boldsymbol{R}|\right), \tag{40}$$

where the sign $\langle \cdots \rangle$ means that we are summing over all nearest-neighbour pairs, $\boldsymbol{R}$ and $\boldsymbol{R'}$, on the lattice. ϵ is the on-site energy, or the bound-state energy. t is the hopping integral.

2.3.2 Energy eigenstates

If we apply the tight binding Hamiltonian to the electron state

$$\begin{aligned}\hat{H}\left|\psi\right\rangle =&\epsilon \sum_{\boldsymbol{R},\boldsymbol{S}} c_{\boldsymbol{R}} \left|\boldsymbol{S}\right\rangle \left\langle \boldsymbol{S}|\boldsymbol{R}\right\rangle - t \sum_{\boldsymbol{R},\langle \boldsymbol{S},\boldsymbol{S'}\rangle} c_{\boldsymbol{R}}(\left|\boldsymbol{S}\right\rangle \left\langle \boldsymbol{S'}|\boldsymbol{R}\right\rangle + \left|\boldsymbol{S'}\right\rangle \left\langle \boldsymbol{S}|\boldsymbol{R}\right\rangle) \\ =&\epsilon \sum_{\boldsymbol{S}} c_{\boldsymbol{S}} \left|\boldsymbol{S}\right\rangle - t \sum_{\langle \boldsymbol{S},\boldsymbol{S'}\rangle} (c_{\boldsymbol{S'}} \left|\boldsymbol{S}\right\rangle + c_{\boldsymbol{S}} \left|\boldsymbol{S'}\right\rangle).\end{aligned} \tag{41}$$

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

$$\left\langle \boldsymbol{R}\right| \hat{H}\left|\psi\right\rangle = \epsilon c_{\boldsymbol{R}} - t \sum_{\langle \boldsymbol{S},\boldsymbol{S'}\rangle} (c_{\boldsymbol{S'}}\delta_{\boldsymbol{R},\boldsymbol{S}} + c_{\boldsymbol{S}}\delta_{\boldsymbol{R},\boldsymbol{S'}}) = \epsilon c_{\boldsymbol{R}} - t \sum_{\boldsymbol{\delta}} c_{\boldsymbol{R}+\boldsymbol{\delta}}, \tag{42}$$

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

$$\epsilon c_{\boldsymbol{R}} - t \sum_{\boldsymbol{\delta}} c_{\boldsymbol{R}+\boldsymbol{\delta}} = E c_{\boldsymbol{R}}, \tag{43}$$

where $c_{\boldsymbol{R}} = \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}}$. So the energy can be expressed as

$$E_{\boldsymbol{k}} = \epsilon - t \sum_{\boldsymbol{\delta}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{\delta}}. \tag{44}$$

For a 2-dimensional square lattice model with lattice spacing a, the energy spectrum is

$$E_{\boldsymbol{k}} = \epsilon - 2t[\cos(k_x a) + \cos(k_y a)]. \tag{45}$$

3 Tight binding chains

In this chapter, we talk about the 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

$$\hat{H} = -\sum_n v_n \left(|n\rangle \langle n+1| + |n+1\rangle \langle n| \right) \tag{46}$$

where v_n is the hopping integral for the link between site n and $n+1$. The number operator at site n is $\hat{n}_m = |m\rangle \langle m|$. 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

$$\frac{\partial \langle \hat{N}_L \rangle}{\partial t} = \frac{i}{\hbar} \langle [\hat{H}, \hat{N}_L] \rangle = -\langle \hat{J}_{n_L} \rangle \tag{47}$$

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 $[\hat{H}_L, \hat{N}_L]$:

$$\begin{aligned}
[\hat{H}_L, \hat{N}_L] &= \sum_{n<n_L} v_n [|n\rangle \langle n+1|, \hat{N}_L] \\
&= \sum_{n<n_L} \sum_{m \leq n_L} v_n \left[|n\rangle \langle n+1|, |m\rangle \langle m| \right] \\
&= \sum_{n<n_L} \sum_{m \leq n_L} v_n (|n\rangle \langle n+1|m\rangle \langle m| - |m\rangle \langle m|n\rangle \langle n+1|) \\
&= \sum_{n<n_L} v_n (|n\rangle \langle n+1| - |n\rangle \langle n+1|) = 0.
\end{aligned} \tag{48}$$

