$= n - m$

$z = re^{i\theta}$ · $\oint d\theta = \oint (\nabla\theta) \cdot dl$

总结：<u>Geometry phase</u> $\xrightarrow{\text{Stokes定理}}$ TKNN 1
构造参数空间物理

$n = \oint d\vec{S} \cdot \vec{B}$

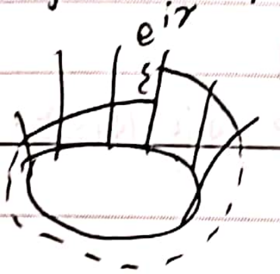
$G = e^2/h \, n$

↳ monopole

↳ Wu-Yang

回顾

$\gamma = i\int \langle \psi_{\vec{R}} | \nabla_R | \psi_{\vec{R}} \rangle \cdot d\vec{R}$



$e^{i\gamma}$ ← fibre $U(1)$ 纤维丛

几何相 ⟵ AB effect ⟵ monopole $\oint \vec{B} \cdot d\vec{S} \in \mathbb{Z}$

Topo insulator: k space monopole

几何相 ⟶ Zak phase (1989)

1d 固体 Bloch能带

$\gamma = i\oint \langle \psi_k | \nabla_k | \psi_k \rangle dk$ ~ polarization

} 在Wannier基下做

Topological insulator

{ Haldane Model (1988)

{ Qi-Wu-Zhang Model

材料实现

↳ Hall effect $G = n e^2/h$ Hall 电导 1981

量子化几何相 ⇒ 测精细结构常数 α

↓ Laughlin argument

作业：1. 量子化基本的推导

2. 阅读的文献

① Laughlin Nobel lecture 1998

② Laughlin PRB, 23, 5632 (1981) 直观图像

③ Haldane 1988 PRL gauge potential 更本质

计算/数值方法

$$\gamma = i\int \langle \psi(R)|\nabla_R|\psi(R)\rangle\, dR$$

$$= i\sum_i \frac{\langle\psi_i|(|\psi_{i+1}\rangle - |\psi_i\rangle)}{\delta R}\delta R$$

$$= i\sum(\langle\psi_i|\psi_{i+1}\rangle - 1)$$

计算发现不收敛

$e^{i\gamma}$ $\gamma\in[0,2\pi)$ well-defined

$\gamma = i\sum(\langle\psi_i|\psi_{i+1}\rangle - 1) \mod 2\pi$ 也不对

因为 $|\psi_i\rangle \to |\psi_i\rangle e^{i\theta_i}$ $|\psi_{i+1}\rangle$, $|\psi_i\rangle$ 存在相位差

正确方法：

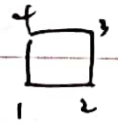
$$e^{i\gamma} = e^{-\int\langle\psi_R|\nabla_R|\psi_R\rangle\cdot dR}$$

$$= e^{-i\sum_i(\underbrace{\langle\psi_i|\psi_{i+1}\rangle}_{\approx 1} - 1)}$$ 成立条件：已知光滑 Gauge

$$= \prod_i e^{1-\langle\psi_i|\psi_{i+1}\rangle}$$

$$= \prod_i(2 - \langle\psi_i|\psi_{i+1}\rangle)$$

修正 $= \prod\langle\psi_i|\psi_{i+1}\rangle$



$$\langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_3\rangle\langle\psi_3|\psi_4\rangle\langle\psi_4|\psi_1\rangle$$
$$e^{i\theta_2}\quad e^{-i\theta_2}$$

$\prod_i\langle\psi_i|\psi_{i+1}\rangle$ $\quad |\psi_{i+1}\rangle = |\psi_i\rangle + (\partial|\psi_i\rangle)dR$

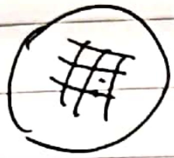
$$= \prod_i(1 + \langle\psi_i|\partial|\psi_i\rangle dR)$$

$$= \prod_i e^{\langle\psi_i|\partial|\psi_i\rangle dR}$$

$$= e^{\int\langle\psi|\partial|\psi\rangle dR}$$

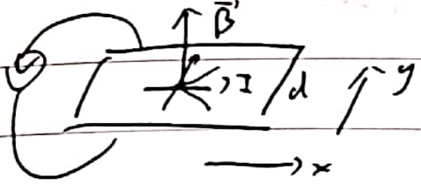
$$= e^{i\gamma}$$

Fukui（日本）



$$\int_{\Sigma} \vec{B}\cdot d\vec{S} = \sum_i \int_{\Sigma_i} \vec{B}\cdot d\vec{S}$$

