1. identity 的证明
2. 证明"equ:3.2tJ_3"[1]和"equ:3.2tJ_1"[2]是等价的.
3. 两格点 Hubbard 模型的精确对角化.
4. Hubbard 模型的旋转不变性.

前两题关注的是 t-J 模型(Hubbard 模型的大 U 极限)的三个形式之间的互相转换的推导.

后两题关注 Hubbard 模型本身.

3.4.1 identity 的证明

$$P_s\left[\sum_{ss'} c_{is}^{\dagger} c_{js} n_{j\uparrow} n_{j\downarrow} c_{js'}^{\dagger} c_{is'}\right] P_s = -2 P_s\left[\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4}\right] P_s$$

最直接的想法是利用我们曾经证明过的自旋算符点乘的恒等式"equ:spin_operator"[3], 将等号右边化简为

$$\begin{aligned}
-2 P_s\left[\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4}\right] P_s &= -2 P_s\left[-\frac{1}{2} c_{is}^{\dagger} c_{js'}^{\dagger} c_{is'} c_{js} - \frac{n_i n_j}{2}\right] P_s \\
&= P_s\left[\sum_{ss'} c_{is}^{\dagger} c_{js'}^{\dagger} c_{is'} c_{js} + n_i n_j\right] P_s
\end{aligned}$$

然后通过各种对易关系将等号左边化简成上式, 就证明完毕了. 但我胡乱尝试了很久都没有成功. 后面看网上的讲义找灵感, 找到了中间的一步, 就试出来了. 证明如下:

$$\begin{aligned}
\sum_{ss'} c_{is}^{\dagger} c_{js} n_{j\uparrow} n_{j\downarrow} c_{js'}^{\dagger} c_{is'} &= \sum_s c_{is}^{\dagger} c_{js} n_{j\uparrow} n_{j\downarrow} c_{j-s}^{\dagger} c_{i-s} + \sum_s c_{is}^{\dagger} c_{js} n_{j\uparrow} n_{j\downarrow} c_{js}^{\dagger} c_{is} \\
&= \sum_s c_{is}^{\dagger} c_{js} n_{js} n_{j-s} c_{j-s}^{\dagger} c_{i-s} + \sum_s c_{is}^{\dagger} c_{js} n_{js} n_{j-s} c_{js}^{\dagger} c_{is} \\
&= -\sum_s c_{is}^{\dagger} c_{i-s} c_{j-s}^{\dagger} c_{js} + \sum_s n_{is} n_{j-s} \\
&= -2\left(S_i^x S_j^x + S_i^y S_j^y\right) + \frac{n_i n_j}{2} - 2 S_i^z S_j^z \\
&= \frac{n_i n_j}{2} - 2 \mathbf{S}_i \cdot \mathbf{S}_j
\end{aligned}$$

- 第一个等号: 将原先的二重求和拆成了两项, 对应 $s' = -s$ 和 $s' = s$. 这样的拆法是具有物理意义的, 代表两种不同的过程: 从 i 跳到 j 和从 j 跳回 i 的两个电子可以是不同自旋的.
- 第二个等号: 由于夹在中间的 $n_{j\uparrow}$ 和 $n_{j\downarrow}$ 是可以互相交换的, 可以赋予它们指标.
- 第三个等号: 这是重要的一个中间结果, 会用到一些对易关系和前后的投影矩阵 P_S

$$
\begin{aligned}
c_{is}^{\dagger}c_{js}n_{js}n_{j-s}c_{j-s}^{\dagger}c_{i-s} &= c_{is}^{\dagger}c_{js}c_{j-s}^{\dagger}c_{j-s}n_{js}c_{j-s}^{\dagger}c_{i-s} \\
&= -c_{is}^{\dagger}c_{j-s}^{\dagger}c_{js}c_{j-s}n_{js}c_{j-s}^{\dagger}c_{i-s} \\
&= -c_{is}^{\dagger}c_{j-s}^{\dagger}c_{js}n_{js}\left(1-c_{j-s}^{\dagger}c_{j-s}\right)c_{i-s} \\
&= -c_{is}^{\dagger}c_{j-s}^{\dagger}c_{js}n_{js}\left(1-n_{j-s}\right)c_{i-s} \\
{\color{red}=} &- c_{is}^{\dagger}c_{j-s}^{\dagger}{\color{red}c_{js}n_{js}}c_{i-s}{\color{red}=}-c_{is}^{\dagger}c_{j-s}^{\dagger}c_{js}c_{i-s} \\
&= -c_{is}^{\dagger}c_{i-s}c_{j-s}^{\dagger}c_{js}
\end{aligned}
$$

$$
\begin{aligned}
c_{is}^{\dagger}c_{js}n_{js}n_{j-s}c_{js}^{\dagger}c_{is} &= n_{j-s}c_{is}^{\dagger}c_{js}n_{js}c_{js}^{\dagger}c_{is} \\
&= n_{j-s}c_{js}n_{js}c_{js}^{\dagger}c_{is}^{\dagger}c_{is} \\
&= n_{j-s}\left(n_{js}c_{js}+c_{js}\right)c_{js}^{\dagger}n_{is} \\
&= n_{j-s}\left(n_{js}+1\right)\left(1-c_{js}^{\dagger}c_{js}\right)n_{is} \\
{\color{red}=} & n_{j-s}\left(1-n_{js}\right)n_{is}{\color{red}=}n_{is}n_{j-s}
\end{aligned}
$$

其中标红的等号用了投影矩阵 P_S 的性质, 也就是前后的态都是单占据态.

- 第四个等号: 利用了自旋算符的两个恒等式

$$
\sum_{\sigma} a_{j-\sigma}^{\dagger}a_{i\sigma}^{\dagger}a_{i-\sigma}a_{j\sigma} = \sum_{\sigma} a_{i\sigma}^{\dagger}a_{i-\sigma}a_{j-\sigma}^{\dagger}a_{j\sigma} = S_i^{+}S_j^{-}+S_i^{-}S_j^{+} = 2\left(S_i^{x}S_j^{x}+S_i^{y}S_j^{y}\right)
$$

$$
\begin{aligned}
\frac{n_i n_j}{4}-S_i^{z}S_j^{z} &= \frac{1}{4}\left[\left(n_{i\uparrow}+n_{i\downarrow}\right)\left(n_{j\uparrow}+n_{j\downarrow}\right)-\left(n_{i\uparrow}-n_{i\downarrow}\right)\left(n_{j\uparrow}-n_{j\downarrow}\right)\right] \\
&= \frac{1}{2}\left[n_{i\uparrow}n_{j\downarrow}+n_{i\downarrow}n_{j\uparrow}\right] = \frac{1}{2}\sum_{\sigma} n_{i\sigma}n_{j-\sigma}
\end{aligned}
$$

3.4.2 t-J 模型的正规排序形式

$$
\mathcal{H}^{t-J} = P_s\left[\mathcal{T}-\frac{1}{U}\sum_{ijk}t_{ij}t_{jk}\left(c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}-c_{i\downarrow}^{\dagger}c_{j\uparrow}^{\dagger}\right)\left(c_{j\downarrow}c_{k\uparrow}-c_{j\uparrow}c_{k\downarrow}\right)\right]P_s
$$

