

《高等量子力学》第 23 讲

4. 坐标表象中的力学量算符

消灭产生算符 $\hat{\psi}_\sigma(\vec{r})$, $\hat{\psi}_\sigma^+(\vec{r})$ 。

1) 动能算符

动能算符是可加性单粒子算符，坐标本征态不是动能的本征态，故在坐标表象动能是一个二阶张量，

$$\begin{aligned}\hat{T} &= \sum_{\sigma\sigma'} \int d^3\vec{r} d^3\vec{r}' \hat{\psi}_\sigma^+(\vec{r}) \hat{\psi}_{\sigma'}(\vec{r}') \langle \vec{r}, \sigma | \frac{\hat{p}^2}{2m} | \vec{r}', \sigma' \rangle \\ &= -\frac{\hbar^2}{2m} \sum_{\sigma\sigma'} \int d^3\vec{r} d^3\vec{r}' \hat{\psi}_\sigma^+(\vec{r}) \hat{\psi}_{\sigma'}(\vec{r}') \vec{\nabla}_r^2 \delta(\vec{r} - \vec{r}') \delta_{\sigma\sigma'} \\ &\quad \underline{\text{两次分部积分}} -\frac{\hbar^2}{2m} \sum_{\sigma\sigma'} \int d^3\vec{r} d^3\vec{r}' (\vec{\nabla}_r^2 \hat{\psi}_\sigma^+(\vec{r})) \hat{\psi}_{\sigma'}(\vec{r}') \delta(\vec{r} - \vec{r}') \delta_{\sigma\sigma'} \\ &= -\frac{\hbar^2}{2m} \sum_{\sigma} \int d^3\vec{r} (\vec{\nabla}_r^2 \hat{\psi}_\sigma^+(\vec{r})) \hat{\psi}_\sigma(\vec{r}) \\ &\quad \underline{\text{分部积分}} \frac{\hbar^2}{2m} \sum_{\sigma} \int d^3\vec{r} \vec{\nabla}_r \hat{\psi}_\sigma^+(\vec{r}) \cdot \vec{\nabla}_r \hat{\psi}_\sigma(\vec{r})\end{aligned}$$

2) 无相互作用费米气体的力学量

先考虑粒子数密度算符的平均值。

基态 $|\Phi_0\rangle = |1, \dots, 1_{p_F}, 0, \dots\rangle$ ：费米面以下 $p < p_F$ 的单粒子态全部占满，而 $p > p_F$ 的态全空。在基态（动量本征态）的密度算符平均值：

$$\bar{\rho}(\vec{r}) = \langle \Phi_0 | \hat{\rho}(\vec{r}) | \Phi_0 \rangle = \langle \Phi_0 | \sum_{\sigma} \hat{\psi}_\sigma^+(\vec{r}) \hat{\psi}_\sigma(\vec{r}) | \Phi_0 \rangle$$

把消灭产生算符从坐标表象到动量表象进行表象变换，并且动量表象的消灭产生算符要作用在同一个态上，即配对成粒子数算符 $\hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma(\vec{p})$ 才能使矩阵元不为零。利用

$$\hat{\psi}_{\sigma}^{+}(\vec{p})\hat{\psi}_{\sigma}(\vec{p})|\Phi_0\rangle=n_{\sigma}(\vec{p})|\Phi_0\rangle$$

和归一化条件

$$\langle\Phi_0|\Phi_0\rangle=1,$$

以及对于费米子

$$n_{\sigma}(\vec{p})=\begin{cases} 1 & p < p_F \\ 0 & p > p_F \end{cases},$$

有

$$\begin{aligned}\bar{\rho}(\vec{r}) &= \sum_{\sigma} \int \frac{d^3\vec{p}d^3\vec{p}'}{(2\pi\hbar)^3} e^{-\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot\vec{r}} \langle\Phi_0|\hat{\psi}_{\sigma}^{+}(\vec{p})\hat{\psi}_{\sigma}(\vec{p}')|\Phi_0\rangle \\ &= \sum_{\sigma} \int \frac{d^3\vec{p}d^3\vec{p}'}{(2\pi\hbar)^3} e^{-\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot\vec{r}} \langle\Phi_0|\hat{\psi}_{\sigma}^{+}(\vec{p})\hat{\psi}_{\sigma}(\vec{p})|\Phi_0\rangle \delta(\vec{p}-\vec{p}') \\ &= \sum_{\sigma} \int \frac{d^3\vec{p}}{(2\pi\hbar)^3} n(\vec{p}) = \sum_{\sigma} \int_{p < p_F} \frac{d^3\vec{p}}{(2\pi\hbar)^3} = n = \frac{p_F^3}{3\hbar^3\pi^2}\end{aligned}$$