Hall Conductance $G = \frac{1}{R}$

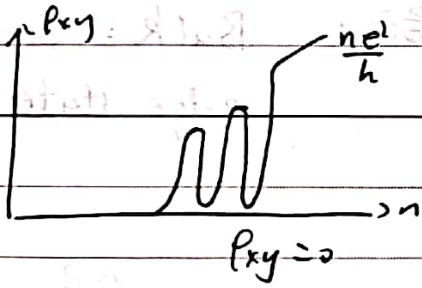


$R = \frac{U}{I}$ $\quad G = \frac{I_x}{V_y} = \rho_{xy}$

$eE = evB$

$I = nevd$ $\quad G = \frac{I_x}{V_y} = \frac{nev}{E} = \frac{ne}{B}$

实验：

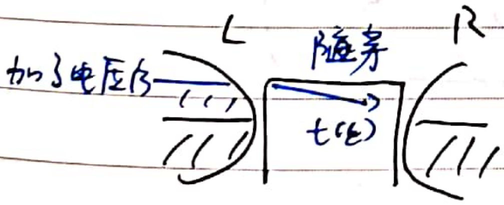


$G = \frac{ne^2}{h}$ $\quad$ n: 整数或分数

Landau 能级与电子

$G=0$ for insulator $\Rightarrow$ 导电 $\Rightarrow$ ~~G~~

$\rho(\varepsilon) \neq 0$ density of state

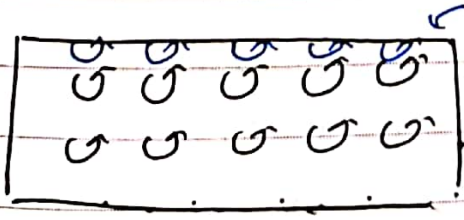


Fermi surface

$$\int \rho_L(\varepsilon+V)\,(1-\rho_R(\varepsilon))\,t(\varepsilon)\,d\varepsilon$$

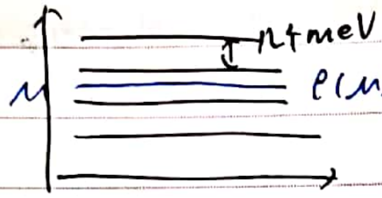
Landau 能级

边界可以导电



$\Rightarrow I_x$?

电子原地转圈，不会贡献电流



非平凡

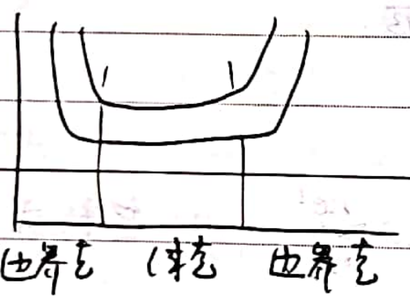
① Landau level ⇒ Insulator 但 $\begin{cases} I \neq 0 \\ \sigma \neq 0 \end{cases}$

② $\sigma = \frac{ne}{B} \longrightarrow \mathbb{Z} \times \frac{e^2}{h}$

n: 密度 ⟶ 整数？

③ $n \longrightarrow p/q$ 分数

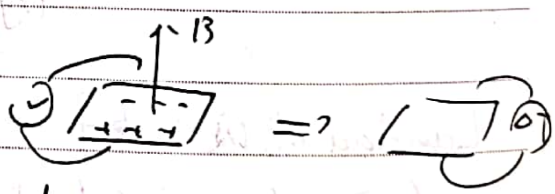
计算得到的能级

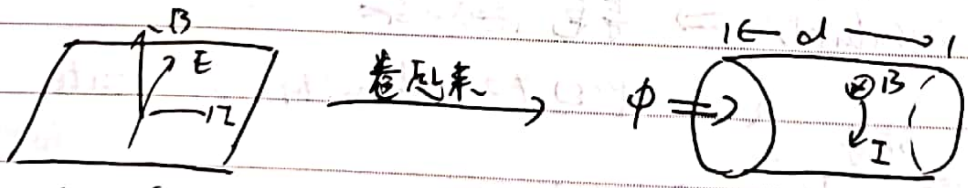


启示： Bulk: Insulator

edge state

Laughlin argument：应用于边界





$\phi = \oint \vec{A}\cdot d\vec{l} = AL$

第一个公式 $I = c\frac{\partial U}{\partial \phi}$

量纲分析 单位 $\frac{eV}{T\cdot m^2}$

$I = c\left(\frac{\partial U}{\partial \phi}\right) = c\frac{\delta U}{\delta \phi}$