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 $\hat{H}_{LR} = -v_{n_L}(|n_L\rangle \langle n_L+1| + |n_L+1\rangle \langle n_L|)$.

$$\begin{aligned}
\left[|n_L\rangle \langle n_L+1|, \hat{N}_L \right] &= \sum_{m \leq n_L} \left(|n_L\rangle \langle n_L+1|m\rangle \langle m| - |m\rangle \langle m|n_L\rangle \langle n_L+1| \right) \\
&= -|n_L\rangle \langle n_L+1|,
\end{aligned} \tag{49}$$

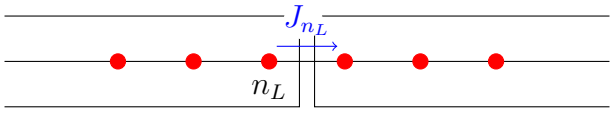

Figure 1: An infinite one-dimensional chain.

$$
\begin{aligned}
\left[|n_L+1\rangle\langle n_L|, \hat{N}_L\right] &= \sum_{m\le n_L} \left(|n_L+1\rangle\langle n_L|m\rangle\langle m| - |m\rangle\langle m|n_L+1\rangle\langle n_L|\right) \\
&= |n_L+1\rangle\langle n_L| .
\end{aligned} \tag{50}
$$

So the commutator is

$$
[\hat{H}, \hat{N}_L] = [\hat{H}_{LR}, \hat{N}_L] = -v_{n_L}(|n_L+1\rangle\langle n_L| - |n_L\rangle\langle n_L+1|), \tag{51}
$$

and the current operator is given by

$$
\hat{J}_n = \frac{i}{\hbar} v_n \left(|n+1\rangle\langle n| - |n\rangle\langle n+1|\right). \tag{52}
$$

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

$$
\begin{aligned}
\langle\psi_k|\hat{J}_n|\psi_k\rangle =& \frac{iv_n}{\hbar N}\sum_{m,m'} \mathrm{e}^{ik(m-m')a}\langle m'|\left(|n+1\rangle\langle n| - |n\rangle\langle n+1|\right)|m\rangle \\
=& \frac{iv_n}{\hbar N}\left(\mathrm{e}^{-ika} - \mathrm{e}^{ika}\right) = \frac{2v_n}{\hbar N}\sin(ka) \\
=& \underbrace{\frac{1}{Na}}_{\text{number density}} \times \underbrace{2v_n a \sin(ka)}_{\text{velocity}} .
\end{aligned} \tag{53}
$$

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

$$
\hat{H}_{\text{alt}} = -\sum_n \left[v(|n,A\rangle\langle n,B| + \text{h.c.}) + w(|n,B\rangle\langle n+1,A| + \text{h.c.})\right]. \tag{54}
$$

The eigenstate is given by

$$
|\psi\rangle = \sum_n (c_{n,A}|n,A\rangle + c_{n,B}|n,B\rangle), \tag{55}
$$

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

$$
Ec_{n,A} = -wc_{n-1,B} - vc_{n,B}, \tag{56}
$$

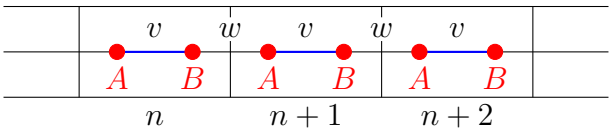

Figure 2: An one-dimensional alternating chain.

$$Ec_{n,B} = -wc_{n+1,A} - vc_{n,A}, \tag{57}$$

which equivalent to

$$-\begin{pmatrix} 0 & v + we^{-ika} \\ v + we^{ika} & 0 \end{pmatrix} \begin{pmatrix} c_A \\ c_B \end{pmatrix} = E \begin{pmatrix} c_A \\ c_B \end{pmatrix}. \tag{58}$$