> 证明上面的形式相当于要证明:
>
> $$
> P_s\sum_{ss'}c_{is}^{\dagger}c_{js}n_{j\uparrow}n_{j\downarrow}c_{js'}^{\dagger}c_{ks'}P_s = P_s\left(c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}-c_{i\downarrow}^{\dagger}c_{j\uparrow}^{\dagger}\right)\left(c_{j\downarrow}c_{k\uparrow}-c_{j\uparrow}c_{k\downarrow}\right)P_s
> $$
>
> 等号左右两边都是四项，可以根据 $c_{is}^{\dagger}$ 和 c_{ks} 来锁死互相的对应, 下面用四种颜色来标记了互相对应关系

$$
\begin{aligned}
&\left(c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}-c_{i\downarrow}^{\dagger}c_{j\uparrow}^{\dagger}\right)\left(c_{j\downarrow}c_{k\uparrow}-c_{j\uparrow}c_{k\downarrow}\right)\\
&=c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}c_{j\downarrow}c_{k\uparrow}-c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}c_{j\uparrow}c_{k\downarrow}-c_{i\downarrow}^{\dagger}c_{j\uparrow}^{\dagger}c_{j\downarrow}c_{k\uparrow}+c_{i\downarrow}^{\dagger}c_{j\uparrow}^{\dagger}c_{j\uparrow}c_{k\downarrow}
\end{aligned}
$$

$$
\begin{aligned}
&\sum_{ss'}c_{is}^{\dagger}c_{js}n_{j\uparrow}n_{j\downarrow}c_{js'}^{\dagger}c_{ks'}\\
&=c_{i\uparrow}^{\dagger}c_{j\uparrow}n_{j\uparrow}n_{j\downarrow}c_{j\uparrow}^{\dagger}c_{k\uparrow}+c_{i\uparrow}^{\dagger}c_{j\uparrow}n_{j\uparrow}n_{j\downarrow}c_{j\downarrow}^{\dagger}c_{k\downarrow}+c_{i\downarrow}^{\dagger}c_{j\downarrow}n_{j\uparrow}n_{j\downarrow}c_{j\uparrow}^{\dagger}c_{k\uparrow}+c_{i\downarrow}^{\dagger}c_{j\downarrow}n_{j\uparrow}n_{j\downarrow}c_{j\downarrow}^{\dagger}c_{k\downarrow}
\end{aligned}
$$

要处理的只是中间四个 j 相关的算符, 以第一项(红色项)为例:

$$
c_{j\uparrow}n_{j\uparrow}n_{j\downarrow}c_{j\uparrow}^{\dagger}=\left(n_{j\uparrow}+1\right)c_{j\uparrow}n_{j\downarrow}c_{j\uparrow}^{\dagger}=\left(n_{j\uparrow}+1\right)n_{j\downarrow}c_{j\uparrow}c_{j\uparrow}^{\dagger}=n_{j\downarrow}\left(1-c_{j\uparrow}^{\dagger}c_{j\uparrow}\right)=n_{j\downarrow}\left(1-n_{j\uparrow}\right)=n_{j\downarrow}
$$

其中两个**标红的等号利用了投影矩阵 的性质**, 即前后都会作用到单占据态上. 后面三项的推导是类似的:

$$
c_{j\uparrow}n_{j\uparrow}n_{j\downarrow}c_{j\downarrow}^{\dagger}=\left(n_{j\uparrow}+1\right)c_{j\uparrow}c_{j\downarrow}^{\dagger}\left(n_{j\downarrow}+1\right)=-c_{j\downarrow}^{\dagger}\left(n_{j\downarrow}+1\right)\left(n_{j\uparrow}+1\right)c_{j\uparrow}=-c_{j\downarrow}^{\dagger}c_{j\uparrow}
$$

$$
c_{j\downarrow}n_{j\uparrow}n_{j\downarrow}c_{j\uparrow}^{\dagger}=n_{j\uparrow}c_{j\downarrow}c_{j\uparrow}^{\dagger}n_{j\downarrow}=-n_{j\uparrow}c_{j\uparrow}^{\dagger}c_{j\downarrow}n_{j\downarrow}=-c_{j\uparrow}^{\dagger}\left(n_{j\uparrow}+1\right)\left(n_{j\downarrow}+1\right)c_{j\downarrow}=-c_{j\uparrow}^{\dagger}c_{j\downarrow}
$$

$$
c_{j\downarrow}n_{j\uparrow}n_{j\downarrow}c_{j\downarrow}^{\dagger}=n_{j\uparrow}c_{j\downarrow}n_{j\downarrow}c_{j\downarrow}^{\dagger}=n_{j\uparrow}\left(n_{j\downarrow}+1\right)c_{j\downarrow}c_{j\downarrow}^{\dagger}=n_{j\uparrow}\left(1-n_{j\downarrow}\right)=n_{j\uparrow}
$$

3.4.3 两格点 Hubbard 模型

找到电子数量分别为 $N_e=1,2,3$ 时的两格点 Hubbard 模型的本征能量和本征态. 根据 Hubbard 模型的一般表达式"equ:3.1Hubbard_model"[4], 我们得到哈密顿量:

$$
\begin{aligned}
\mathcal{H}&=-\sum_{i,j=1,i\neq j}^{2}t_{ij}\sum_{s}\mathrm{c}_{is}^{\dagger}c_{js}+U\sum_{i=1}^{2}n_{i\uparrow}n_{i\downarrow}\\
&=\sum_{s}\left(t_{12}\mathrm{c}_{1s}^{\dagger}c_{2s}+t_{21}\mathrm{c}_{2s}^{\dagger}c_{1s}\right)+U\left(n_{1\uparrow}n_{1\downarrow}+n_{2\uparrow}n_{2\downarrow}\right)
\end{aligned}
$$

首先讨论三个情形相关的 Fock space:

- $N_e=1$: 共有四种可能的态 $\mathrm{c}_{1\uparrow}^{\dagger}|\Omega\rangle,\mathrm{c}_{2\uparrow}^{\dagger}|\Omega\rangle,\mathrm{c}_{1\downarrow}^{\dagger}|\Omega\rangle,\mathrm{c}_{2\downarrow}^{\dagger}|\Omega\rangle$, 各自本身并不是本征态, 可以线性组合出本征态.
- $N_e=2$: 半填充情形, 共有六个可能的态:
    - Two **spin-polarized states** $a_{1\uparrow}^{\dagger}a_{2\uparrow}^{\dagger}|\Omega\rangle,a_{1\downarrow}^{\dagger}a_{2\downarrow}^{\dagger}|\Omega\rangle$, are **zero energy eigenstates.**
        - According to Pauli principle, the hopping between site 1 and site2 is inhibited, and then double occupacy in one site is also inhibited.

  - So Hubbard Hamiltonina acts on the two states and get 0.
- Four states that satisfy $S^z_{\text{total}} = 0$, $|s_1\rangle = a^\dagger_{1\uparrow} a^\dagger_{2\downarrow}|\Omega\rangle, |s_2\rangle = a^\dagger_{2\uparrow} a^\dagger_{1\downarrow}|\Omega\rangle, |d_1\rangle = a^\dagger_{1\uparrow} a^\dagger_{1\downarrow}|\Omega\rangle$, and $|d_2\rangle = a^\dagger_{2\uparrow} a^\dagger_{2\downarrow}|\Omega\rangle$
  - $|s_i\rangle$: **singly occupied** subspaces, with projector $\hat{P}_s = \sum_{i=1,2}|s_i\rangle\langle s_i|$
  - $|d_i\rangle$: **doubly occupied** subspaces, with projector $\hat{P}_d = \sum_{i=1,2}|d_i\rangle\langle d_i|$

  其中自旋极化态的能量为 0, 是本征态; 双占据态和单占据态本身并不是本征态, 但可以线性组合出能量非零的本征态.