再定义 **粒子数密度矩阵**

$$\begin{aligned}\bar{\rho}(\vec{r}-\vec{r}') &= \langle\Phi_0|\hat{\rho}(\vec{r}-\vec{r}')|\Phi_0\rangle \\ &= \langle\Phi_0|\sum_{\sigma}\hat{\psi}_{\sigma}^{+}(\vec{r})\hat{\psi}_{\sigma}(\vec{r}')|\Phi_0\rangle \\ &= \sum_{\sigma} \int \frac{d^3\vec{p}d^3\vec{p}'}{(2\pi\hbar)^3} e^{-\frac{i}{\hbar}(\vec{p}\cdot\vec{r}-\vec{p}'\cdot\vec{r}')} \langle\Phi_0|\hat{\psi}_{\sigma}^{+}(\vec{p})\hat{\psi}_{\sigma}(\vec{p}')|\Phi_0\rangle \\ &= \sum_{\sigma} \int_{p < p_F} \frac{d^3\vec{p}}{(2\pi\hbar)^3} e^{-\frac{i}{\hbar}\vec{p}\cdot(\vec{r}-\vec{r}')} \\ &= 3n \frac{\sin(p_F|\vec{r}-\vec{r}'|)-p_F|\vec{r}-\vec{r}'|\cos(p_F|\vec{r}-\vec{r}'|)}{p_F|\vec{r}-\vec{r}'|}\end{aligned}$$

当 $\vec{r}-\vec{r}'\rightarrow 0$ 时, 有

$$\lim_{\vec{r}-\vec{r}'\rightarrow 0} \bar{\rho}(\vec{r}-\vec{r}') \rightarrow \bar{\rho}(\vec{r}) = n.$$

现在考虑**两粒子关联函数**：在 \vec{r}, σ 处发现一个粒子同时又在 \vec{r}', σ' 发现另一个粒子的几率。由于在 \vec{r}, σ 处发现一个粒子的几率为

$$\langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{r}) \hat{\psi}_\sigma(\vec{r}) | \Phi_0 \rangle = \left(\langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{r}) \right) \left(\hat{\psi}_\sigma(\vec{r}) | \Phi_0 \rangle \right),$$

故在此基础上又在 \vec{r}', σ' 发现另一个粒子的几率为

$$\left(\langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{r}) \right) \hat{\psi}_{\sigma'}^+(\vec{r}') \hat{\psi}_{\sigma'}(\vec{r}') \left(\hat{\psi}_\sigma(\vec{r}) | \Phi_0 \rangle \right) = \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{r}) \hat{\psi}_{\sigma'}^+(\vec{r}') \hat{\psi}_{\sigma'}(\vec{r}') \hat{\psi}_\sigma(\vec{r}) | \Phi_0 \rangle$$

通过表象变换,

$$\begin{aligned} & \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{r}) \hat{\psi}_{\sigma'}^+(\vec{r}') \hat{\psi}_{\sigma'}(\vec{r}') \hat{\psi}_\sigma(\vec{r}) | \Phi_0 \rangle \\ &= \int \frac{d^3 \vec{p} d^3 \vec{p}' d^3 \vec{q} d^3 \vec{q}'}{(2\pi\hbar)^6} e^{-\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot\vec{r}} e^{-\frac{i}{\hbar}(\vec{q}-\vec{q}')\cdot\vec{r}'} \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_{\sigma'}^+(\vec{q}) \hat{\psi}_{\sigma'}(\vec{q}') \hat{\psi}_\sigma(\vec{p}') | \Phi_0 \rangle \end{aligned}$$

只有当 4 个消灭产生算符配对成 2 个作用在不同状态上的粒子数算符

$\hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma(\vec{p})$ 和 $\hat{\psi}_{\sigma'}^+(\vec{q}) \hat{\psi}_{\sigma'}(\vec{q})$ 时矩阵元才不为零。

