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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

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

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

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

We prepare the system in eigenstate

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

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

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

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

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

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

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

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

Then we have

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

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

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

Rearranging this equation and then

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

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

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

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

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

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 introduce 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

For any eigenstate $\psi(\boldsymbol{r})$ of a periodic system

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

$$\psi_{\alpha\boldsymbol{k}}(\boldsymbol{r}) = \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}}\phi_{\alpha\boldsymbol{k}}(\boldsymbol{r}) \tag{39}$$

where $\phi_{\alpha\boldsymbol{k}}(\boldsymbol{r}) = \phi_{\alpha\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{R})$.

2.2 Nearly free electron model

The nearly free electron model (NFE model) is a theoretical framework in solid-state physics that 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 is a theoretical framework in solid-state physics used to describe the behavior of electrons in crystals, particularly effective for insulators and semiconductors. Unlike the Nearly Free Electron Model, the Tight Binding Model focuses on the strong coupling between electrons and one or more atomic nuclei, especially when electrons are confined close to atomic or molecular orbitals.

We can write the electron state as

$$|\psi\rangle = \sum_{\boldsymbol{R}} c_{\boldsymbol{R}} \, |\boldsymbol{R}\rangle \, , \tag{40}$$

where $c_{\boldsymbol{R}}$ is the probability amplitude for finding the electron at site $\boldsymbol{R}$. Then the binding model can be defined by the Hamiltonian

$$\hat{H} = \epsilon_\alpha \sum_{\boldsymbol{R}} |\boldsymbol{R}\rangle \langle \boldsymbol{R}| - t_\alpha \sum_{\langle \boldsymbol{R},\boldsymbol{R}'\rangle} (|\boldsymbol{R}\rangle \langle \boldsymbol{R}'| + |\boldsymbol{R}'\rangle \langle \boldsymbol{R}|), \tag{41}$$

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 means the on-site energy, or the bound-state energy. t

means the hopping integral. Applying the Hamiltonian to the electron state

$$\begin{aligned}\hat{H}\left|\psi\right\rangle =&\epsilon_\alpha \sum_{\boldsymbol{R},\boldsymbol{S}} c_{\boldsymbol{R}}\left|\boldsymbol{S}\right\rangle \left\langle \boldsymbol{S}|\boldsymbol{R}\right\rangle - t_\alpha \sum_{\boldsymbol{R},\langle \boldsymbol{S},\boldsymbol{S}'\rangle} c_{\boldsymbol{R}}(\left|\boldsymbol{S}\right\rangle \left\langle \boldsymbol{S}'|\boldsymbol{R}\right\rangle + \left|\boldsymbol{S}'\right\rangle \left\langle \boldsymbol{S}|\boldsymbol{R}\right\rangle)\\ =&\epsilon_\alpha \sum_{\boldsymbol{S}} c_{\boldsymbol{S}}\left|\boldsymbol{S}\right\rangle - t_\alpha \sum_{\langle \boldsymbol{S},\boldsymbol{S}'\rangle} (c_{\boldsymbol{S}'}\left|\boldsymbol{S}\right\rangle + c_{\boldsymbol{S}}\left|\boldsymbol{S}'\right\rangle).\end{aligned} \tag{42}$$

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

$$\left\langle \boldsymbol{R}\right|\hat{H}\left|\psi\right\rangle = \epsilon_\alpha c_{\boldsymbol{R}} - t_\alpha \sum_{\langle \boldsymbol{S},\boldsymbol{S}'\rangle} (c_{\boldsymbol{S}'}\delta_{\boldsymbol{R},\boldsymbol{S}} + c_{\boldsymbol{S}}\delta_{\boldsymbol{R},\boldsymbol{S}'}) = \epsilon_\alpha c_{\boldsymbol{R}} - t_\alpha \sum_{\boldsymbol{\delta}} c_{\boldsymbol{R}+\boldsymbol{\delta}}, \tag{43}$$

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 $\left\langle \boldsymbol{R}\right|\hat{H}\left|\psi\right\rangle = E\left\langle \boldsymbol{R}|\psi\right\rangle$, then

$$\epsilon_\alpha c_{\boldsymbol{R}} - t_\alpha \sum_{\boldsymbol{\delta}} c_{\boldsymbol{R}+\boldsymbol{\delta}} = E c_{\boldsymbol{R}}. \tag{44}$$

The system with N sites under periodic boundary conditions has eigenstates

$$\left|\psi_{\alpha\boldsymbol{k}}\right\rangle = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}}\left|\boldsymbol{R},\alpha\right\rangle, \tag{45}$$

and the energy is

$$E_{\alpha\boldsymbol{k}} = \epsilon_\alpha - t_\alpha \sum_{\boldsymbol{\delta}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{\delta}}, \tag{46}$$

where $\boldsymbol{k}$ is in the first Brillouin zone.