用量子化电子 $\delta\phi = \_\_$

$H(\phi)$

$H|\psi(\phi)\rangle = |\psi(\phi)\rangle E(\phi)$

Feynman - Hellman 定理

$$\langle\psi(\phi)|\frac{\partial H}{\partial \phi}|\psi(\phi)\rangle = \frac{\partial}{\partial \phi}\langle\psi(\phi)|H(\phi)|\psi(\phi)\rangle = \frac{\partial U}{\partial \phi}$$

另一方面 $\frac{\partial H}{\partial \phi} = \frac{1}{L}\frac{\partial H}{\partial A}$

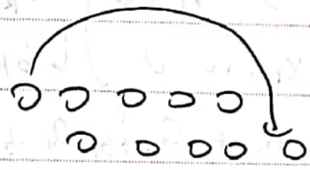
电流的中 $\mathcal{L} \to \mathcal{L}_0 + \vec{j}\cdot\vec{A}$ minimal coupling

$$H = \frac{(p-eA)^2}{2m} + U(r)$$

$$\frac{\partial H}{\partial \phi} = \frac{1}{L}\frac{p-eA}{m}e = \frac{1}{Lm}\Pi e \sim \frac{e}{L}u \sim j$$

因此 $I = c\frac{\partial H}{\partial \phi}$ 确实对应于电流

图像:



$\delta U = neV$

$\delta\phi = \frac{hc}{e}$

$G = \frac{I}{V} = n\frac{e^2}{h}$

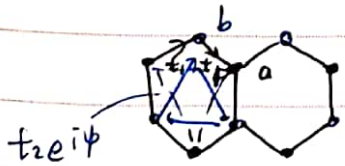
作业: 推导 Laughlin 文章中的 Landau 能级

Haldane Model 1988   QHE without LL $\Rightarrow$ Gauge potential

$G = \frac{ne^2}{h}$

Honeycomb lattice: a, b sublattice (a_k, b_k)

只有 $t_1 \Rightarrow$ Graphene $\Rightarrow$ Dirac cone



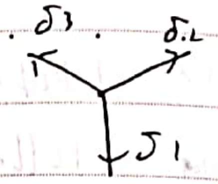
$$H = \begin{pmatrix} m & p_x - ip_y \\ p_x + ip_y & -m \end{pmatrix}$$

$t_2 e^{i\phi} \Rightarrow \Delta$ 累积 3ϕ 相位

$t_2 e^{-i\phi} \Rightarrow -3\phi$

写出来 nearest neighboring

$$H_{NN} = -t_1\sum_i (a_i^\dagger b_{i+\delta_1} + a_i^\dagger b_{i+\delta_2} + a_i^\dagger b_{i+\delta_3}) + h.c.$$



$\delta_1 = (0,-1)$
$\delta_2 = (\frac{\sqrt{3}}{2}, \frac{1}{2})$
$\delta_3 = (-\frac{\sqrt{3}}{2}, \frac{1}{2})$

Fourier transformation

$$\begin{cases} a_i = \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\cdot\vec{R}_i^a} a_k \\ b_i = \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\cdot\vec{R}_i^b} b_k \end{cases}$$

动量 k well-defined

$$\sum_{ij} c(i-j)\, a_i^\dagger a_j = \sum_{kq}\sum_{ij} c(i-j)\, a_k^\dagger a_q\, e^{-ik\cdot i + iq\cdot j} \frac{1}{N}$$

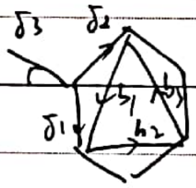
$$= \sum_{kq} \Big(\sum_d c(d) e^{-ikd}\Big) \underbrace{\frac{1}{N}\sum_j e^{-i(k-q)j}}_{\delta_{k-q}}\, a_k^\dagger a_q$$

t

$$H_{NN} = -t \sum_k (a_k^\dagger b_k)\Big(\sum_{\delta_i} e^{ik\cdot\delta_i}\Big) \longrightarrow x_1 + i x_2$$

$$= -t\,(a_k^\dagger \;\; b_k^\dagger) \begin{pmatrix} 0 & x_1 - i x_2 \\ x_1 + i x_2 & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

$$H_{NNN}^a = -t_2 e^{i\phi} \sum_i \big(a_i^\dagger a_{i+b_1} + a_{i+b_1}^\dagger a_{i-b_3} + a_{i-b_3}^\dagger a_i\big) + h.c.$$