- $N_e = 3$: 有一个格点上必定是双占据, 另一个格点上单占据, 共有四个可能的态 $\mathrm{c}^\dagger_{1\uparrow}\mathrm{c}^\dagger_{1\downarrow}\mathrm{c}^\dagger_{2\uparrow}|\Omega\rangle, \mathrm{c}^\dagger_{1\uparrow}\mathrm{c}^\dagger_{1\downarrow}\mathrm{c}^\dagger_{2\downarrow}|\Omega\rangle, \mathrm{c}^\dagger_{2\uparrow}\mathrm{c}^\dagger_{2\downarrow}\mathrm{c}^\dagger_{1\uparrow}|\Omega\rangle, \mathrm{c}^\dagger_{2\uparrow}\mathrm{c}^\dagger_{2\downarrow}\mathrm{c}^\dagger_{1\downarrow}|\Omega\rangle$, 各自本身都不是本征态, 但可以线性组合出本征态.

要找到所有的本征态, 需要将哈密顿量对角化, 或者慢慢试出来.对角化的代码见 2siteHubbard.nb.pdf

$N_e = 1$

Fock space 中有四个相关的态, 因此哈密顿量的矩阵形式是 4×4 的, 可以将矩阵元一一求出来, 进而得到哈密顿量

$$|1\rangle = \mathrm{c}^\dagger_{1\uparrow}|\Omega\rangle, |2\rangle = \mathrm{c}^\dagger_{1\downarrow}|\Omega\rangle, |3\rangle = \mathrm{c}^\dagger_{2\uparrow}|\Omega\rangle, |4\rangle = \mathrm{c}^\dagger_{2\downarrow}|\Omega\rangle$$

$$\mathcal{H}_{ij} = \langle i|\mathcal{H}|j\rangle$$

$$\mathcal{H} = \begin{pmatrix} 0 & 0 & t_{12} & 0 \\ 0 & 0 & 0 & t_{12} \\ t_{21} & 0 & 0 & 0 \\ 0 & t_{21} & 0 & 0 \end{pmatrix}$$

设 $t_{12} = t_{21}$, 最终的四个本征态就是其中两个态的平权叠加, 比如说考虑第一行, 第三列是非零的, 说明有一个本征态是 $|1\rangle$ 和 $|3\rangle$ 的平权线性叠加. 四个本征态及对应的能量如下:

$$\begin{cases} |e_1\rangle = \frac{1}{\sqrt{2}}(0,-1,0,1) = \frac{1}{\sqrt{2}}(|4\rangle - |2\rangle), E_1 = -t \\ |e_2\rangle = \frac{1}{\sqrt{2}}(-1,0,1,0) = \frac{1}{\sqrt{2}}(|3\rangle - |1\rangle), E_2 = -t \\ |e_3\rangle = \frac{1}{\sqrt{2}}(0,1,0,1) = \frac{1}{\sqrt{2}}(|2\rangle + |4\rangle), E_3 = t \\ |e_4\rangle = \frac{1}{\sqrt{2}}(1,0,1,0) = \frac{1}{\sqrt{2}}(|1\rangle + |3\rangle), E_4 = t \end{cases}$$

$N_e = 2$

Fock space 中有六个相关的态

$$
\begin{cases}
|1\rangle = c_{1\uparrow}^{\dagger} c_{2\uparrow}^{\dagger} |\Omega\rangle, |2\rangle = c_{1\downarrow}^{\dagger} c_{2\downarrow}^{\dagger} |\Omega\rangle \\
|3\rangle = c_{1\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} |\Omega\rangle, |4\rangle = c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger} |\Omega\rangle \\
|5\rangle = c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} |\Omega\rangle, |6\rangle = c_{2\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} |\Omega\rangle
\end{cases}
$$

$$
\mathcal{H} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & t_{21} & t_{12} \\
0 & 0 & 0 & 0 & -t_{21} & t_{12} \\
0 & 0 & t_{12} & -t_{12} & U & 0 \\
0 & 0 & t_{21} & t_{21} & 0 & U
\end{pmatrix}
$$

> $$
\begin{aligned}
\langle 3|\mathcal{H}|5\rangle &= \langle 3|t_{21} c_{2\downarrow}^{\dagger} c_{1\downarrow} c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} |\Omega\rangle = -t_{21} \langle 3|c_{2\downarrow}^{\dagger} c_{1\uparrow}^{\dagger} c_{1\downarrow} c_{1\downarrow}^{\dagger} |\Omega\rangle \\
&= -t_{21} \langle 3|c_{2\downarrow}^{\dagger} c_{1\uparrow}^{\dagger} \left(1 - c_{1\downarrow}^{\dagger} c_{1\downarrow}\right) |\Omega\rangle = t_{21} \langle 3|c_{1\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} |\Omega\rangle = t_{21}
\end{aligned}
$$
>
> $$
\begin{aligned}
\langle 3|\mathcal{H}|6\rangle &= \langle 3|t_{12} c_{1\uparrow}^{\dagger} c_{2\uparrow} c_{2\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} |\Omega\rangle = t_{12} \langle 3|c_{1\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} |\Omega\rangle = t_{12} \\
\langle 4|\mathcal{H}|5\rangle &= \langle 4|t_{21} c_{2\uparrow}^{\dagger} c_{1\uparrow} c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} |\Omega\rangle = \langle 4|t_{21} c_{2\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} |\Omega\rangle = -t_{21} \\
\langle 4|\mathcal{H}|6\rangle &= \langle 4|t_{12} c_{1\downarrow}^{\dagger} c_{2\uparrow} c_{2\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} |\Omega\rangle = \langle 4|t_{12} c_{1\downarrow}^{\dagger} c_{2\downarrow}^{\dagger} |\Omega\rangle = t_{12}
\end{aligned}
$$

由于两个自旋极化态 $|1\rangle, |2\rangle$ 本身就是能量本征态, 不会和另外四个态相跃迁, 实际上处理的还是一个 4×4 的矩阵

$$
\mathcal{H} = \begin{pmatrix}
0 & 0 & t_{21} & t_{12} \\
0 & 0 & -t_{21} & t_{12} \\
t_{12} & -t_{12} & U & 0 \\
t_{21} & t_{21} & 0 & U
\end{pmatrix}
$$

$$
\begin{cases}
|e_1\rangle = \left(-\frac{U+\sqrt{8t^2+U^2}}{4t}, -\frac{U+\sqrt{8t^2+U^2}}{4t}, 0, 1\right), E_1 = \frac{1}{2}\left(U - \sqrt{8t^2+U^2}\right) \\
|e_2\rangle = \left(-\frac{U+\sqrt{8t^2+U^2}}{4t}, \frac{U+\sqrt{8t^2+U^2}}{4t}, 0, 1\right), E_2 = \frac{1}{2}\left(U - \sqrt{8t^2+U^2}\right) \\
|e_3\rangle = \left(-\frac{U-\sqrt{8t^2+U^2}}{4t}, -\frac{U-\sqrt{8t^2+U^2}}{4t}, 0, 1\right), E_3 = \frac{1}{2}\left(U + \sqrt{8t^2+U^2}\right) \\
|e_4\rangle = \left(-\frac{U-\sqrt{8t^2+U^2}}{4t}, \frac{U-\sqrt{8t^2+U^2}}{4t}, 0, 1\right), E_4 = \frac{1}{2}\left(U + \sqrt{8t^2+U^2}\right)
\end{cases}
$$