当 $\sigma \neq \sigma'$ 时, 只有一种可能配对方法, 即 $\vec{p}' = \vec{p}$, $\vec{q}' = \vec{q}$,

$$\begin{aligned} & \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_{\sigma'}^+(\vec{q}) \hat{\psi}_{\sigma'}(\vec{q}) \hat{\psi}_\sigma(\vec{p}) | \Phi_0 \rangle \\ &= \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_{\sigma'}^+(\vec{q}) \hat{\psi}_{\sigma'}(\vec{q}) \hat{\psi}_\sigma(\vec{p}) | \Phi_0 \rangle \delta(\vec{p} - \vec{p}') \delta(\vec{q} - \vec{q}') \end{aligned}$$

两粒子关联函数

$$\begin{aligned} & \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{r}) \hat{\psi}_{\sigma'}^+(\vec{r}') \hat{\psi}_{\sigma'}(\vec{r}') \hat{\psi}_\sigma(\vec{r}) | \Phi_0 \rangle \\ &= \int \frac{d^3 \vec{p} d^3 \vec{q}}{(2\pi\hbar)^6} \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_{\sigma'}^+(\vec{q}) \hat{\psi}_{\sigma'}(\vec{q}) \hat{\psi}_\sigma(\vec{p}) | \Phi_0 \rangle \\ &= \int \frac{d^3 \vec{p} d^3 \vec{q}}{(2\pi\hbar)^6} \langle \Phi_0 | \hat{\psi}_{\sigma'}^+(\vec{q}) \hat{\psi}_{\sigma'}(\vec{q}) \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma(\vec{p}) | \Phi_0 \rangle \quad (\text{反对易关系}) \\ &= \int \frac{d^3 \vec{p} d^3 \vec{q}}{(2\pi\hbar)^6} n_\sigma(\vec{p}) n_{\sigma'}(\vec{q}) = \left(\frac{n}{2} \right)^2 \quad \left(\int \frac{d^3 \vec{p}}{(2\pi\hbar)^3} n_\sigma(\vec{p}) = \frac{n}{2} \right) \end{aligned}$$

当 $\sigma = \sigma'$ 时, 有两种可能的配对方法 $\vec{p}' = \vec{q}$, $\vec{q}' = \vec{p}$ 或 $\vec{p}' = \vec{p}$, $\vec{q}' = \vec{q}$, 矩阵元都不为零,

$$\begin{aligned} & \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma^+(\vec{q}) \hat{\psi}_\sigma(\vec{q}') \hat{\psi}_\sigma(\vec{p}') | \Phi_0 \rangle \\ &= \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma^+(\vec{q}) \hat{\psi}_\sigma(\vec{q}) \hat{\psi}_\sigma(\vec{p}) | \Phi_0 \rangle \delta(\vec{p} - \vec{p}') \delta(\vec{q} - \vec{q}') \\ &+ \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma^+(\vec{q}) \hat{\psi}_\sigma(\vec{p}) \hat{\psi}_\sigma(\vec{q}) | \Phi_0 \rangle \delta(\vec{p} - \vec{q}') \delta(\vec{q} - \vec{p}') \end{aligned}$$

两粒子关联函数

$$\begin{aligned} & \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{r}) \hat{\psi}_\sigma^+(\vec{r}') \hat{\psi}_\sigma(\vec{r}') \hat{\psi}_\sigma(\vec{r}) | \Phi_0 \rangle \\ &= \int \frac{d^3 \vec{p} d^3 \vec{q}}{(2\pi\hbar)^6} \langle \Phi_0 | \left[\hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma^+(\vec{q}) \hat{\psi}_\sigma(\vec{q}) \hat{\psi}_\sigma(\vec{p}) + e^{-\frac{i}{\hbar}(\vec{p}-\vec{q})\cdot(\vec{r}-\vec{r}')} \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma^+(\vec{q}) \hat{\psi}_\sigma(\vec{p}) \hat{\psi}_\sigma(\vec{q}) \right] | \Phi_0 \rangle \\ &= \int \frac{d^3 \vec{p} d^3 \vec{q}}{(2\pi\hbar)^6} \langle \Phi_0 | \left[\hat{\psi}_\sigma^+(\vec{q}) \hat{\psi}_\sigma(\vec{q}) \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma(\vec{p}) - e^{-\frac{i}{\hbar}(\vec{p}-\vec{q})\cdot(\vec{r}-\vec{r}')} \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma(\vec{p}) \hat{\psi}_\sigma^+(\vec{q}) \hat{\psi}_\sigma(\vec{q}) \right] | \Phi_0 \rangle \\ &= \int \frac{d^3 \vec{p} d^3 \vec{q}}{(2\pi\hbar)^6} \left(1 - e^{-\frac{i}{\hbar}(\vec{p}-\vec{q})\cdot(\vec{r}-\vec{r}')} \right) n_\sigma(\vec{p}) n_\sigma(\vec{q}) \\ &= \left(\frac{n}{2} \right)^2 - \frac{1}{2} \bar{\rho}(\vec{r} - \vec{r}') \end{aligned}$$