$\vec{b}_1 = \delta_1 - \delta_2$
$\vec{b}_2 = \delta_2 - \delta_3$
$\vec{b}_3 = \delta_3 - \delta_1$

$$H_{NNN}^b = -t_2 e^{-i\phi} \sum_i \big(b_i^\dagger b_{i-b_3} + b_{i-b_3}^\dagger b_{i+\delta_2} + b_{i+\delta_2}^\dagger b_i\big)$$

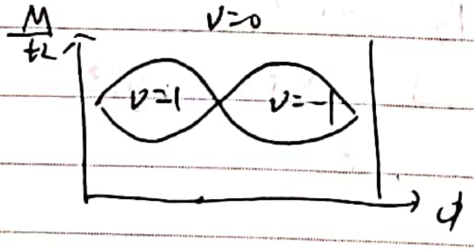
Fourier 变换 $\Longrightarrow$ $H_{NNN}^a = \sum_k E_k^a(\phi)\, a_k^\dagger a_k$

$H_{NNN}^b = \sum_k E_k^b(\phi)\, b_k^\dagger b_k$

会打开 gap

$$a_k^\dagger a_k \Big(\sum_i e^{i\vec{k}\cdot\vec{b}_i + i\phi}\Big) + h.c.$$

$$b_k^\dagger b_k \Big(\sum_i e^{i\vec{k}\cdot\vec{b}_i - i\phi}\Big) + h.c.$$



Q-W-Z Model

$$H = a_k\sigma_x + b_k\sigma_y + c_k\sigma_z$$

$$E = \pm\sqrt{a_k^2 + b_k^2 + c_k^2}$$

$$H = \underbrace{v(k_x\sigma_x + k_y\sigma_y)}_{SOC} + (M - \boxed{Bk^2})\sigma_z$$

S.Q. Shen Modified Dirac equation

紧束缚模型

$$H = -\sum_{ij}(t_{ij}c_i^\dagger c_j + t_{ji}c_j^\dagger c_i) + \sum V_i c_i^\dagger c_i$$

$$H^\dagger = H \Rightarrow t_{ij}^* = t_{ji}, \quad V_i = V_i^*$$

晶格中只有一种原子，$V_i = const$

$\Rightarrow H = -\sum(t_{ij}c_i^\dagger c_j + t_{ij}^* c_j^\dagger c_i) + VN$ 常数，可去

若只考虑最近邻 $H = -t\sum_{\langle ij\rangle}(c_i^\dagger c_j + c_j^\dagger c_i) = -t\sum c_i^\dagger c_{i+1} + h.c.$

Fourier 变换 （k 连续）

$$c_k = \frac{\sqrt{a}}{\sqrt{2\pi}}\sum c_i e^{-ikx}$$

$$c_i = \frac{\sqrt{a}}{\sqrt{2\pi}}\int_{BZ} dk\, c_k e^{ikx}$$

由于 $\{c_i, c_j^\dagger\} = \delta_{ij} \Rightarrow \{c_k, c_{k'}^\dagger\} = \cdots = \sum_i \frac{1}{2\pi/a} e^{-i(k-k')ia} = a\delta((k-k')a) = \delta(k-k')$

将 $H = -t\sum c_i^\dagger c_{i+1} + h.c.$ 变换到 k 空间中

$$\sum_j c_j^\dagger c_{j+1} = \sum_j \frac{1}{\sqrt{2\pi/a}}\int_{BZ} dk\, c_k^\dagger e^{-ikaj} \frac{1}{\sqrt{2\pi/a}}\int_{BZ} dk'\, c_{k'} e^{ik'(j+1)a}$$

$$= \sum_j \frac{1}{2\pi/a}\int_{BZ}\int_{BZ} dk\,dk'\, c_k^\dagger c_{k'} e^{ik'a} e^{-i(k-k')aj} = \int_{BZ}\int_{BZ} dk\,dk'\, c_k^\dagger c_{k'} e^{ik'a}\, \delta(k-k')$$

$$= \int_{BZ} dk\, c_k^\dagger c_k e^{ika}$$

$$H = -t\sum c_i^\dagger c_{i+1} + h.c. = -t\int_{BZ} dk\, c_k^\dagger c_k e^{ika} - t\int_{BZ} dk\, c_k^\dagger c_k e^{-ika}$$