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

$$E_k = \pm\sqrt{v^2 + w^2 + 2vw\cos ka}, \tag{59}$$

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

$$E_k = \pm 2t\cos(ka/2) \tag{60}$$

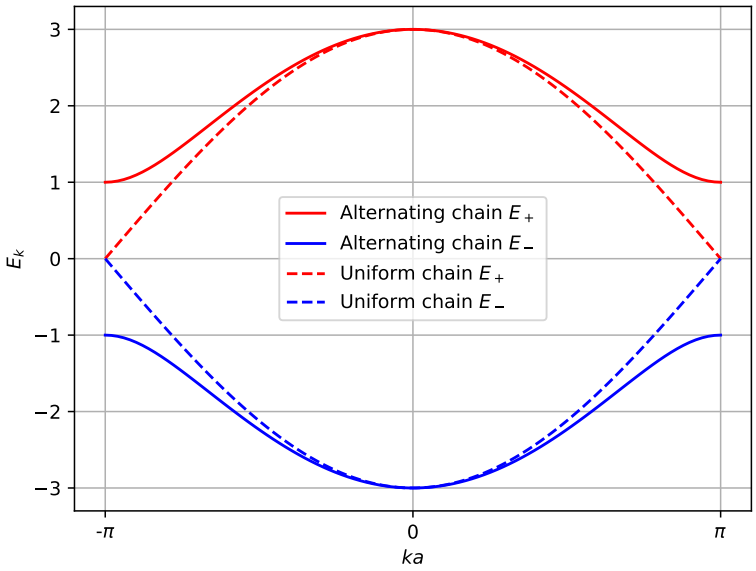

Figure 3: Energy spectrum for a tight binding chain. The dashed line corresponds to an uniform chain with hopping integral $t = 1.5$. The solid line corresponds to an alternating chain with hopping integrals $v = 1.0$ and $w = 2.0$. This has a band gap of $2|v - w| = 2.0$.

3.2.2 Sublattice symmetry

The dispersion relations of the two energy bands of the alternating chain are exactly symmetric under reflection in the $E = 0$ axis. Let an eigenstate at energy E be

$$|\psi\rangle = \sum_n (c_{n,A}\,|n, A\rangle + c_{n,B}\,|n, B\rangle). \tag{61}$$

For this system,

$$-wc_{n-1,B} - vc_{n,B} = Ec_{n,A}, \quad -wc_{n+1,A} - vc_{n,A} = Ec_{n,B}. \tag{62}$$

If we change sign on every other site, i.e., $_{n,A} = c_{n,A}$ and $_{n,B} = -c_{n,B}$, then

$$-w\tilde{c}_{n-1,B} - v\tilde{c}_{n,B} = -E\tilde{c}_{n,A}, \quad -v\tilde{c}_{n,A} - w\tilde{c}_{n+1,A} = -E\tilde{c}_{n,B}, \tag{63}$$

and the new state

$$|\tilde{\psi}\rangle = \sum_n (\tilde{c}_{n,A}\,|n,A\rangle + \tilde{c}_{n,B}\,|n,B\rangle) = \sum_n (c_{n,A}\,|n,A\rangle - c_{n,B}\,|n,B\rangle) \tag{64}$$

is also an eigenstate with energy $-E$.

3.3 Polyacetylene

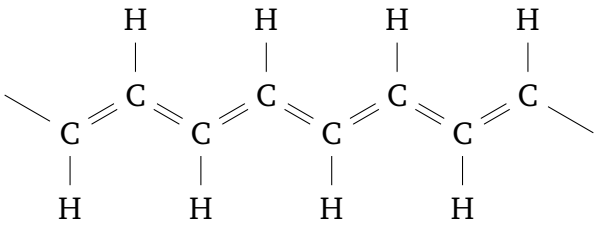

Figure 4: polyacetylene

3.4 Peierls instability

4 Edge states on SSH chain

In this chapter we talk about semi-infinite alternating chain.

4.1 Edge states of a dimerized chain

4.2 Exact solution: 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

$$\hat{H} = -\sum_{n=0} \left[v(|n,A\rangle \langle n,B| + |n,B\rangle \langle n,A|) + w(|n,B\rangle \langle n+1,A| + |n+1,A\rangle \langle n,B|) \right]. \tag{65}$$

The eigenstate at energy E

$$|\psi\rangle = \sum_{n=0} (c_{n,A} |n,A\rangle + c_{n,B} |n,B\rangle), \tag{66}$$

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

$$\begin{aligned}
\hat{H}|\psi\rangle =& -\sum_{m,n=0} \big[v(|m,A\rangle \langle m,B| + |m,B\rangle \langle m,A|) \\
&+ w(|m,B\rangle \langle m+1,A| + |m+1,A\rangle \langle m,B|) \big] (c_{n,A}|n,A\rangle + c_{n,B}|n,B\rangle) \\
=& -\sum_{n=0} (v c_{n,B}|n,A\rangle + v c_{n,A}|n,B\rangle + w c_{n,A}|n-1,B\rangle + w c_{n,B}|n+1,A\rangle) \\
=& -\sum_{n=0} (v c_{n,B}|n,A\rangle + v c_{n,A}|n,B\rangle + w c_{n+1,A}|n,B\rangle + w c_{n-1,B}|n,A\rangle) \\
=& E \sum_{n=0} (c_{n,A}|n,A\rangle + c_{n,B}|n,B\rangle).
\end{aligned} \tag{67}$$