注意: 4 个消灭产生算符都作用在同一个态上是不行的, 因为 Pauli 不相容原理,

$$\begin{aligned} & \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma^+(\vec{p}) \hat{\psi}_\sigma(\vec{p}) \hat{\psi}_\sigma(\vec{p}) | \Phi_0 \rangle \\ &= \langle \Phi_0 | \hat{\psi}_\sigma^+(\vec{p}) (1 - \hat{\psi}_\sigma(\vec{p}) \hat{\psi}_\sigma^+(\vec{p})) \hat{\psi}_\sigma(\vec{p}) | \Phi_0 \rangle \\ &= n_\sigma(\vec{p}) (1 - n_\sigma(\vec{p})) = 0 \end{aligned}$$

3) 无相互作用玻色气体的力学量

考虑自旋为零的玻色气体。对于态 $|\Phi_0\rangle = |n_1, n_2, \dots, n_i, \dots\rangle$, 表象变换以后的两粒子关联函数

$$\begin{aligned} & \langle \Phi_0 | \hat{\psi}^+(\vec{r}) \hat{\psi}^+(\vec{r}') \hat{\psi}(\vec{r}') \hat{\psi}(\vec{r}) | \Phi_0 \rangle \\ &= \int \frac{d^3 \vec{p} d^3 \vec{p}' d^3 \vec{q} d^3 \vec{q}'}{(2\pi\hbar)^6} e^{-\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot\vec{r}} e^{-\frac{i}{\hbar}(\vec{q}-\vec{q}')\cdot\vec{r}'} \langle \Phi_0 | \hat{\psi}^+(\vec{p}) \hat{\psi}^+(\vec{q}) \hat{\psi}(\vec{q}') \hat{\psi}(\vec{p}') | \Phi_0 \rangle \end{aligned}$$

只有当消灭产生算符配对成 2 个作用在不同状态上的粒子数算符 $\hat{\psi}_\sigma^+(\vec{p})\hat{\psi}_\sigma(\vec{p})$ 和 $\hat{\psi}_\sigma^+(\vec{q})\hat{\psi}_\sigma(\vec{q})$, 即 $\vec{p}'=\vec{p}$, $\vec{q}'=\vec{q}$ 或 $\vec{p}'=\vec{q}$, $\vec{q}'=\vec{p}$ 但 $\vec{p}\neq\vec{q}$ 时, 矩阵元不为零,

$$\begin{aligned} & \langle \Phi_0 | \hat{\psi}^+(\vec{p}) \hat{\psi}^+(\vec{q}) \hat{\psi}(\vec{q}') \hat{\psi}(\vec{p}') | \Phi_0 \rangle \\ &= [1-\delta(\vec{p}-\vec{q})] \{ \langle \Phi_0 | \hat{\psi}^+(\vec{p}) \hat{\psi}^+(\vec{q}) \hat{\psi}(\vec{q}) \hat{\psi}(\vec{p}) | \Phi_0 \rangle \delta(\vec{p}-\vec{p}') \delta(\vec{q}-\vec{q}') \\ & \quad + \langle \Phi_0 | \hat{\psi}^+(\vec{p}) \hat{\psi}^+(\vec{q}) \hat{\psi}(\vec{p}) \hat{\psi}(\vec{q}) | \Phi_0 \rangle \delta(\vec{p}-\vec{q}') \delta(\vec{q}-\vec{p}') \} \end{aligned}$$