$$= \int_{BZ} dk\,(-2t\cos ka)\, c_k^\dagger c_k$$

对于固体，$E = \sum_n \int_{BZ} dk\, \varepsilon_n(k)\, n_n(k)$ n 为能带，$n_n(k)$ 为占据数，$\varepsilon_n(k)$ 为色散关系，在二次量子化中，$H = \sum_n \int_{BZ} dk\, \varepsilon_n(k)\, \gamma_{nk}^\dagger \gamma_{nk}$，$\gamma_{nk}^\dagger$ 为 Bloch 波函数 $\psi_{n,k}(r) = u_{n,k}(r)e^{ikr}$ 的生成算符。因此，$c_k^\dagger$ 实际上是 Bloch 波函数的生成算符

Fourier 变换.（k 离散）

定义 ~~$\tilde{f}_k = \frac{1}{\sqrt{N}}\sum_j f_j e^{-ikaj}$~~ $f_j = \frac{1}{\sqrt{N}}\sum_k \tilde{f}_k e^{ikaj}$

$f_{N+i} = f_N \Rightarrow k = \frac{2\pi m}{Na} = \frac{2\pi m}{L}$

可以证明 $\tilde{f}_k = \frac{1}{\sqrt{N}}\sum_j f_j e^{-ikaj}$

定义 $k_m = \frac{2\pi m}{L}$，则 $\tilde{f}_{k_{m+N}} = \tilde{f}_{k_m}$，可以选取 $-\frac{N}{2} \le m < \frac{N}{2}$，即

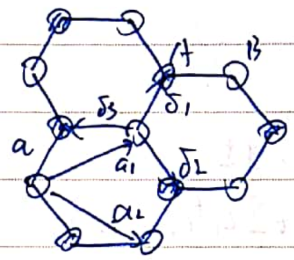
$-\frac{\pi}{a} \le k < \frac{\pi}{a}$，对应于第一 Brillouin区

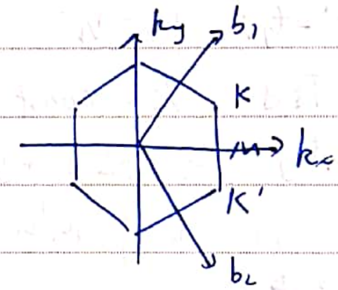
$\boxed{\text{公式}}$

$$\frac{1}{N}\sum_k e^{ikaj} e^{-ikaj'} = \delta_{jj'}$$

$$\frac{1}{N}\sum_j e^{ikaj} e^{-ik'aj} = \delta_{kk'}$$

石墨烯的紧束缚模型





$\vec{a}_1 = \frac{a}{2}(3, \sqrt{3})$

$\vec{a}_2 = \frac{a}{2}(3, -\sqrt{3})$

$\vec{\delta}_1 = \frac{a}{2}(1, \sqrt{3})$ $\vec{\delta}_2 = \frac{a}{2}(1, -\sqrt{3})$ $\vec{\delta}_3 = -a(1, 0)$

$\vec{K} = \frac{2\pi}{3\sqrt{3}a}(\sqrt{3}, 1)$ $\vec{K}' = \frac{2\pi}{3\sqrt{3}a}(\sqrt{3}, -1)$

最近邻近似：

$$\hat{H} = -t\sum_{\langle ij\rangle}(\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i)$$

$$\sum_{\langle ij\rangle}(\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i) = \sum_{i\in A}\sum_{\delta}(\hat{a}_i^\dagger \hat{b}_{i+\delta} + \hat{b}_{i+\delta}\hat{a}_i)$$

A 的阵点个数为 $N/2$

$\hat{a}_i^\dagger = \frac{1}{\sqrt{N/2}}\sum_k e^{i\vec{k}\cdot\vec{r}_i}\hat{a}_{\vec{k}}^\dagger$ $\hat{b}_{i+\delta} = --$ 代入 H 中

$$H = -\frac{t}{N/2}\sum_{i\in A}\sum_{\delta,k,k'}\left[e^{i(\vec{k}-\vec{k}')\cdot\vec{r}_i} e^{-i\vec{k}'\cdot\vec{\delta}}\hat{a}_{\vec{k}}^\dagger \hat{b}_{\vec{k}'} + h.c.\right]$$

$$= -t\sum_{\delta,k}(e^{-i\vec{k}\cdot\vec{\delta}}\hat{a}_{\vec{k}}^\dagger \hat{b}_{\vec{k}} + h.c.)$$

$$= -t\sum_{\delta,k}(e^{-i\vec{k}\cdot\vec{\delta}}\hat{a}_{\vec{k}}^\dagger \hat{b}_{\vec{k}} + e^{i\vec{k}\cdot\vec{\delta}}\hat{b}_{\vec{k}}^\dagger \hat{a}_{\vec{k}})$$