单重态和三重态之间的能量劈裂

- 单重态: $(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)/\sqrt{2}$
- 三重态: 包括两个能量为零的自旋极化态和 $(|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle)/\sqrt{2}$;

$$
\begin{aligned}
\mathcal{H}^{(2)} &= J\mathbf{S}_1\cdot\mathbf{S}_2 = J\left(S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z\right) \\
&= \frac{J}{2}\left(S_1^- S_2^+ + S_2^- S_1^+\right) + JS_1^z S_2^z \\
&= \frac{2t^2}{U}\left(S_1^- S_2^+ + S_2^- S_1^+\right) + \frac{4t^2}{U}S_1^z S_2^z
\end{aligned}
$$

其中第二个等号利用了

$$
\begin{aligned}
S_1^- S_2^+ &= \left(S_1^x - iS_1^y\right)\left(S_2^x + iS_2^y\right) = S_1^x S_2^x + S_1^y S_2^y + i\left(S_1^x S_2^y - S_1^y S_2^x\right) \\
S_2^- S_1^+ &= \left(S_2^x - iS_2^y\right)\left(S_1^x + iS_1^y\right) = S_1^x S_2^x + S_1^y S_2^y + i\left(S_2^x S_1^y - S_2^y S_1^x\right) \\
&\Rightarrow S_1^- S_2^+ + S_2^- S_1^+ = 2\left(S_1^x S_2^x + S_1^y S_2^y\right)
\end{aligned}
$$

利用这个表达式可以轻易得到:

$$
\left\langle\uparrow,\downarrow\left|\mathcal{H}^{(2)}\right|\downarrow,\uparrow\right\rangle = \left\langle\downarrow,\uparrow\left|\mathcal{H}^{(2)}\right|\uparrow,\downarrow\right\rangle = \frac{2t^2}{U}
$$

$$
\left\langle\downarrow,\uparrow\left|\mathcal{H}^{(2)}\right|\downarrow,\uparrow\right\rangle = \left\langle\uparrow,\downarrow\left|\mathcal{H}^{(2)}\right|\uparrow,\downarrow\right\rangle = -\frac{t^2}{U}
$$

$$
\left\langle\downarrow,\downarrow\left|\mathcal{H}^{(2)}\right|\downarrow,\downarrow\right\rangle = \left\langle\uparrow,\uparrow\left|\mathcal{H}^{(2)}\right|\uparrow,\uparrow\right\rangle = +\frac{t^2}{U}
$$

从后面两个式子看到, 两个单占据态的能量比两个自旋极化态的能量要低 $2t^2/U$, 和前面的"交换路径解释"[5]是一致的. 简并度部分解除之后, 单占据态才是基态.

$N_e = 3$

$$
|1\rangle = \mathrm{c}_{1\uparrow}^\dagger \mathrm{c}_{1\downarrow}^\dagger \mathrm{c}_{2\uparrow}^\dagger|\Omega\rangle, |2\rangle = \mathrm{c}_{1\uparrow}^\dagger \mathrm{c}_{1\downarrow}^\dagger \mathrm{c}_{2\downarrow}^\dagger|\Omega\rangle, |3\rangle = \mathrm{c}_{2\uparrow}^\dagger \mathrm{c}_{2\downarrow}^\dagger \mathrm{c}_{1\uparrow}^\dagger|\Omega\rangle, |4\rangle = \mathrm{c}_{2\uparrow}^\dagger \mathrm{c}_{2\downarrow}^\dagger \mathrm{c}_{1\downarrow}^\dagger|\Omega\rangle
$$

仔细观察可发现, $|1\rangle$ 和 $|3\rangle$ 之间可以通过一次 hopping 转换, $|2\rangle$ 和 $|4\rangle$ 之间也可以.

$$
\mathcal{H} = \begin{pmatrix} U & 0 & -t_{12} & 0 \\ 0 & U & 0 & -t_{12} \\ -t_{21} & 0 & U & 0 \\ 0 & -t_{21} & 0 & U \end{pmatrix}
$$

$$
\begin{aligned}
\langle 1|\mathcal{H}|3\rangle &= \langle 1|t_{12}\mathrm{c}_{1\downarrow}^\dagger c_{2\downarrow}\mathrm{c}_{2\uparrow}^\dagger \mathrm{c}_{2\downarrow}^\dagger \mathrm{c}_{1\uparrow}^\dagger|\Omega\rangle = -t_{12}\langle 1|\mathrm{c}_{1\downarrow}^\dagger \mathrm{c}_{2\uparrow}^\dagger c_{2\downarrow}\mathrm{c}_{2\downarrow}^\dagger \mathrm{c}_{1\uparrow}^\dagger|\Omega\rangle \\
&= -t_{12}\langle 1|\mathrm{c}_{1\downarrow}^\dagger \mathrm{c}_{2\uparrow}^\dagger \mathrm{c}_{1\uparrow}^\dagger|\Omega\rangle = -t_{12}\langle 1|\mathrm{c}_{1\uparrow}^\dagger \mathrm{c}_{1\downarrow}^\dagger \mathrm{c}_{2\uparrow}^\dagger|\Omega\rangle = -t_{12}
\end{aligned}
$$

$$
\begin{aligned}
\langle 2|\mathcal{H}|4\rangle &= \langle 2|t_{12}\mathrm{c}_{1\uparrow}^\dagger c_{2\uparrow}\mathrm{c}_{2\uparrow}^\dagger \mathrm{c}_{2\downarrow}^\dagger \mathrm{c}_{1\downarrow}^\dagger|\Omega\rangle = t_{12}\langle 2|\mathrm{c}_{1\uparrow}^\dagger \mathrm{c}_{2\downarrow}^\dagger \mathrm{c}_{1\downarrow}^\dagger|\Omega\rangle \\
&= -t_{12}\langle 2|\mathrm{c}_{1\uparrow}^\dagger \mathrm{c}_{1\downarrow}^\dagger \mathrm{c}_{2\downarrow}^\dagger|\Omega\rangle = -t_{12}
\end{aligned}
$$

$$\begin{cases} |e_1\rangle = \frac{1}{\sqrt{2}}(0,1,0,1) = \frac{1}{\sqrt{2}}(|2\rangle + |4\rangle), E_1 = -t+U \\ |e_2\rangle = \frac{1}{\sqrt{2}}(1,0,1,0) = \frac{1}{\sqrt{2}}(|1\rangle + |3\rangle), E_2 = -t+U \\ |e_3\rangle = \frac{1}{\sqrt{2}}(0,-1,0,1) = \frac{1}{\sqrt{2}}(-|2\rangle + |4\rangle), E_3 = t+U \\ |e_4\rangle = \frac{1}{\sqrt{2}}(-1,0,1,0) = \frac{1}{\sqrt{2}}(-|1\rangle + |3\rangle), E_4 = t+U \end{cases}$$

推广到 extended lattice: 4×4 的晶格

- $N_e = 1$: $C_{16}^1 \times 2 = 32 = C_{32}^1$, 哈密顿量为一个很稀疏的 32×32 的矩阵, 比如说第 i 列, 经历一次 hopping 只能跳到上下左右四个格点之中, $i-4$, $i-1$, $i+1$, $i+4$ 四行上的矩阵元非零.
- $N_e = 2$: $C_{16}^2 \times 2^2 + C_{16}^1 = 480 + 16 = 496 = C_{32}^2$
- $N_e = 3$: $C_{16}^3 \times 2^3 + C_{16}^1 (C_{15}^1 \times 2) = 4960 = C_{32}^3$

这告诉我们, 对于大晶格, 这种严格对角化的方法是越来越难做的. 设晶格的格点数为 L, 则固定电子数 N_e 的 Hilbert 空间大小为$C_{2L}^{N_e}$.