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

$$E c_{n,A} = 0 = -v c_{n,B} - w c_{n-1,B}, \tag{68}$$

$$E c_{n,B} = 0 = -v c_{n,A} - w c_{n+1,A}, \tag{69}$$

at zero-energy state. Then we have

$$c_{n,B} = -\frac{w}{c} c_{n-1,B}, \qquad c_{n+1,A} = -\frac{v}{w} c_{n,A}, \qquad c_{0,A} = 0, \tag{70}$$

at $E = 0$. These equations gives the following results

$$c_{n,A} = 0, \qquad c_{n,B} = c_{0,B} \left(-\frac{w}{v}\right)^n = c_{0,B} (-1)^n \mathrm{e}^{-n/\xi} \tag{71}$$

where $\xi = 1/\ln(v/w)$.

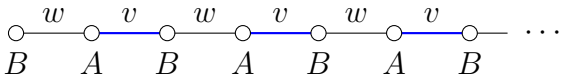

Figure 5: Caption

5 Adiabatic transport

5.1 Adiabatic cycle on a dimerized chain

5.1.1 Rice-Mele model

$$\hat{H}_{\text{RM}} = \hat{H}_{\text{alt}} + u \sum_n \left(|n, A\rangle \langle n, A| - |n, B\rangle \langle n, B| \right) \tag{72}$$

5.1.2 Charge pump cycle

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

5.2 Thouless adiabatic current

first Chern number

$$Q = \frac{1}{2\pi i} \int_0^T \mathrm{d}t \oint_{\text{BZ}} \mathrm{d}k (\langle \partial_k \nu | \partial_t \nu \rangle - \langle \partial_t \nu | \partial_k \nu \rangle) \tag{73}$$

5.3 Adiabatic charge transport in a filled band

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 $\boldsymbol{A}$ and the scalar potential ϕ

$$\hat{H} = \frac{1}{2m}(-i\hbar\boldsymbol{\nabla} - q\boldsymbol{A})^2 + q\phi, \tag{74}$$

where $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$ is the magnetic field and $\boldsymbol{E} = -\boldsymbol{\nabla}\phi - \partial\boldsymbol{A}/\partial t$ 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 $\boldsymbol{B}$ and $\boldsymbol{E}$) 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. $\boldsymbol{B}$ and $\boldsymbol{E}$ is invarent under the transformation

$$\boldsymbol{A} \to \boldsymbol{A}' = \boldsymbol{A} + \boldsymbol{\nabla}\varphi, \quad \phi \to \phi' = \phi - \frac{\partial\varphi}{\partial t}. \tag{75}$$

And the Hamiltonian also transforms

$$\hat{H} \to \hat{H}' = \frac{1}{2m}(-i\hbar\boldsymbol{\nabla} - q\boldsymbol{A} - q\boldsymbol{\nabla}\varphi)^2 + q\phi - q\frac{\partial\varphi}{\partial t}. \tag{76}$$

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

$$\psi \to \psi' = \mathrm{e}^{iq\varphi/\hbar}\psi. \tag{77}$$

Now we examine the Shrödinger 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

$$\begin{aligned}(-i\hbar\boldsymbol{\nabla} - q\boldsymbol{A} - q\boldsymbol{\nabla}\varphi)\psi' =& (-i\hbar\boldsymbol{\nabla} - q\boldsymbol{A} - q\boldsymbol{\nabla}\varphi)\mathrm{e}^{iq\varphi/\hbar}\psi \\ =& q(\boldsymbol{\nabla}\varphi)\mathrm{e}^{iq\varphi/\hbar}\psi - i\hbar(\boldsymbol{\nabla}\psi)\mathrm{e}^{iq\varphi/\hbar} - q\boldsymbol{A}\mathrm{e}^{iq\varphi/\hbar}\psi - q(\boldsymbol{\nabla}\varphi)\mathrm{e}^{iq\varphi/\hbar}\psi \\ =& -i\hbar(\boldsymbol{\nabla}\psi)\mathrm{e}^{iq\varphi/\hbar} - q\boldsymbol{A}\mathrm{e}^{iq\varphi/\hbar}\psi \\ =& \mathrm{e}^{iq\varphi/\hbar}(-i\hbar\boldsymbol{\nabla} - q\boldsymbol{A})\psi.\end{aligned} \tag{78}$$