其中 $1-\delta(\vec{p}-\vec{q})$ 的作用是保证 2 个粒子数算符作用在不同状态上。

对于玻色子, 当消灭产生算符配对成 2 个作用在同一态上的粒子数算符

$\hat{\psi}^+(\vec{p})\hat{\psi}^+(\vec{p})\hat{\psi}(\vec{p})\hat{\psi}(\vec{p})$, 即 $\vec{p}=\vec{q}$ 时, 矩阵元也不为零,

$$\begin{aligned} & \langle \Phi_0 | \hat{\psi}^+(\vec{p}) \hat{\psi}^+(\vec{q}) \hat{\psi}(\vec{q}') \hat{\psi}(\vec{p}') | \Phi_0 \rangle \\ &= \langle \Phi_0 | \hat{\psi}^+(\vec{p}) \hat{\psi}^+(\vec{p}) \hat{\psi}(\vec{p}) \hat{\psi}(\vec{p}) | \Phi_0 \rangle \delta(\vec{p}-\vec{q}) \delta(\vec{p}-\vec{p}') \delta(\vec{q}-\vec{q}') \end{aligned}$$

故两粒子关联函数

$$\begin{aligned} & \langle \Phi_0 | \hat{\psi}^+(\vec{r}) \hat{\psi}^+(\vec{r}') \hat{\psi}(\vec{r}') \hat{\psi}(\vec{r}) | \Phi_0 \rangle \\ &= \int \frac{d^3 \vec{p} d^3 \vec{q}}{(2\pi\hbar)^6} (1-\delta(\vec{p}-\vec{q})) \langle \Phi_0 | \hat{\psi}^+(\vec{p}) \hat{\psi}^+(\vec{q}) \hat{\psi}(\vec{q}) \hat{\psi}(\vec{p}) \\ & \quad + e^{-\frac{i}{\hbar}(\vec{p}-\vec{q})\cdot(\vec{r}-\vec{r}')} \hat{\psi}^+(\vec{p}) \hat{\psi}^+(\vec{q}) \hat{\psi}(\vec{p}) \hat{\psi}(\vec{q}) | \Phi_0 \rangle + \int \frac{d^3 \vec{p}}{(2\pi\hbar)^6} \langle \Phi_0 | \hat{\psi}^+(\vec{p}) \hat{\psi}^+(\vec{p}) \hat{\psi}(\vec{p}) \hat{\psi}(\vec{p}) | \Phi_0 \rangle \end{aligned}$$

对于最后一项, 利用对易关系, 有

$$\hat{\psi}^+(\vec{p})\hat{\psi}^+(\vec{p})\hat{\psi}(\vec{p})\hat{\psi}(\vec{p}) = \hat{\psi}^+(\vec{p})\left(\hat{\psi}(\vec{p})\hat{\psi}^+(\vec{p})-1\right)\hat{\psi}(\vec{p})$$

故

$$\begin{aligned}
& \langle \Phi_0 | \hat{\psi}^+(\vec{r}) \hat{\psi}^+(\vec{r}') \hat{\psi}(\vec{r}') \hat{\psi}(\vec{r}) | \Phi_0 \rangle \\
&= \int \frac{d^3 \vec{p} d^3 \vec{q}}{(2\pi\hbar)^6} (1 - \delta(\vec{p} - \vec{q})) n(\vec{p}) n(\vec{q}) \left(1 + e^{-\frac{i}{\hbar}(\vec{p}-\vec{q})\cdot(\vec{r}-\vec{r}')} \right) + \int \frac{d^3 \vec{p}}{(2\pi\hbar)^6} n(\vec{p}) (n(\vec{p}) - 1) \\
&= \left(\int \frac{d^3 \vec{p}}{(2\pi\hbar)^3} n(\vec{p}) \right)^2 + \left| \int \frac{d^3 \vec{p}}{(2\pi\hbar)^3} n(\vec{p}) e^{-\frac{i}{\hbar} \vec{p} \cdot (\vec{r} - \vec{r}')} \right|^2 - 2 \int \frac{d^3 \vec{p}}{(2\pi\hbar)^6} n^2(\vec{p}) + \int \frac{d^3 \vec{p}}{(2\pi\hbar)^6} n(\vec{p}) (n(\vec{p}) - 1) \\
&= \left(\int \frac{d^3 \vec{p}}{(2\pi\hbar)^3} n(\vec{p}) \right)^2 + \left| \int \frac{d^3 \vec{p}}{(2\pi\hbar)^3} n(\vec{p}) e^{-\frac{i}{\hbar} \vec{p} \cdot (\vec{r} - \vec{r}')} \right|^2 - \int \frac{d^3 \vec{p}}{(2\pi\hbar)^6} n(\vec{p}) (n(\vec{p}) + 1)
\end{aligned}$$