3 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

$$\hat{H} = -\sum_n v_n \left(|n\rangle \langle n+1| + |n+1\rangle \langle n| \right) \tag{47}$$

where v_n is the hopping integral1 for the link between site n and $n+1$. The number operator at site n is $\hat{n} = |n\rangle \langle n|$. 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

$$\frac{\partial \langle \hat{N}_L \rangle}{\partial t} = \frac{i}{\hbar} \langle [\hat{H}, \hat{N}_L] \rangle = -\langle \hat{J}_{n_L} \rangle \tag{48}$$

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 block R only, $\hat{H}_L$ involves links inside block L only, and $\hat{H}_{LR}$ contains the link joining the left and right blocks together.

$$\begin{aligned}
\left[\sum_{n<n_L} v_n |n\rangle \langle n+1| , \hat{N}_L \right] &= \sum_{n<n_L} \sum_{m \leq n_L} v_n \left[|n\rangle \langle n+1| , |m\rangle \langle m| \right] \\
&= \sum_{n<n_L} \sum_{m \leq n_L} v_n (|n\rangle \langle n+1|m\rangle \langle m| - |m\rangle \langle m|n\rangle \langle n+1|) \\
&= \sum_{n<n_L} v_n (|n\rangle \langle n+1| - |n\rangle \langle n+1|) = 0
\end{aligned} \tag{49}$$

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

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

$$\begin{aligned}
\left[|n_L+1\rangle \langle n_L| , \hat{N}_L \right] &= \sum_{m \leq n_L} (|n_L+1\rangle \langle n_L|m\rangle \langle m| - |m\rangle \langle m|n_L+1\rangle \langle n_L|) \\
&= |n_L+1\rangle \langle n_L| .
\end{aligned} \tag{51}$$

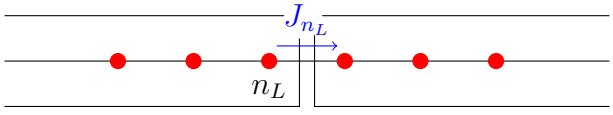

Figure 1: Caption

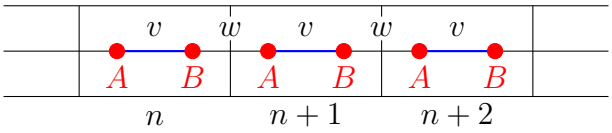

Figure 2: Caption

So the commutator

$$[\hat{H}, \hat{N}_L] = -v_{n_L}(|n_L+1\rangle\langle n_L| - |n_L\rangle\langle n_L+1|), \tag{52}$$

and the current operator

$$\hat{J}_n = \frac{i}{\hbar} v_n \left(|n+1\rangle\langle n| - |n\rangle\langle n+1|\right). \tag{53}$$

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

$$\begin{aligned}\langle\psi_k|\hat{J}_n|\psi_k\rangle =& \frac{iv_n}{\hbar N}\sum_{m,m'} \mathrm{e}^{ik(m-m')a}\langle m'|\left(|n+1\rangle\langle n| - |n\rangle\langle n+1|\right)|m\rangle \\ =& \frac{iv_n}{\hbar N}\left(\mathrm{e}^{-ika} - \mathrm{e}^{ika}\right) = \frac{2v_n}{\hbar N}\sin(ka) \\ =& \underbrace{\frac{1}{Na}}_{\text{number density}} \times \underbrace{2v_n a \sin(ka)}_{\text{velocity}}.\end{aligned} \tag{54}$$

3.2 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

$$\hat{H} = -\sum_{n=-\infty}^{\infty}\left[v(|n,A\rangle\langle n,B| + |n,B\rangle\langle n,A|) + w(|n,B\rangle\langle n+1,A| + |n+1,A\rangle\langle n,B|)\right], \tag{55}$$

with the eigenstate

$$|\psi\rangle = \sum_n (c_{n,A}|n,A\rangle + c_{n,B}|n,B\rangle), \tag{56}$$

where $c_{n,A} = c_A \mathrm{e}^{iknа}$, $c_{n,B} = c_B \mathrm{e}^{iknа}$ based on the Bloch theorem. The eigenfunction $\hat{H}|\psi\rangle = E|\psi\rangle$ gives

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

$$Ec_{n,B} = -wc_{n+1,A} - vc_{nA}, \tag{58}$$

which equivalent to

$$-\begin{pmatrix} 0 & v + w\mathrm{e}^{-ika} \\ v + w\mathrm{e}^{ika} & 0 \end{pmatrix}\begin{pmatrix} c_A \\ c_B \end{pmatrix} = E\begin{pmatrix} c_A \\ c_B \end{pmatrix}. \tag{59}$$

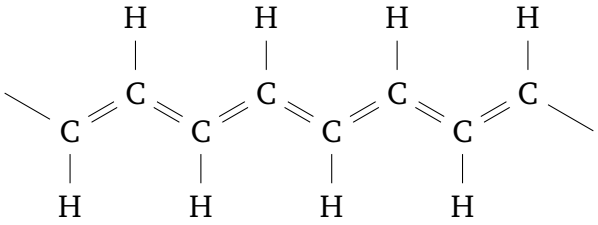

Figure 3: polyacetylene

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

$$E_k = \pm\sqrt{v^2 + w^2 + 2vw\cos ka}, \tag{60}$$

with k in the first Brillouin zoom, i.e., $-\pi/a < k < \pi/a$.

3.3 Uniform chain

For uniform chain, we have $v = w = t$, then the band energy

$$E_k = \pm 2t\cos(ka/2) \tag{61}$$

3.4 Example: polyacetylene

3.5 Peierls instability