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

$$(-i\hbar\boldsymbol{\nabla} - q\boldsymbol{A} - q\boldsymbol{\nabla}\varphi)^2\psi' = \mathrm{e}^{iq\varphi/\hbar}(-i\hbar\boldsymbol{\nabla} - q\boldsymbol{A})^2\psi. \tag{79}$$

So the right handside of the Schrödinger equation is

$$\text{RHS} = \hat{H}'\psi' = \mathrm{e}^{iq\varphi/\hbar}\left[\frac{1}{2m}(-i\hbar\boldsymbol{\nabla} - q\boldsymbol{A})^2\psi + q\phi - q\frac{\partial\varphi}{\partial t}\right]\psi = \mathrm{e}^{iq\varphi/\hbar}H\psi. \tag{80}$$

The left handside of the equation is

$$\text{LHS} = i\hbar\frac{\partial\psi'}{\partial t} = \mathrm{e}^{iq\varphi/\hbar}i\hbar\frac{\partial\psi}{\partial t}. \tag{81}$$

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

6.2 Current in a vector potential

The current density in the absence of a vector potential is

$$\boldsymbol{J} = \frac{1}{2m}[\psi^*(-i\hbar\boldsymbol{\nabla})\psi + \psi(i\hbar\boldsymbol{\nabla})\psi^*]. \tag{82}$$

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

$$\begin{aligned}\boldsymbol{J} =& \frac{1}{2m}[\psi^*(-i\hbar\boldsymbol{\nabla} - q\boldsymbol{A})\psi + \psi(i\hbar\boldsymbol{\nabla} - q\boldsymbol{A})\psi^*] \\ =& -\frac{i\hbar}{2m}(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*) - \frac{q\boldsymbol{A}}{2m}|\psi|^2.\end{aligned} \tag{83}$$

The current is gauge invarience and we can examine this:

$$\begin{aligned}\boldsymbol{J}' =& -\frac{i\hbar}{2m}[(\psi')^*\boldsymbol{\nabla}\psi' - \psi'\boldsymbol{\nabla}(\psi')^*] - \frac{q\boldsymbol{A}'}{2m}|\psi'|^2 \\ =& \frac{1}{2m}[\psi^*(-i\hbar\boldsymbol{\nabla} + q\boldsymbol{\nabla}\varphi)\psi + \psi(i\hbar\boldsymbol{\nabla} + q\boldsymbol{\nabla}\varphi)\psi^*] - \frac{q}{2m}(\boldsymbol{A} + \boldsymbol{\nabla}\varphi)|\psi|^2 \\ =& -\frac{i\hbar}{2m}(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*) - \frac{q\boldsymbol{A}}{2m}|\psi|^2 = \boldsymbol{J}.\end{aligned} \tag{84}$$

6.3 Aharonov-Bohm effect

6.3.1 Adiabatic derivation

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

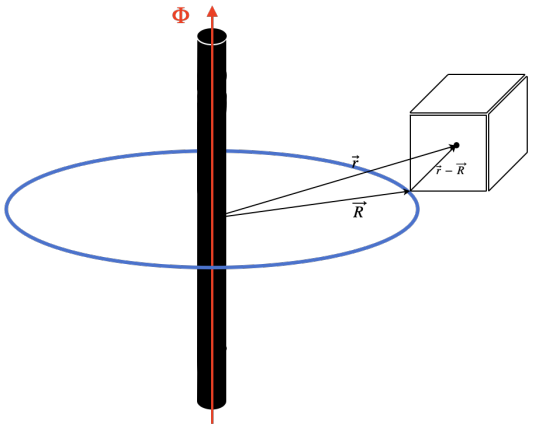

Figure 6: A particle is confined to a ox at position $R(t)$ which is moved adiabatically along path C around an infinite solenoid carrying flux Φ. The box does not move through any region with non-zero magnetic field.