Grand-canonical Hubbard model

Grand-canonical potential form of Hubbard model:

$$\mathcal{H} - \mu\hat{N} = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu)\, \hat{n}_{\mathbf{k}\sigma} + U \sum_{\mathbf{j}} \hat{n}_{\mathbf{j}\uparrow}\hat{n}_{\mathbf{j}\downarrow}$$

- $\hat{N} = \sum_{\mathbf{k}\sigma} \hat{n}_{\mathbf{k}\sigma}$: the operator of the total number of particles

When should we use this form? In fact, it's the question that whether we choose $\mathcal{F}^N$ or $\mathcal{F} = \otimes_N \mathcal{F}^N$ as our Hilbert space.

- This form is suitable if we wish to work in the 4^L-dimensional Hilbert space (L is the number of sites, and every site has "four possible state"[6]) comprising the states with **all possible values** of the total number of electrons.
- The Hilbert space for a **fixed number N
** of the electrons has the much lower dimensionality C_{2L}^N.

3.4.4 Hubbard 模型的旋转不变性

证明 Hubbard 模型"equ:3.1Hubbard_model"[4]满足旋转不变性, 也就是和总自旋算符 $\mathbf{S}_{\text{tot}} = \sum_i \mathbf{S}_i$ 对易.

考虑一个具有 $\mathcal{N}$ 个格点和周期性边界条件的一维环(ring), 可以用什么量子数来对本征态进行分类? 一般就是角动量量子数m

1.
2.
3.
4.
5.
   - $|a\rangle, |b\rangle = |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle$: 二阶能量修正是 $-2t^2/U < 0$, 两条交换路径如下, 最后都会变成 $|\downarrow,\uparrow\rangle$.
   - $|\uparrow,\downarrow\rangle \xrightarrow{\hat{H}^t} |\uparrow\downarrow,0\rangle \xrightarrow{\hat{H}^t} |\downarrow,\uparrow\rangle$: 贡献为 $-t^2/U$
   - $|\uparrow,\downarrow\rangle \xrightarrow{\hat{H}^t} |0,\uparrow\downarrow\rangle \xrightarrow{\hat{H}^t} |\downarrow,\uparrow\rangle$: 贡献同样是 $-t^2/U$
   - 对于自旋极化态 $|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$, 经历一次 hopping 之后就会变成零, 因此二阶修正为零.
6.
   1. $|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ is empty
   2. $|\uparrow\rangle_{\mathbf{j}} = c^{\dagger}_{\mathbf{j}\uparrow}|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ occupied by an $\uparrow$-electron
   3. $|\downarrow\rangle_{\mathbf{j}} = c^{\dagger}_{\mathbf{j}\downarrow}|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ occupied by an $\downarrow$-electron
   4. $|d\rangle_{\mathbf{j}} = c^{\dagger}_{\mathbf{j}\uparrow}c^{\dagger}_{\mathbf{j}\downarrow}|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ is doubly occupied
      1. The definition of $|d\rangle_{\mathbf{j}}$ fixes a convention about the order of the two creation operators.
      2. Merely saying that the site is doubly occupied would be *ambiguous* : it could also be understood to mean $c^{\dagger}_{\mathbf{j}\downarrow}c^{\dagger}_{\mathbf{j}\uparrow}|0\rangle_{\mathbf{j}} = -c^{\dagger}_{\mathbf{j}\uparrow}c^{\dagger}_{\mathbf{j}\downarrow}|0\rangle_{\mathbf{j}} = -|d\rangle_{\mathbf{j}}$.

Ch.4 Mott Transition and Hubbard Model

4.3 The Hubbard Model

$$\mathcal{H}=-t\sum_{\langle\mathbf{j},\mathbf{l}\rangle}\sum_{\sigma}\left(c_{\mathbf{j}\sigma}^{\dagger}c_{\mathbf{l}\sigma}+c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{j}\sigma}\right)+U\sum_{\mathbf{j}}\hat{n}_{\mathbf{j}\uparrow}\hat{n}_{\mathbf{j}\downarrow}$$

$$\mathcal{H}_{\text{band}}=-t\sum_{\langle\mathbf{j},\mathbf{l}\rangle}\sum_{\sigma}\left(c_{\mathbf{j}\sigma}^{\dagger}c_{\mathbf{l}\sigma}+c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{j}\sigma}\right)=\sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}\hat{n}_{\mathbf{k}\sigma}$$

$$\mathcal{H}_{U}=U\sum_{\mathbf{j}}\hat{n}_{\mathbf{j}\uparrow}\hat{n}_{\mathbf{j}\downarrow}$$

$$U=\int d\mathbf{r}_1\int d\mathbf{r}_2\left|\phi\left(\mathbf{r}_1-\mathbf{R}_{\mathbf{j}}\right)\right|^2\frac{e^2}{\left|\mathbf{r}_1-\mathbf{r}_2\right|}\left|\phi\left(\mathbf{r}_2-\mathbf{R}_{\mathbf{j}}\right)\right|^2$$

Grand-canonical Hubbard model

Grand-canonical potential form of Hubbard model:

$$\mathcal{H}-\mu\hat{N}=\sum_{\mathbf{k}\sigma}\left(\epsilon_{\mathbf{k}}-\mu\right)\hat{n}_{\mathbf{k}\sigma}+U\sum_{\mathbf{j}}\hat{n}_{\mathbf{j}\uparrow}\hat{n}_{\mathbf{j}\downarrow}$$

- $\hat{N}=\sum_{\mathbf{k}\sigma}\hat{n}_{\mathbf{k}\sigma}$: the operator of the total number of particles

When should we use this form? In fact, it's the question that whether we choose $\mathcal{F}^N$ or $\mathcal{F}=\otimes_N\mathcal{F}^N$ as our Hilbert space.

- This form is suitable if we wish to work in the 4^L-dimensional Hilbert space (L is the number of sites, and every site has "four possible state"[1]) comprising the states with **all possible values** of the total number of electrons.
- The Hilbert space for a **fixed number N
** of the electrons has the much lower dimensionality C_{2L}^N.

Lattice models and Continuum models

- The Hubbard model is the most-studied **lattice fermion model**.
    - Other lattice models of interest
        - the **periodic Anderson model** allows us to study homogeneous valence mixing, and the arising of a heavy Fermi liquid in certain !-electron systems (Ch. 11)

- **two-band and many-band Hubbard models** might be relevant for itinerant ferromagnetism (Ch. 7) and maybe for high-temperature superconductivity
- (Ch. 1) a **spinless fermion model** for Wigner crystallization

$$
\mathcal{H}=\mathcal{H}_{\text{hop}}+\mathcal{H}_{\text{el}-\text{el}}=-t\sum_{<\mathbf{i},\mathbf{j}>}\left(c_{\mathbf{i}}^{\dagger}c_{\mathbf{j}}+c_{\mathbf{j}}^{\dagger}c_{\mathbf{i}}\right)+V\sum_{<\mathbf{i},\mathbf{j}>}\hat{n}_{\mathbf{i}}\hat{n}_{\mathbf{j}}
$$

- A common feature of lattice models: the existence of **certain magic values of the band filling** where **new correlated phases** may appear.
  - We expect a Mott insulator only if n is an integer;
  - Wigner crystallization was associated with $n=1/2$.
- Loosely speaking, at a magic filling a density wave of the electron system is in registry with the underlying lattice; such **commensurability effects** can arise only in lattice models.
  - This statement seems to be contradicted with the finding of an **incompressible Laughlin state** at $\nu=1/3$ in a continuum model (Sec. 12.4.1). We can argue that there the external magnetic field gave rise to a **length scale**, and thus to the possibility of magic values of filling.

