《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 $\hat{\psi}_\sigma\left(\vec{r}\right)$，$\hat{\psi}_\sigma^+\left(\vec{r}\right)$。

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，

$$\hat{\mathrm{T}}=\sum_{\sigma\sigma'}\int d^3\vec{r}d^3\vec{r}\,'\hat{\psi}_\sigma^+(\vec{r})\hat{\psi}_{\sigma'}(\vec{r}\,')\left\langle\vec{r},\sigma\left|\frac{\hat{\vec{p}}^2}{2m}\right|\vec{r}\,',\sigma'\right\rangle$$

$$=-\frac{\hbar^2}{2m}\sum_{\sigma\sigma'}\int d^3\vec{r}d^3\vec{r}\,'\hat{\psi}_\sigma^+(\vec{r})\hat{\psi}_{\sigma'}(\vec{r}\,')\vec{\nabla}_r^2\delta\left(\vec{r}-\vec{r}\,'\right)\delta_{\sigma\sigma'}$$

$$\underline{\underline{\text{两次分部积分}}}-\frac{\hbar^2}{2m}\sum_{\sigma\sigma'}\int d^3\vec{r}d^3\vec{r}\,'\left(\vec{\nabla}_r^2\hat{\psi}_\sigma^+(\vec{r})\right)\hat{\psi}_{\sigma'}(\vec{r}\,')\delta\left(\vec{r}-\vec{r}\,'\right)\delta_{\sigma\sigma'}$$

$$=-\frac{\hbar^2}{2m}\sum_{\sigma}\int d^3\vec{r}\left(\vec{\nabla}_r^2\hat{\psi}_\sigma^+(\vec{r})\right)\hat{\psi}_\sigma(\vec{r})$$

$$\underline{\underline{\text{分部积分}}}\frac{\hbar^2}{2m}\sum_{\sigma}\int d^3\vec{r}\vec{\nabla}_r\hat{\psi}_\sigma^+(\vec{r})\cdot\vec{\nabla}_r\hat{\psi}_\sigma(\vec{r})$$

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 $\left|\Phi_0\right\rangle=\left|1,\ldots1_{p_F},0,\ldots\right\rangle$：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：

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

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

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

和归一化条件 $\left\langle\Phi_0\middle|\Phi_0\right\rangle = 1$，

以及对于费米子

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

有

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

再定义粒子数密度矩阵

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

当 $\vec{r}-\vec{r}\,' \to 0$ 时，有

$$\lim_{\vec{r}-\vec{r}\,'\to 0} \overline{\rho}(\vec{r}-\vec{r}\,') \to \overline{\rho}(\vec{r}) = n\text{。}$$

现在考虑两粒子关联函数：在$\vec{r},\sigma$处发现一个粒子同时又在$\vec{r}\,',\sigma'$发现另一个粒子的几率。由于在$\vec{r},\sigma$处发现一个粒子的几率为

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

故在此基础上又在$\vec{r}\,',\sigma'$发现另一个粒子的几率为

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

通过表象变换，

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

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$\vec{p}\,'=\vec{p}$，$\vec{q}\,'=\vec{q}$，

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

两粒子关联函数

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

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，

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

两粒子关联函数

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

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,

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

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 $\left|\Phi_0\right\rangle=\left|n_1,n_2,\ldots n_i,\ldots\right\rangle$，表象变换以后的两粒子关联函数

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

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

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，

$$\left\langle\Phi_0\left|\hat{\psi}^+(\vec{p})\hat{\psi}^+(\vec{q})\hat{\psi}(\vec{q}\,')\hat{\psi}(\vec{p}\,')\right|\Phi_0\right\rangle$$

$$=\left[1\text{-}\delta\left(\vec{p}-\vec{q}\right)\right]\{\left\langle\Phi_0\left|\hat{\psi}^+(\vec{p})\hat{\psi}^+(\vec{q})\hat{\psi}(\vec{q})\hat{\psi}(\vec{p})\right|\Phi_0\right\rangle\delta\left(\vec{p}-\vec{p}\,'\right)\delta\left(\vec{q}-\vec{q}\,'\right)$$
$$+\left\langle\Phi_0\left|\hat{\psi}^+(\vec{p})\hat{\psi}^+(\vec{q})\hat{\psi}(\vec{p})\hat{\psi}(\vec{q})\right|\Phi_0\right\rangle\delta\left(\vec{p}-\vec{q}\,'\right)\delta\left(\vec{q}-\vec{p}\,'\right)\}$$

其中 $1\text{-}\delta\left(\vec{p}-\vec{q}\right)$ 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，

$$\left\langle\Phi_0\left|\hat{\psi}^+(\vec{p})\hat{\psi}^+(\vec{q})\hat{\psi}(\vec{q}\,')\hat{\psi}(\vec{p}\,')\right|\Phi_0\right\rangle$$

$$=\left\langle\Phi_0\left|\hat{\psi}^+(\vec{p})\hat{\psi}^+(\vec{p})\hat{\psi}(\vec{p})\hat{\psi}(\vec{p})\right|\Phi_0\right\rangle\delta\left(\vec{p}-\vec{q}\right)\delta\left(\vec{p}-\vec{p}\,'\right)\delta\left(\vec{q}-\vec{q}\,'\right)$$