5. Hartree-Fock 平均场方法

在任意表象 A ，设全同费米子体系的能量包含动能和两体相互作用部分，忽略其它多体相互作用，

$$\hat{H} = \sum_{ij} T_{ij} \hat{a}_i^+ \hat{a}_j + \frac{1}{2} \sum_{ijmn} V_{ijmn} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_m \hat{a}_n。$$

下面把四体相互作用近似用二体相互作用来表示（Wick 定理）。把四体关联 $\hat{a}_i^+ \hat{a}_j^+ \hat{a}_m \hat{a}_n$ 中的二体关联 $\hat{a}_i^+ \hat{a}_j$ 分成经典部分（平均场部分） $\langle \Phi_0 | \hat{a}_i^+ \hat{a}_j | \Phi_0 \rangle$ 和量子涨落部分 $\delta(\hat{a}_i^+ \hat{a}_j)$ ，

$$\hat{a}_i^+ \hat{a}_j = \langle \Phi_0 | \hat{a}_i^+ \hat{a}_j | \Phi_0 \rangle + \delta(\hat{a}_i^+ \hat{a}_j)，$$

考虑 $\hat{a}_i^+ \hat{a}_j^+ \hat{a}_m \hat{a}_n$ 中所有可能的二体关联的分解，利用费米子的反对易关系，有

$$\begin{aligned}
\hat{a}_i^+ \hat{a}_j^+ \hat{a}_m \hat{a}_n &= \langle \Phi_0 | \hat{a}_j^+ \hat{a}_m | \Phi_0 \rangle \langle \Phi_0 | \hat{a}_i^+ \hat{a}_n | \Phi_0 \rangle + \langle \Phi_0 | \hat{a}_i^+ \hat{a}_n | \Phi_0 \rangle \hat{a}_j^+ \hat{a}_m \\
&\quad + \langle \Phi_0 | \hat{a}_j^+ \hat{a}_m | \Phi_0 \rangle \hat{a}_i^+ \hat{a}_n - \langle \Phi_0 | \hat{a}_j^+ \hat{a}_n | \Phi_0 \rangle \hat{a}_i^+ \hat{a}_m \\
&\quad - \langle \Phi_0 | \hat{a}_i^+ \hat{a}_m | \Phi_0 \rangle \hat{a}_j^+ \hat{a}_n + \hat{a}_i^+ \hat{a}_j^+ \hat{a}_m \hat{a}_n
\end{aligned}$$

这里已经把右边的量子涨落 $\delta(\hat{a}_i^+ \hat{a}_j)$ 用 $\hat{a}_i^+ \hat{a}_j$ 来表示。

忽略完全量子涨落项，即四体算符 $\hat{a}_i^+ \hat{a}_j^+ \hat{a}_m \hat{a}_n$ ，只保留二体部分，

$$\begin{aligned}\hat{H} = & \sum_{ij} T_{ij} \hat{a}_i^+ \hat{a}_j + \frac{1}{2} \sum_{ijmn} V_{ijmn} [\langle \Phi_0 | \hat{a}_j^+ \hat{a}_m | \Phi_0 \rangle \langle \Phi_0 | \hat{a}_i^+ \hat{a}_n | \Phi_0 \rangle \\ & + \langle \Phi_0 | \hat{a}_i^+ \hat{a}_n | \Phi_0 \rangle \hat{a}_j^+ \hat{a}_m + \langle \Phi_0 | \hat{a}_j^+ \hat{a}_m | \Phi_0 \rangle \hat{a}_i^+ \hat{a}_n \\ & - \langle \Phi_0 | \hat{a}_j^+ \hat{a}_n | \Phi_0 \rangle \hat{a}_i^+ \hat{a}_m - \langle \Phi_0 | \hat{a}_i^+ \hat{a}_m | \Phi_0 \rangle \hat{a}_j^+ \hat{a}_n]\end{aligned}$$

利用 V_{ijmn} 的定义，

$$V_{ijmn} = \langle a_i | \langle a_j | \hat{V} | a_m \rangle | a_n \rangle = \langle \dots 1_j \dots 1_i \dots | \hat{V} | \dots 1_n \dots 1_m \dots \rangle = \langle 0 | \hat{a}_i \hat{a}_j \hat{V} \hat{a}_m^+ \hat{a}_n^+ | 0 \rangle$$