- **Continuum models**: an interacting electron fluid is moving on a uniform background of positive charge.
  - Fermi liquid theory
- It is reasonable to expect that at **low band fillings**, the lattice models behave like continuum models.
  - Even the typical strong correlation features (heavy mass, etc.) found in the immediate vicinity of n = 1 for the Hubbard model can be reformulated in the Fermi liquid terminology.

4.3.1 Local Basis

Hubbard model is a four-state model, i.e. each lattice site can be found in any of the following four local basis state:

1. $|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ is empty
2. $|\uparrow\rangle_{\mathbf{j}}=c_{\mathbf{j}\uparrow}^{\dagger}|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ occupied by an $\uparrow$-electron
3. $|\downarrow\rangle_{\mathbf{j}}=c_{\mathbf{j}\downarrow}^{\dagger}|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ occupied by an $\downarrow$-electron
4. $|d\rangle_{\mathbf{j}}=c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}^{\dagger}|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ is doubly occupied

1. The definition of $|d\rangle_{\mathrm{j}}$ fixes a convention about the order of the two creation operators.
2. Merely saying that the site is doubly occupied would be *ambiguous* : it could also be understood to mean $c_{\mathrm{j}\downarrow}^{\dagger} c_{\mathrm{j}\uparrow}^{\dagger}|0\rangle_{\mathrm{j}}=-c_{\mathrm{j}\uparrow}^{\dagger} c_{\mathrm{j}\downarrow}^{\dagger}|0\rangle_{\mathrm{j}}=-|d\rangle_{\mathrm{j}}$.

It's useful to define corresponding **local projectors**:

$$
\begin{aligned}
\hat{P}_{\mathrm{j}0} &= |0\rangle_{\mathrm{jj}}\langle 0|=\left(1-\hat{n}_{\mathrm{j}\uparrow}\right)\left(1-\hat{n}_{\mathrm{j}\downarrow}\right) \\
\hat{P}_{\mathrm{j}\uparrow} &= |\uparrow\rangle_{\mathrm{jj}}\langle\uparrow|=\hat{n}_{\mathrm{j}\uparrow}\left(1-\hat{n}_{\mathrm{j}\downarrow}\right) \\
\hat{P}_{\mathrm{j}\downarrow} &= |\downarrow\rangle_{\mathrm{jj}}\langle\downarrow|=\hat{n}_{\mathrm{j}\downarrow}\left(1-\hat{n}_{\mathrm{j}\uparrow}\right) \\
\hat{P}_{\mathrm{j}d} &= |d\rangle_{\mathrm{jj}}\langle d|=\hat{n}_{\mathrm{j}\uparrow}\hat{n}_{\mathrm{j}\downarrow}
\end{aligned}
$$

- The completeness of the local basis

$$
\hat{P}_{\mathrm{j}0}+\hat{P}_{\mathrm{j}\uparrow}+\hat{P}_{\mathrm{j}\downarrow}+\hat{P}_{\mathrm{j}d}=\hat{1}
$$

- "correlations are strong" means that an $\uparrow$-spin electron observes very carefully whether it is sharing a lattice site with a $\downarrow$-spin electron.
  - The local projectors provide a tool to keep track of these local events.

4.5 Symmetries

假设 U 在每个格点上都是一样的, 那么 $\mathcal{H}_U$ 在晶格的各种对称操作之下都是不变的, Hubbard 模型的对称性取决于 $\mathcal{H}_{\text{band}}$. 除了这种纯几何对称性之外, 还有更多的对称性需要考虑.

- 连续自旋旋转不变性 (continuous spin-rotational invariance): 在对本征态进行分类上十分重要, 且磁序的出现可以理解为这个对称性的自发破缺.
- 电子-空穴对称性 (the electron-hole symmetry): 一大类的 Hubbard 模型都具有这个重要的离散对称性.
- 时间反演不变性 (time-reversal invariance): 当磁场不存在时, Hubbard 模型会展现出时间反演不变性.

4.5.1 自旋旋转不变性 (spin-rotational invariance)

Hubbard 模型本身导出的时候就是和电子的自旋自由度完全无关的:

- Hopping term: 代表电子的动能
- Interaction term: 源于电子之间的库伦相互作用, 只依赖于电子之间的距离

因此, 我们理所当然地认为 Hubbard 哈密顿量是在所有自旋同时旋转时不变的. 下面我们在数学上证明这个事情, 即证明 "Hubbard 哈密顿量"[2]和集体自旋算符是对易的.

集体自旋算符为:

$$\mathbf{S}_{\text{tot}}=\sum_{\mathbf{j}}\mathbf{S}_{\mathbf{j}}=\frac{1}{2}\sum_{\mathbf{j}}\mathbf{c}_{\mathbf{j}}^{\dagger}\boldsymbol{\sigma}_{\mathbf{j}}\mathbf{c}_{\mathbf{j}}$$

具体地, 其中每个格点上的"自旋算符的各个分量"[3]写为:

$$\begin{cases} S_{\mathbf{j}}^{x}=\frac{1}{2}\left(c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}+c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}\right)\\ S_{\mathbf{j}}^{y}=\frac{i}{2}\left(-c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}+c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}\right)\\ S_{\mathbf{j}}^{z}=\frac{1}{2}\left(c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\uparrow}-c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\downarrow}\right)=\frac{1}{2}\left(n_{\mathbf{j}\uparrow}-n_{\mathbf{j}\downarrow}\right)\end{cases}$$

$\mathcal{H}_{\text{band}}$ 和总自旋算符的对易

$$\mathcal{H}_{\text{band}}=-t\sum_{\langle\mathbf{j},\mathbf{l}\rangle}\sum_{\sigma}\left(c_{\mathbf{j}\sigma}^{\dagger}c_{\mathbf{l}\sigma}+c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{j}\sigma}\right)=\sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}\hat{n}_{\mathbf{k}\sigma}$$

这一项代表电子的动能, 物理上看来, 不同格点之间 hopping 的电子是不区分其自旋的, 自然是对易的. 数学上的证明如下, 首先看 $\mathcal{H}_{\text{band}}$ 和 x 方向自旋的对易子:

$$\begin{aligned}
[\mathcal{H}_{\text{band}},S_{\text{tot}}^{x}]&=\left[-t\sum_{\langle\mathbf{m},\mathbf{l}\rangle}\sum_{\sigma}\left(c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma}+c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{m}\sigma}\right),\sum_{\mathbf{j}}\frac{1}{2}\left(c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}+c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}\right)\right]\\
&=-\frac{1}{2}t\sum_{\langle\mathbf{m},\mathbf{l}\rangle}\sum_{\mathbf{j}}\sum_{\sigma}\left[\left(c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma}+c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{m}\sigma}\right),\left(c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}+c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}\right)\right]\\
&=-\frac{1}{2}t\sum_{\mathbf{j}}\left\{\begin{array}{c}\left[\sum_{\langle\mathbf{m},\mathbf{l}\rangle,\sigma}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma},c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}\right]+\left[\sum_{\langle\mathbf{m},\mathbf{l}\rangle,\sigma}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma},c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}\right]\\+\left[\sum_{\langle\mathbf{m},\mathbf{l}\rangle,\sigma}c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{m}\sigma},c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}\right]+\left[\sum_{\langle\mathbf{m},\mathbf{l}\rangle,\sigma}c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{m}\sigma},c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}\right]\end{array}\right\}\\
&=-\frac{1}{2}t\sum_{\mathbf{j}}\left\{\begin{array}{c}\sum_{\langle\mathbf{m}\rangle_{\mathbf{j}}}\left(c_{\mathbf{m}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}+c_{\mathbf{m}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}+c_{\mathbf{m}\downarrow}c_{\mathbf{j}\uparrow}^{\dagger}+c_{\mathbf{m}\uparrow}c_{\mathbf{j}\downarrow}^{\dagger}\right)\\+\sum_{\langle\mathbf{l}\rangle_{\mathbf{j}}}\left(c_{\mathbf{l}\downarrow}c_{\mathbf{j}\uparrow}^{\dagger}+c_{\mathbf{l}\uparrow}c_{\mathbf{j}\downarrow}^{\dagger}+c_{\mathbf{l}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}+c_{\mathbf{l}\uparrow}^{\dagger}c_{\mathbf{j}\uparrow}\right)\end{array}\right\}\\
&=-t\sum_{\langle\mathbf{m},\mathbf{j}\rangle}\left(c_{\mathbf{m}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}+c_{\mathbf{m}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}-c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{m}\downarrow}-c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{m}\uparrow}\right)\\
&=-t\sum_{\langle\mathbf{m},\mathbf{j}\rangle}\left(c_{\mathbf{m}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}+c_{\mathbf{m}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}\right)-t\sum_{\langle\mathbf{m},\mathbf{j}\rangle}\left(c_{\mathbf{m}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}+c_{\mathbf{m}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}\right)\\
&=0
\end{aligned}$$