令 $\Psi = \begin{pmatrix}\hat{a}_{\vec{k}} \\ \hat{b}_{\vec{k}}\end{pmatrix}$ $\Delta_{\vec{k}} = \sum_\delta e^{i\vec{k}\cdot\vec{\delta}}$ $h(\vec{k}) = -t\begin{pmatrix}0 & \Delta_{\vec{k}} \\ \Delta_{\vec{k}}^* & 0\end{pmatrix}$

$$H = \sum_k \Psi^\dagger h(\vec{k})\Psi$$

写成 Pauli 矩阵的形式

$\Delta_{\vec{k}} = \sum_{\delta} e^{i\vec{k}\cdot\vec{\delta}} = \sum_{\delta}[\cos(\vec{k}\cdot\vec{\delta}) + i\sin(\vec{k}\cdot\vec{\delta})]$

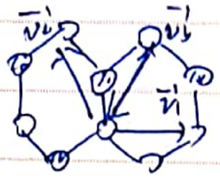
$h(\vec{k}) = -t\sum_{\delta}[\cos(\vec{k}\cdot\vec{\delta})\sigma_x + -\sin(\vec{k}\cdot\vec{\delta})\sigma_y]$

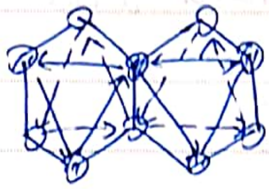
若考虑 inversion-symmetry-breaking on-site energy +M on A and −M on B，之间的VN跃迁就不能直接忽略，最终结果为

$$h_M(\vec{k}, M) = -t\sum_{\delta}[\cos(\vec{k}\cdot\vec{\delta})\sigma_x - \sin(\vec{k}\cdot\vec{\delta})\sigma_y + M\sigma_z]$$

$$= -t\sum_{\delta}\begin{pmatrix} M & \cos(\vec{k}\cdot\vec{\delta}) + i\sin(\vec{k}\cdot\vec{\delta}) \\ \cos(\vec{k}\cdot\vec{\delta}) - i\sin(\vec{k}\cdot\vec{\delta}) & -M \end{pmatrix}$$

H_{NNN} hopping：





$$H_{NNN} = -t'e^{i\phi}\sum_i a^\dagger_{r_i} a_{r_i+v_1} - t'\sum_i a^\dagger_{r_i+v_1} a_{r_i-v_3} - t'e^{i\phi}\sum_i a^\dagger_{r_i-v_3} a_{r_i} + h.c. + (a\to b \text{ and } \phi\to-\phi)$$

$\vec{v}_1 = (\sqrt{3}a, 0)$ $\quad\vec{v}_2 = (-\sqrt{3}/2\,a, 3/2\,a)$ $\quad\vec{v}_3 = (-\sqrt{3}/2\,a, -3/2\,a)$

换成k空间

$$H = -t'e^{i\phi}\sum_k a_k^\dagger a_k(e^{-ik\cdot v_1} + e^{-ik\cdot v_2} + e^{-ik\cdot v_3}) + h.c. + (a\to b \text{ and } \phi\to-\phi)$$

$$= \sum_k (a_k^\dagger\ \ b_k^\dagger)\begin{pmatrix} -2t'(\cos(k\cdot v_1-\phi)+\cos(k\cdot v_2-\phi)+\cos(k\cdot v_3-\phi)) & 0 \\ 0 & -2t'(\cos(k\cdot v_1+\phi)+\cos(k\cdot v_2+\phi)+\cos(k\cdot v_3+\phi)) \end{pmatrix}\begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

或写成 Pauli 矩阵形式

$$H_{NNN} = 2t_2\cos\phi\left(\sum_i\cos(\vec{k}\cdot\vec{v}_i)\right)I + (-2t_2)\sin\phi\left(\sum_i\sin(\vec{k}\cdot\vec{v}_i)\right)\sigma_z$$

回顾：

① 几何相数值计算

$e^{i\gamma} = \prod_i \langle\psi_i|\psi_{i+1}\rangle$ ← 联络矩阵

好处：1) Gauge Invariant

2) 便于实验研究