outside the solenoid is zero). With the relation

$$\oint_C \boldsymbol{A}\cdot \mathrm{d}\boldsymbol{r} = \int_S \boldsymbol{B}\cdot \mathrm{d}\boldsymbol{S} = \Phi, \tag{85}$$

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 $V(\boldsymbol{r}-\boldsymbol{R})$ centered at $\boldsymbol{R}$ far away from the solenoid. The Hamiltonian of the particle is

$$\hat{H} = \frac{1}{2m}(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{r}} - q\boldsymbol{A}(\boldsymbol{r}))^2 + V(\boldsymbol{r}-\boldsymbol{R}). \tag{86}$$

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

$$i\hbar\frac{\partial\psi}{\partial t} = \left[\frac{1}{2m}(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{r}} - q\boldsymbol{A}(\boldsymbol{r}))^2 + V(\boldsymbol{r}-\boldsymbol{R}(t))\right]\psi. \tag{87}$$

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

$$\psi_{\boldsymbol{R}}(r) = \mathrm{e}^{i\chi_{\boldsymbol{R}}(\boldsymbol{r})}u(\boldsymbol{r}-\boldsymbol{R}), \quad \chi_{\boldsymbol{R}}(\boldsymbol{r}) = \frac{q}{\hbar}\int_{\boldsymbol{R}}^{\boldsymbol{r}} \boldsymbol{A}(\boldsymbol{r}')\cdot \mathrm{d}\boldsymbol{r}'. \tag{88}$$

Now we examine the solutions given in Eq.(88). Let's begin with the relation

$$(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{r}} - q\boldsymbol{A})\mathrm{e}^{i\chi(\boldsymbol{r})}u(\boldsymbol{r}-\boldsymbol{R}) = \mathrm{e}^{i\chi(\boldsymbol{r})}(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{r}} + \hbar\boldsymbol{\nabla}\chi - q\boldsymbol{A})u(\boldsymbol{r}-\boldsymbol{R}). \tag{89}$$

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

$$(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{r}} - q\boldsymbol{A})\mathrm{e}^{i\chi(\boldsymbol{r})}u(\boldsymbol{r}-\boldsymbol{R}) = \mathrm{e}^{i\chi(\boldsymbol{r})}(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{r}})u(\boldsymbol{r}-\boldsymbol{R}), \tag{90}$$

$$(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{r}} - q\boldsymbol{A})^2\mathrm{e}^{i\chi(\boldsymbol{r})}u(\boldsymbol{r}-\boldsymbol{R}) = \mathrm{e}^{i\chi(\boldsymbol{r})}(-i\hbar\boldsymbol{\nabla}_{\boldsymbol{r}})^2u(\boldsymbol{r}-\boldsymbol{R}). \tag{91}$$

So we have

$$\hat{H}(\boldsymbol{A})\psi_{\boldsymbol{R}}(\boldsymbol{r}) = \mathrm{e}^{i\chi(\boldsymbol{r})}\hat{H}(\boldsymbol{A}=0)u(\boldsymbol{r}-\boldsymbol{R}) = \mathrm{e}^{i\chi(\boldsymbol{r})}Eu(\boldsymbol{r}-\boldsymbol{R}) = E\psi_{\boldsymbol{R}}(\boldsymbol{r}). \tag{92}$$

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

$$\gamma_{\text{geom}} = \oint_C \boldsymbol{a}(\boldsymbol{R})\cdot\mathrm{d}\boldsymbol{R}, \tag{93}$$

where the Berry connection is

$$\boldsymbol{a}(\boldsymbol{R}) = i\left\langle\psi_{\boldsymbol{R}}\right|\boldsymbol{\nabla}_{\boldsymbol{R}}\left|\psi_{\boldsymbol{R}}\right\rangle = i\left[-i\frac{q}{\hbar}\boldsymbol{A}(\boldsymbol{R})\right] + i\left\langle u_{\boldsymbol{R}}\right|\boldsymbol{\nabla}_{\boldsymbol{R}}\left|u_{\boldsymbol{R}}\right\rangle = \frac{q}{\hbar}\boldsymbol{A}(\boldsymbol{R}). \tag{94}$$

So the Berry phase is

$$\gamma_{\text{geom}} = \frac{q}{\hbar}\oint_C \boldsymbol{A}(\boldsymbol{R})\cdot\mathrm{d}\boldsymbol{R} = \frac{q}{\hbar}\Phi. \tag{95}$$

6.3.2 Aharonov-Bohm interferometry

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

$$\Delta(\text{phase}) = \frac{q}{\hbar}\int_{C_L}\boldsymbol{A}(\boldsymbol{R})\cdot\mathrm{d}\boldsymbol{R} - \frac{q}{\hbar}\int_{C_R}\boldsymbol{A}(\boldsymbol{R})\cdot\mathrm{d}\boldsymbol{R} = \frac{q\Phi}{\hbar}. \tag{96}$$

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

$$\Phi = \frac{h}{2e}(2n+1), \tag{97}$$

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 $h/2e$.

