补充内容：二次量子化 · 规则 → 紧束缚能带计算

(0) Motivation：化简计算 → 形形色色晶格系统

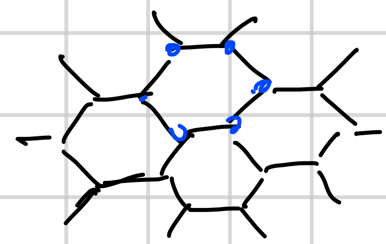
声子，电子

b_k^+ $\quad (c_j^+, c_k^+)$

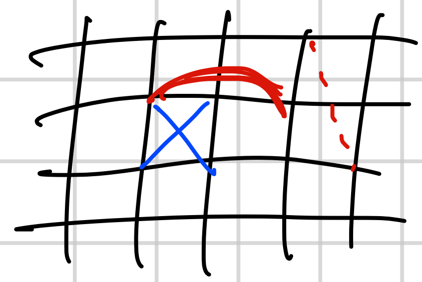
⇓

二维常见格子 三维常见格子

↳ 紧束缚能带求解(?) 去调包



生成：Git lab



(1) 费米子单粒子基底

平面波 $|\vec{k}\rangle$: $\frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$

布洛赫波 $|nk\rangle$: $e^{ikr}u_k(r)$

瓦尼尔函数 $|nj\rangle$: $a_{nj}(\vec{r}-\vec{R})$

(2) 产生湮灭算符规则

$|0\rangle$ 真空态 $\qquad a_j^+|0\rangle = |1_j\rangle \qquad a_j^+|1_j\rangle = 0$

$(a_j)^2 = 0 \qquad\qquad (= a_j^+ a_j^+ |0\rangle)$

$(a_j^+)^2 = 0$

$a_1^+ a_2^+ |0\rangle = |1_1, 1_2\rangle$ （多粒子）

$a_1^+ a_2^+ = -a_2^+ a_1^+$ 费米子产生湮灭算符反对易

$$a_j^+ |\cdots n_{j-1}, n_j, n_{j+1}, \cdots\rangle = \begin{cases} |\cdots n_{j-1}\ 1_j\ n_{j+1} \cdots\rangle (-1)^{n_j} & n_j = 0 \\ 0 & n_j = 1 \end{cases}$$

$$a_j |\cdots n_{j-1}, n_j, n_{j+1}, \cdots\rangle = \begin{cases} 0 & n_j = 0 \\ |\cdots n_{j-1}\ 0_j\ n_{j+1} \cdots\rangle (-1)^{n_j} & n_j = 1 \end{cases}$$

多粒子基

验证 多粒子态 ⟺ 反对易自洽

(3) $(a_1^+)^1 (a_2^+)^0 (a_3^+)^1 (a_4^+)^1 (a_5^+)^0 |0\rangle = |1_1, 0_2, 1_3, 1_4, 0_5\rangle$

$\Rightarrow |\cdots n_{j-1}, n_j, n_{j+1} \cdots\rangle = \prod_j (a_j^+)^{n_j} |0\rangle$

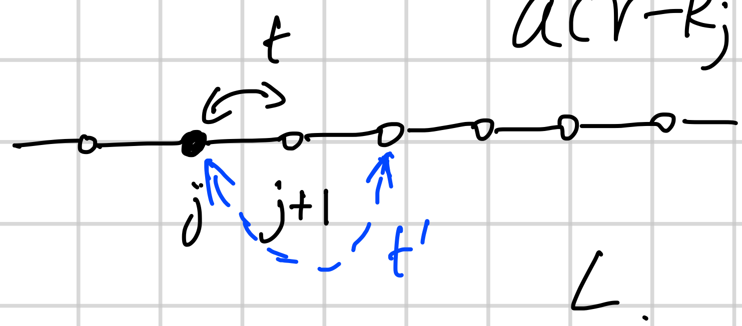
(4) 二次量子化写出，能带Hamiltonian ☆

$$\hat{H} = \sum_{n,k} \varepsilon_{nk} C^{+}_{nk} C_{nk}$$ 对角(粒子数)

$N_{nk} = C^{+}_{nk} C_{nk}$ 表示(n,k)布洛赫轨道上的粒子数

$a(\vec{r}-\vec{R}_j)$

(5) 一维晶格



TBM: Wannier function

$$H = -t_1 \sum_j \left(C_j^{+} C_{j+1} + C_{j+1}^{+} C_j\right)$$ 紧束缚模型

$$-t_2 \sum_j \left(C_j^{+} C_{j+2} + h.c.\right) + \cdots$$

$$\Rightarrow t_m = -\langle a(\vec{r}) | \Delta V | a(\vec{r}-\vec{R}_m) \rangle \simeq J_m$$

(6) 求解：傅利叶变换

$$\begin{cases} C_j^{+} = \sum_k e^{-ikja} \cdot C_k^{+} \cdot \frac{1}{\sqrt{L}} \\ C_j = \sum_k e^{ikja} \cdot C_k \cdot \frac{1}{\sqrt{L}} \end{cases}$$

$$H = -t_1 \sum_j \sum_k \sum_{k'} \left[e^{-ikja} C_k^{+} \cdot e^{ik'ja} C_{k'} e^{ik'a} + h.c. \right] \frac{1}{L}$$

$$= -t_1 \sum_{k,k'} \sum_j \left[C_k^{+} C_{k'} e^{i(k'-k)j\cdot a} \cdot e^{ik'a} + h.c. \right] \frac{1}{L}$$