其中第四个等号的过程如下:

$$
\begin{aligned}
\left[c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma}, c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}\right] &= c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma}c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow} - c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma} \\
&= \begin{cases}
\mathbf{m},\mathbf{l}\neq\mathbf{j}: c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma} - c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma} = 0 \\
\mathbf{m}\neq\mathbf{j},\mathbf{l}=\mathbf{j},\sigma=\uparrow: c_{\mathbf{m}\sigma}^{\dagger}\left(-c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{l}\sigma}+1\right)c_{\mathbf{j}\downarrow} - c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma} = c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{j}\downarrow} \\
\mathbf{m}\neq\mathbf{j},\mathbf{l}=\mathbf{j},\sigma=\downarrow: c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma} - c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma} = 0 \\
\mathbf{m}=\mathbf{j},\mathbf{l}\neq\mathbf{j},\sigma=\uparrow: c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma} - c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma} = 0 \\
\mathbf{m}=\mathbf{j},\mathbf{l}\neq\mathbf{j},\sigma=\downarrow: -c_{\mathbf{j}\uparrow}^{\dagger}\left(-c_{\mathbf{j}\downarrow}c_{\mathbf{m}\sigma}^{\dagger}+1\right)c_{\mathbf{l}\sigma} - c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma} = c_{\mathbf{l}\sigma}c_{\mathbf{j}\uparrow}^{\dagger}
\end{cases} \\
&= c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{j}\downarrow}\delta_{\mathbf{l}\mathbf{j}}\delta_{\sigma\uparrow} + c_{\mathbf{l}\sigma}c_{\mathbf{j}\uparrow}^{\dagger}\delta_{\mathbf{m}\mathbf{j}}\delta_{\sigma\downarrow}
\end{aligned}
$$

$$
\begin{aligned}
\left[c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma}, c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}\right] &= c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma}c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow} - c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma} \\
&= \delta_{\mathbf{l}\mathbf{j}}\delta_{\sigma\downarrow}\left[c_{\mathbf{m}\sigma}^{\dagger}\left(-c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{l}\sigma}+1\right)c_{\mathbf{j}\uparrow} - c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma}\right] \\
&\quad + \delta_{\mathbf{m}\mathbf{j}}\delta_{\sigma\uparrow}\left[-c_{\mathbf{j}\downarrow}^{\dagger}\left(-c_{\mathbf{j}\uparrow}c_{\mathbf{m}\sigma}^{\dagger}+1\right)c_{\mathbf{l}\sigma} - c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{l}\sigma}\right] \\
&= c_{\mathbf{m}\sigma}^{\dagger}c_{\mathbf{j}\uparrow}\delta_{\mathbf{l}\mathbf{j}}\delta_{\sigma\downarrow} + c_{\mathbf{l}\sigma}c_{\mathbf{j}\downarrow}^{\dagger}\delta_{\mathbf{m}\mathbf{j}}\delta_{\sigma\uparrow}
\end{aligned}
$$

$$
\begin{aligned}
\left[c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{m}\sigma}, c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}\right] &= c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{m}\sigma}c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow} - c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{m}\sigma} \\
&= \delta_{\mathbf{l}\mathbf{j}}\delta_{\sigma\downarrow}\left[-c_{\mathbf{j}\uparrow}^{\dagger}\left(-c_{\mathbf{j}\downarrow}c_{\mathbf{l}\sigma}^{\dagger}+1\right)c_{\mathbf{m}\sigma} - c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{m}\sigma}\right] \\
&\quad + \delta_{\mathbf{m}\mathbf{j}}\delta_{\sigma\uparrow}\left[c_{\mathbf{l}\sigma}^{\dagger}\left(-c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{m}\sigma}+1\right)c_{\mathbf{j}\downarrow} - c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{m}\sigma}\right] \\
&= c_{\mathbf{m}\sigma}c_{\mathbf{j}\uparrow}^{\dagger}\delta_{\mathbf{l}\mathbf{j}}\delta_{\sigma\downarrow} + c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{j}\downarrow}\delta_{\mathbf{m}\mathbf{j}}\delta_{\sigma\uparrow}
\end{aligned}
$$

$$
\left[c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{m}\sigma}, c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}\right] = c_{\mathbf{m}\sigma}c_{\mathbf{j}\downarrow}^{\dagger}\delta_{\mathbf{l}\mathbf{j}}\delta_{\sigma\uparrow} + c_{\mathbf{l}\sigma}^{\dagger}c_{\mathbf{j}\uparrow}\delta_{\mathbf{m}\mathbf{j}}\delta_{\sigma\downarrow}
$$

$\mathcal{H}_{\mathrm{band}}$ 和 y 方向自旋的对易子可以直接根据上面的计算经验得到是零. $S_{\mathbf{j}}^{y}$ 和 $S_{\mathbf{j}}^{x}$ 定义上的区别就在于小括号里面的两项 $c_{\mathbf{j}\uparrow}^{\dagger}c_{\mathbf{j}\downarrow}, c_{\mathbf{j}\downarrow}^{\dagger}c_{\mathbf{j}\uparrow}$ 是相减还是相加, 但实际上我们上面的计算表明, $\mathcal{H}_{\mathrm{band}}$ 和这两项分别都是对易的.