7 Electrons in a magnetic field

7.1 Electrons in a uniform magnetic field - Landau levels

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

$$\frac{mv^2}{r} = eBv, \tag{98}$$

gives the **cyclotron frequency**

$$\omega_c = \frac{v}{r} = \frac{eB}{m}. \tag{99}$$

The Hamiltonian of the electron

$$\hat{H} = \frac{1}{2m}(-i\hbar\boldsymbol{\nabla} + e\boldsymbol{A})^2 + V(z) \tag{100}$$

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

$$\hat{H} = \frac{1}{2m}\left[-i\hbar\left(\partial_x, \partial_y, \partial_z\right) + e\left(-By, 0, 0\right)\right]^2 + V(z) = \hat{H}_{xy} + \hat{H}_z, \tag{101}$$

where

$$\hat{H}_{xy} = \frac{1}{2m}\left[-\hbar^2\frac{\partial^2}{\partial y^2} + \left(-i\hbar\frac{\partial}{\partial x} - eBy\right)^2\right], \quad \hat{H}_z = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V(z). \tag{102}$$

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

$$\hat{H}_{xy}\psi(x, y) = E_{xy}\psi(x, y), \quad \hat{H}_z u(z) = E_z u(z), \quad E = E_{xy} + E_z. \tag{103}$$

Now we focus on the xy-plane. In the 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: $\psi(x, y) = \mathrm{e}^{ik_x x}v_{k_x}(y)$. Then

$$\hat{H}_{xy}\mathrm{e}^{ik_x x}v_{k_x}(y) = \frac{\hbar^2}{2m}\left[-\partial_y^2 + \left(k_x - \frac{y}{l_B^2}\right)^2\right]\mathrm{e}^{ik_x x}v_{k_x}(y) = E_{xy}\mathrm{e}^{ik_x x}v_{k_x}(y), \tag{104}$$

or

$$\hat{H}_{k_x}v_{k_x}(y) = \frac{\hbar^2}{2m}\left[-\partial_y^2 + \left(k_x - \frac{y}{l_B^2}\right)^2\right]v_{k_x}(y) = E_{xy}v_{k_x}(y), \tag{105}$$

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

$$\hat{H}_{\text{SHO}} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{1}{2}m\omega_0^2(y - y_k)^2 = \frac{\hbar^2}{2m}\left[-\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{m^2\omega_0^2}{\hbar^2}(y - y_k)^2\right]. \tag{106}$$

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

$$\hat{H}_{k_x} = \frac{\hbar^2}{2m}\left[-\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{e^2B^2}{\hbar^2}\left(y - \frac{k_x\hbar}{eB}\right)^2\right], \tag{107}$$

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

$$E_{xy}(k_x) = (n + 1)\hbar\omega_c, \tag{108}$$

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 $n = 0, 1, 2, \ldots$. How many degenerate states at each n?

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

$$\delta y_{k_x} = l_B^2\delta k_x = \frac{2\pi l_B^2}{L_x}. \tag{109}$$

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

$$g = \frac{L_y}{\delta y_{k_x}} = \frac{L_xL_y}{2\pi l_B^2} = \frac{e}{h}BA = \frac{\Phi}{\Phi_0}, \tag{110}$$

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 $\boldsymbol{B}$ in the z direction and an electric field $\boldsymbol{\mathcal{E}}$ in the y-direction. The equation of motion for the electron is

$$m\ddot{x} = -eB\dot{y}, \quad m\ddot{y} = eB\dot{x} - e\mathcal{E}_y. \tag{111}$$