故两粒子关联函数

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

$$=\int\frac{d^3\vec{p}d^3\vec{q}}{\left(2\pi\hbar\right)^6}\left(1\text{-}\delta\left(\vec{p}-\vec{q}\right)\right)\langle\Phi_0|\hat{\psi}^+(\vec{p})\hat{\psi}^+(\vec{q})\hat{\psi}(\vec{q})\hat{\psi}(\vec{p})$$

$$+e^{-\frac{i}{\hbar}(\vec{p}-\vec{q})\cdot(\vec{r}-\vec{r}\,')}\hat{\psi}^+(\vec{p})\hat{\psi}^+(\vec{q})\hat{\psi}(\vec{p})\hat{\psi}(\vec{q})\left|\Phi_0\right\rangle+\int\frac{d^3\vec{p}}{\left(2\pi\hbar\right)^6}\left\langle\Phi_0\left|\hat{\psi}^+(\vec{p})\hat{\psi}^+(\vec{p})\hat{\psi}(\vec{p})\hat{\psi}(\vec{p})\right|\Phi_0\right\rangle$$

对于最后一项，利用对易关系，有

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

故

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

$$=\int \frac{d^3\vec{p}d^3\vec{q}}{(2\pi\hbar)^6}\left(1-\delta(\vec{p}-\vec{q})\right)n(\vec{p})n(\vec{q})\left(1+e^{-\frac{i}{\hbar}(\vec{p}-\vec{q})\cdot(\vec{r}-\vec{r}\,')}\right)+\int \frac{d^3\vec{p}}{(2\pi\hbar)^6}n(\vec{p})\left(n(\vec{p})-1\right)$$

$$=\left(\int \frac{d^3\vec{p}}{(2\pi\hbar)^3}n(\vec{p})\right)^2+\left|\int \frac{d^3\vec{p}}{(2\pi\hbar)^3}n(\vec{p})e^{-\frac{i}{\hbar}\vec{p}\cdot(\vec{r}-\vec{r}\,')}\right|^2-2\int \frac{d^3\vec{p}}{(2\pi\hbar)^3}n^2(\vec{p})+\int \frac{d^3\vec{p}}{(2\pi\hbar)^6}n(\vec{p})\left(n(\vec{p})-1\right)$$

$$=\left(\int \frac{d^3\vec{p}}{(2\pi\hbar)^3}n(\vec{p})\right)^2+\left|\int \frac{d^3\vec{p}}{(2\pi\hbar)^3}n(\vec{p})e^{-\frac{i}{\hbar}\vec{p}\cdot(\vec{r}-\vec{r}\,')}\right|^2-\int \frac{d^3\vec{p}}{(2\pi\hbar)^6}n(\vec{p})\left(n(\vec{p})+1\right)$$

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，

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

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）$\left\langle \Phi_0 \left| \hat{a}_i^+\hat{a}_j \right| \Phi_0 \right\rangle$ 和量子涨落部分 $\delta\left(\hat{a}_i^+\hat{a}_j\right)$，

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

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

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

这里已经把右边的量子涨落 $\delta\left(\hat{a}_i^+\hat{a}_j\right)$ 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，

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

利用V_{ijmn}的定义，

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

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

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

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

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

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$\varepsilon_i$。

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

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

能量算符中的常数项

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

能量算符简化成

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

其中

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

在基态的能量

$$\hat{\mathrm{H}}\left|\Phi_0\right\rangle = E_0\left|\Phi_0\right\rangle,$$

$$E_0 = \left(\frac{1}{2}\sum_{ij}V_{ijji}\delta\left(\vec{p}_F-\vec{p}_j\right)+\sum_i\varepsilon_i\right)\delta\left(\vec{p}_F-\vec{p}_i\right)$$

利用对易关系

$$\left[\hat{\mathrm{H}},\ \hat{a}_m\right]=\sum_i\varepsilon_i\left[\hat{a}_i^+\hat{a}_i,\ \hat{a}_m\right] = \sum_i\varepsilon_i\left(\hat{a}_i^+\hat{a}_i\hat{a}_m-\hat{a}_m\hat{a}_i^+\hat{a}_i\right)$$

$$= -\sum_i\varepsilon_i\left\{\hat{a}_m,\ \hat{a}_i^+\right\}\hat{a}_i = -\varepsilon_m\hat{a}_m$$

$$\left[\hat{\mathrm{H}},\ \hat{a}_m^+\right] = \varepsilon_m\hat{a}_m^+$$

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

$$\hat{\mathrm{H}}\hat{a}_m^+\hat{a}_n\left|\Phi_0\right\rangle = E_1\hat{a}_m^+\hat{a}_n\left|\Phi_0\right\rangle,$$

$$E_1 = E_0+\varepsilon_m-\varepsilon_n$$