$\mathcal{H}_{\mathrm{band}}$ 和 z 方向自旋的对易子可以利用数算符和产生湮灭算符的对易关系"equ:2.1.3number_commute_creani"[4]推出:

$$
\begin{aligned}
\left[\mathcal{H}_{\text{band}}, S_{\mathbf{j}}^{z}\right] &= \left[-t \sum_{\langle \mathbf{m},\mathbf{l}\rangle} \sum_{\sigma} \left(c_{\mathbf{m}\sigma}^{\dagger} c_{\mathbf{l}\sigma} + c_{\mathbf{l}\sigma}^{\dagger} c_{\mathbf{m}\sigma}\right), \sum_{\mathbf{j}} \frac{1}{2}\left(\hat{n}_{\mathbf{j}\uparrow} - \hat{n}_{\mathbf{j}\downarrow}\right)\right] \\
&= -\frac{1}{2} t \sum_{\langle \mathbf{m},\mathbf{l}\rangle} \sum_{\mathbf{j}} \sum_{\sigma} \left[\left(c_{\mathbf{m}\sigma}^{\dagger} c_{\mathbf{l}\sigma} + c_{\mathbf{l}\sigma}^{\dagger} c_{\mathbf{m}\sigma}\right), \left(\hat{n}_{\mathbf{j}\uparrow} - \hat{n}_{\mathbf{j}\downarrow}\right)\right] \\
&= \frac{1}{2} t \sum_{\langle \mathbf{m},\mathbf{l}\rangle} \sum_{\mathbf{j}} \sum_{\sigma} \left\{ \begin{array}{c} \left[\hat{n}_{\mathbf{j}\uparrow}, c_{\mathbf{m}\sigma}^{\dagger} c_{\mathbf{l}\sigma}\right] + \left[\hat{n}_{\mathbf{j}\uparrow}, c_{\mathbf{l}\sigma}^{\dagger} c_{\mathbf{m}\sigma}\right] \\ -\left[\hat{n}_{\mathbf{j}\downarrow}, c_{\mathbf{m}\sigma}^{\dagger} c_{\mathbf{l}\sigma}\right] - \left[\hat{n}_{\mathbf{j}\downarrow}, c_{\mathbf{l}\sigma}^{\dagger} c_{\mathbf{m}\sigma}\right] \end{array} \right\} \\
&= \frac{1}{2} t \sum_{\langle \mathbf{m},\mathbf{l}\rangle} \sum_{\mathbf{j}} \sum_{\sigma} \left\{ \begin{array}{c} c_{\mathbf{m}\sigma}^{\dagger} \left[\hat{n}_{\mathbf{j}\uparrow}, c_{\mathbf{l}\sigma}\right] + \left[\hat{n}_{\mathbf{j}\uparrow}, c_{\mathbf{m}\sigma}^{\dagger}\right] c_{\mathbf{l}\sigma} \\ + c_{\mathbf{l}\sigma}^{\dagger} \left[\hat{n}_{\mathbf{j}\uparrow}, c_{\mathbf{m}\sigma}\right] + \left[\hat{n}_{\mathbf{j}\uparrow}, c_{\mathbf{l}\sigma}^{\dagger}\right] c_{\mathbf{m}\sigma} \\ - c_{\mathbf{m}\sigma}^{\dagger} \left[\hat{n}_{\mathbf{j}\downarrow}, c_{\mathbf{l}\sigma}\right] - \left[\hat{n}_{\mathbf{j}\downarrow}, c_{\mathbf{m}\sigma}^{\dagger}\right] c_{\mathbf{l}\sigma} \\ - c_{\mathbf{l}\sigma}^{\dagger} \left[\hat{n}_{\mathbf{j}\downarrow}, c_{\mathbf{m}\sigma}\right] - \left[\hat{n}_{\mathbf{j}\downarrow}, c_{\mathbf{l}\sigma}^{\dagger}\right] c_{\mathbf{m}\sigma} \end{array} \right\} \\
&= \frac{1}{2} t \sum_{\langle \mathbf{m},\mathbf{l}\rangle} \sum_{\mathbf{j}} \sum_{\sigma} \left\{ \begin{array}{c} {\color{red}-\delta_{\mathbf{jl}} \delta_{\sigma\uparrow} c_{\mathbf{m}\sigma}^{\dagger} c_{\mathbf{l}\sigma}} {\color{blue}+\delta_{\mathbf{mj}} \delta_{\sigma\uparrow} c_{\mathbf{m}\sigma}^{\dagger} c_{\mathbf{l}\sigma}} \\ {\color{blue}-\delta_{\mathbf{mj}} \delta_{\sigma\uparrow} c_{\mathbf{l}\sigma}^{\dagger} c_{\mathbf{m}\sigma}} {\color{red}+\delta_{\mathbf{jl}} \delta_{\sigma\uparrow} c_{\mathbf{l}\sigma}^{\dagger} c_{\mathbf{m}\sigma}} \\ {\color{magenta}+\delta_{\mathbf{jl}} \delta_{\sigma\downarrow} c_{\mathbf{m}\sigma}^{\dagger} c_{\mathbf{l}\sigma}} {\color{green}-\delta_{\mathbf{mj}} \delta_{\sigma\downarrow} c_{\mathbf{m}\sigma}^{\dagger} c_{\mathbf{l}\sigma}} \\ {\color{green}-\delta_{\mathbf{mj}} \delta_{\sigma\downarrow} c_{\mathbf{l}\sigma}^{\dagger} c_{\mathbf{m}\sigma}} {\color{magenta}-\delta_{\mathbf{jl}} \delta_{\sigma\downarrow} c_{\mathbf{l}\sigma}^{\dagger} c_{\mathbf{m}\sigma}} \end{array} \right\} \\
&= 0
\end{aligned}
$$

最后一个等号中, 相同颜色的项互相抵消了. 得证.

$\mathcal{H}_U$ 和总自旋算符的对易

$\mathcal{H}_U$ 这一项看上去包含了特定的自旋符号, 因此我们可能会担心它是否和自旋算符对易. 实际上, 我们可以利用一个恒等式将 $\mathcal{H}_U$ 改写:

> $$\hat{n}_{\mathbf{j}\uparrow} \hat{n}_{\mathbf{j}\downarrow} = \frac{\hat{n}_{\mathbf{j}}}{2} - \frac{2}{3} \mathbf{S}_{\mathbf{j}}^{2}$$

$$\mathcal{H}_U = \sum_{\mathbf{j}} \hat{n}_{\mathbf{j}\uparrow} \hat{n}_{\mathbf{j}\downarrow} = \frac{UN}{2} - \frac{2U}{3} \sum_{\mathbf{j}} \mathbf{S}_{\mathbf{j}}^{2}$$

这就让这一项的自旋旋转不变性显现出来了. 注意到对于格点 $\mathbf{j}$ 的四种不同可能的状态, $\mathbf{S}_{\mathbf{j}}^{2}$ 有不同的取值:

$$\mathbf{S}_{\mathbf{j}}^{2} = \begin{cases} \frac{1}{2}\left(\frac{1}{2}+1\right) = \frac{3}{4} & \text{for} |\uparrow\rangle, |\downarrow\rangle \\ 0 & \text{for} |0\rangle, |d\rangle \end{cases}$$

因此相互作用使得体系更倾向于拥有**无补偿自旋(uncompensated spins)**.

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1. 1. $|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ is empty
   2. $|\uparrow\rangle_{\mathbf{j}} = c_{\mathbf{j}\uparrow}^{\dagger}|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ occupied by an $\uparrow$-electron

3. $|\downarrow\rangle_{\mathbf{j}} = c^{\dagger}_{\mathbf{j}\downarrow}|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ occupied by an $\downarrow$-electron
4. $|d\rangle_{\mathbf{j}} = c^{\dagger}_{\mathbf{j}\uparrow}c^{\dagger}_{\mathbf{j}\downarrow}|0\rangle_{\mathbf{j}}$: site $\mathbf{j}$ is doubly occupied
    1. The definition of $|d\rangle_{\mathbf{j}}$ fixes a convention about the order of the two creation operators.
    2. Merely saying that the site is doubly occupied would be *ambiguous* : it could also be understood to mean $c^{\dagger}_{\mathbf{j}\downarrow}c^{\dagger}_{\mathbf{j}\uparrow}|0\rangle_{\mathbf{j}} = -c^{\dagger}_{\mathbf{j}\uparrow}c^{\dagger}_{\mathbf{j}\downarrow}|0\rangle_{\mathbf{j}} = -|d\rangle_{\mathbf{j}}$.

2.
3.
4.