费米子消灭产生算符的反对易关系导致 V_{ijmn} 的反对易关系

$$V_{ijmn} = -V_{jimn} = -V_{ijnm} = V_{jinm}$$

故

$$\begin{aligned}\hat{H} = & \frac{1}{2} \sum_{ijmn} V_{ijmn} \langle \Phi_0 | \hat{a}_j^+ \hat{a}_m | \Phi_0 \rangle \langle \Phi_0 | \hat{a}_i^+ \hat{a}_n | \Phi_0 \rangle \\ & + \sum_{ij} \left[T_{ij} + 2 \sum_{mn} V_{mijn} \langle \Phi_0 | \hat{a}_m^+ \hat{a}_n | \Phi_0 \rangle \right] \hat{a}_i^+ \hat{a}_j\end{aligned}$$

第一项是常数项，第二项是单体相互作用。

如果选择表象 A 使得单体相互作用项对角化，有

$$T_{ij} + 2 \sum_{mn} V_{mijn} \langle \Phi_0 | \hat{a}_m^+ \hat{a}_n | \Phi_0 \rangle = \varepsilon_i \delta_{ij}.$$

注意：这个使得单体相互作用项对角化的表象 A 不对应一个裸粒子的力学量算符 \hat{A} 。这是一个有效的单体相互作用，已经包含了二体相互作用的贡献，因此表象 A 对应的是一个准粒子的力学量算符。如何找到这个准粒子表象，就是通过矩阵 $T_{ij} + 2 \sum_{mn} V_{mijn} \langle \Phi_0 | \hat{a}_m^+ \hat{a}_n | \Phi_0 \rangle$ 的对角化来确定准粒子的能级 ε_i 。

在按准粒子能量分布的 Fock 空间态 $|\Phi_0\rangle = |1, \dots, 1_{p_F}, 0, \dots\rangle$, 有

$$\langle \Phi_0 | \hat{a}_m^+ \hat{a}_n | \Phi_0 \rangle = \delta_{mn} \delta(\vec{p}_F - \vec{p}_m)$$

能量算符中的常数项

$$\frac{1}{2} \sum_{ijmn} V_{ijmn} \langle \Phi_0 | \hat{a}_j^+ \hat{a}_m | \Phi_0 \rangle \langle \Phi_0 | \hat{a}_i^+ \hat{a}_n | \Phi_0 \rangle = \frac{1}{2} \sum_{ij} V_{ijji} \delta(\vec{p}_F - \vec{p}_i) \delta(\vec{p}_F - \vec{p}_j)$$

能量算符简化成

$$\hat{H} = \frac{1}{2} \sum_{ij} V_{ijji} \delta(\vec{p}_F - \vec{p}_i) \delta(\vec{p}_F - \vec{p}_j) + \sum_i \varepsilon_i \hat{a}_i^+ \hat{a}_i$$

其中

$$\varepsilon_i = T_{ii} + 2 \sum_m V_{mim} \delta(\vec{p}_F - \vec{p}_m)。$$

在基态的能量

$$\begin{aligned} \hat{H} |\Phi_0\rangle &= E_0 |\Phi_0\rangle, \\ E_0 &= \left(\frac{1}{2} \sum_{ij} V_{ijji} \delta(\vec{p}_F - \vec{p}_j) + \sum_i \varepsilon_i \right) \delta(\vec{p}_F - \vec{p}_i) \end{aligned}$$

利用对易关系

$$\begin{aligned} [\hat{H}, \hat{a}_m] &= \sum_i \varepsilon_i [\hat{a}_i^+ \hat{a}_i, \hat{a}_m] = \sum_i \varepsilon_i (\hat{a}_i^+ \hat{a}_i \hat{a}_m - \hat{a}_m \hat{a}_i^+ \hat{a}_i) \\ &= - \sum_i \varepsilon_i \{ \hat{a}_m, \hat{a}_i^+ \} \hat{a}_i = -\varepsilon_m \hat{a}_m \\ [\hat{H}, \hat{a}_m^+] &= \varepsilon_m \hat{a}_m^+ \end{aligned}$$

在单粒子-空穴态 $\hat{a}_m^+ \hat{a}_n |\Phi_0\rangle$ 的能量

$$\begin{aligned} \hat{H} \hat{a}_m^+ \hat{a}_n |\Phi_0\rangle &= E_1 \hat{a}_m^+ \hat{a}_n |\Phi_0\rangle, \\ E_1 &= E_0 + \varepsilon_m - \varepsilon_n \end{aligned}$$