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

$$m\ddot{z} - ieB\dot{z} = -ie\mathcal{E}_y. \tag{112}$$

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

$$\dot{z} = A\mathrm{e}^{i\omega_c t} + \frac{\mathcal{E}_y}{B}, \quad z = z_0\mathrm{e}^{i\omega_c t} + \frac{\mathcal{E}_y t}{B} + z_1 \tag{113}$$

where $\omega_c = eB/m$ is the cyclotron frequency with electric field $\boldsymbol{\mathcal{E}} = 0$, $z_0 = A/i\omega_c$ 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

$$J_x = -nev_x = -(ne/B)\mathcal{E}_y. \tag{114}$$

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

$$R_{\mathrm{H}} = \frac{V_y}{I_x} = \frac{B}{ne}. \tag{115}$$

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

$$\begin{pmatrix} J_x \\ J_y \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{pmatrix} \begin{pmatrix} \mathcal{E}_x \\ \mathcal{E}_y \end{pmatrix}, \tag{116}$$

where the matrix $\boldsymbol{\sigma}$ is the **conductivity tensor**. Note that this is an anti-asymmetric tensor. Conversely, we can define a resistivity tensor

$$\begin{pmatrix} \mathcal{E}_x \\ \mathcal{E}_y \end{pmatrix} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ -\rho_{xy} & \rho_{xx} \end{pmatrix} \begin{pmatrix} J_x \\ J_y \end{pmatrix}, \tag{117}$$

with

$$\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}, \quad \rho_{xy} = -\frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2}. \tag{118}$$

In this way, the Hall effect can be written as

$$\rho_{xy} = -\frac{\mathcal{E}_y}{J_x} = \frac{B}{en}. \tag{119}$$

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

7.3 Interger quantum Hall effect

7.3.1 2D electron gas

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

$$\hat{H} = \frac{1}{2m}\left[-\hbar^2\frac{\partial^2}{\partial y^2} + \left(-i\hbar\frac{\partial}{\partial x} - eBy\right)^2\right] + e\mathcal{E}y. \tag{120}$$

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

$$\hat{H}_{k_x} v_{k_x}(y) = \frac{\hbar^2}{2m}\left[-\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \left(k_x - \frac{y}{l_B^2}\right)^2 + \frac{2me\mathcal{E}y}{\hbar^2}\right] v_{k_x}(y) = E(k_x) v_{k_x}(y). \tag{121}$$

It is a simple harmonic oscillator

$$\hat{H}_{k_x} = \frac{\hbar\omega_c}{2}\left[-l_B^2\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{1}{l_B^2}(y - y_{k_x} + y_\mathcal{E})^2\right] + e\mathcal{E}\left(y_{k_x} - \frac{y_\mathcal{E}}{2}\right), \quad y_\mathcal{E} = \frac{m\mathcal{E}}{eB^2}, \tag{122}$$

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 center has shifted to $y_{k_x} - y_\mathcal{E}$. The eigenenergies are

$$\begin{aligned} E_n(k_x) &= \left(n + \frac{1}{2}\right)\hbar\omega_c + e\mathcal{E}\left(y_{k_x} - \frac{y_\mathcal{E}}{2}\right) \\ &= \left(n + \frac{1}{2}\right)\hbar\omega_c + e\mathcal{E}\left(y_{k_x} - y_\mathcal{E}\right) + \frac{1}{2}m\left(\frac{\mathcal{E}}{B}\right)^2. \end{aligned} \tag{123}$$

The group velocity is

$$v_g(k_x) = \frac{1}{\hbar}\frac{\partial E_n(k_x)}{\partial k_x} = \frac{e\mathcal{E}}{\hbar}\frac{\partial y_{k_x}}{\partial k_x} = \frac{\mathcal{E}}{B}. \tag{124}$$

Recall the degeneracy of the Landau level. the number of electron states in a strip of width L_y is $g = \Phi/\Phi_0 = L_x L_y eB/h$. The total charge current is

$$J_x = -e\frac{g}{L_x L_y} v_g = -e\frac{eB}{h}\frac{\mathcal{E}}{B} = -\frac{e^2}{h}\mathcal{E}. \tag{125}$$

So the conductivity

$$\sigma_{xy} = -\frac{e^2}{h}, \quad \rho_{xy} = \frac{h}{e^2}, \quad \rho_x x = 0, \quad \sigma_{xx} = 0. \tag{126}$$

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 $\sigma_{xy} = -Me^2/h$.

7.3.2 Edge states

7.3.3 Laughlin's gauge argument: adiabatic transport

7.3.4 Hall effect and Landau levels