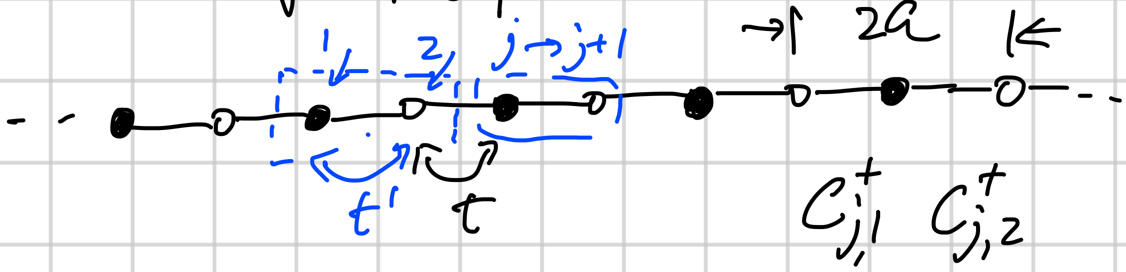
$$= -t_1 \sum_{k,k'} \delta_{k,k'} \left(C_k^{+} C_{k'} e^{ika} + C_{k'}^{+} C_k e^{-ika} \right)$$

$$= -t_1 \sum_k C_k^{+} C_k \left(e^{ika} + e^{-ika} \right)$$

$$= -t_1 \sum_k 2\cos(ka)\, C_k^{+} C_k$$

$$\varepsilon_k = -2t_1 \cos(ka)$$ #

(7) 两周期紧束缚模型



$$H=\sum_j -t'\left(c^+_{j,1}c_{j,2}+c^+_{j,2}c_{j,1}\right)-t\left(c^+_{j,2}c_{j+1,1}+c^+_{j+1,1}c_{j,2}\right)$$

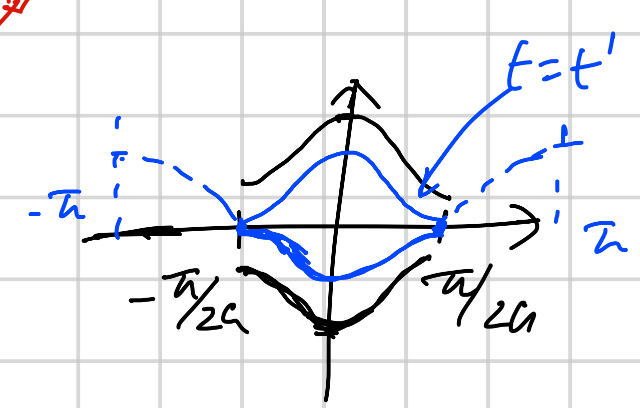
$$\begin{cases} c_{j,1}=\sum_k e^{ikj\cdot 2a}\cdot c_{k,1} \\ c_{j,2}=\sum_k e^{ikj\cdot 2a}\cdot c_{k,2}\end{cases}$$

$$=\sum_j\Big[-t'\sum_{k,k'}\left(e^{-ikj\cdot 2a}c^+_{k,1}\cdot e^{ik'j2a}c_{k',2}+h.c.\right)$$
$$-t\sum_{k,k'}\left(e^{-ikj\cdot 2a}c^+_{k,2}\,e^{ik'(j+1)\cdot 2a}c_{k',1}+h.c.\right)\Big]$$

$$=\sum_{k,k'}-t'\left(c^+_{k,1}c_{k',2}+h.c.\right)\cdot\delta_{k,k'}$$
$$-t\left(c^+_{k,2}c_{k',1}e^{ik\cdot 2a}+h.c.\right)\delta_{k,k'}$$

$$=\sum_k -t'\left(c^+_{k,1}c_{k,2}+h.c.\right)-t\left(c^+_{k,2}c_{k,1}e^{ik\cdot 2a}+c^+_{k,1}c_{k,2}e^{-ik2a}\right)$$

$$\Rightarrow H=\sum_k \varepsilon^1_k c^+_{k,1}c_{k,1}+\varepsilon^2_k c^+_{k,2}c_{k,2}$$



☆ $\tilde{c}_{k,\alpha}=\left(c_{k,1}\cdot A^\alpha_k+c_{k,2}\cdot B^\alpha_k\right)$

$$\begin{array}{ccc} & c_{k,1} & c_{k,2} \\ c^+_{k,1} & & \\ c^+_{k,2} & & \end{array}\begin{pmatrix} 0 & -t'-te^{-ik2a} \\ -t'-te^{ik2a} & 0\end{pmatrix}\Rightarrow \varepsilon_{k\alpha}$$

$$|\varepsilon_{k\alpha}|^2=\left(t'+te^{ik2a}\right)\left(t'+te^{-ik2a}\right)$$
$$=t'^2+t^2+2tt'\cdot\cos(k\cdot 2a)$$

$$\Rightarrow \varepsilon_{k,\pm}=\pm\sqrt{t'^2+t^2+2tt'\cos(k2a)}$$ #