《高等量子力学》第 22 讲

7) 粒子数算符的比例常数

$$\hat{a}_i\left|n_1,\ldots,n_i,n_{i+1}\ldots\right\rangle = c_i\left|n_1,\ldots,n_i-1,n_{i+1}\ldots\right\rangle$$
$$\hat{a}_i^+\left|n_1,\ldots,n_i,n_{i+1}\ldots\right\rangle = d_i\left|n_1,\ldots,n_i+1,n_{i+1}\ldots\right\rangle$$

$c_i,d_i=?$

考虑 Fock 空间的态$\left|0,\ldots 0,n_i,n_{i+1},\ldots\right\rangle$（$n_1=n_2=\ldots\ldots=n_{i-1}=0$）。利用对易关系（类似于谐振子问题的代数解法）有

$$\hat{a}_i\left|0,\ldots 0,n_i,n_{i+1}\ldots\right\rangle = \sqrt{n_i}\left|0,\ldots 0,n_i-1,n_{i+1}\ldots\right\rangle,$$
$$\hat{a}_i^+\left|0,\ldots 0,n_i,n_{i+1}\ldots\right\rangle = \sqrt{n_i+1}\left|0,\ldots 0,n_i+1,n_{i+1}\ldots\right\rangle.$$

由

$$\left|n_1,\ldots,n_i,n_{i+1}\ldots\right\rangle = A(n_1,\ldots n_{i-1})\left(\hat{a}_1^+\right)^{n_1}\left(\hat{a}_2^+\right)^{n_2}\ldots\left(\hat{a}_{i-1}^+\right)^{n_{i-1}}\left|0,\ldots 0,n_i,n_{i+1}\ldots\right\rangle,$$

注意产生算符的次序，$\hat{a}_{i-1}^+$ 比 $\hat{a}_{i-2}^+$ 先作用，对于玻色子，由对易关系，有

$$\begin{aligned}\hat{a}_i\left|n_1,\ldots,n_i,n_{i+1}\ldots\right\rangle &= A(n_1,\ldots n_{i-1})\left(\hat{a}_1^+\right)^{n_1}\left(\hat{a}_2^+\right)^{n_2}\ldots\left(\hat{a}_{i-1}^+\right)^{n_{i-1}}\hat{a}_i\left|0,\ldots,n_i,n_{i+1}\ldots\right\rangle\\ &= A(n_1,\ldots n_{i-1})\left(\hat{a}_1^+\right)^{n_1}\left(\hat{a}_2^+\right)^{n_2}\ldots\left(\hat{a}_{i-1}^+\right)^{n_{i-1}}\sqrt{n_i}\left|0,\ldots,n_i-1,n_{i+1}\ldots\right\rangle\\ &= \sqrt{n_i}\left|n_1,\ldots,n_i-1,n_{i+1}\ldots\right\rangle\end{aligned}$$

$$\hat{a}_i^+\left|n_1,\ldots,n_i,n_{i+1}\ldots\right\rangle = \sqrt{n_i+1}\left|n_1,\ldots,n_i+1,n_{i+1}\ldots\right\rangle$$

对于费米子，由反对易关系，有

$$\begin{aligned}\hat{a}_i\left|n_1,\ldots,n_i,n_{i+1}\ldots\right\rangle &= A(n_1,\ldots n_{i-1})\left(\hat{a}_1^+\right)^{n_1}\left(\hat{a}_2^+\right)^{n_2}\ldots\left(\hat{a}_{i-1}^+\right)^{n_{i-1}}(-1)^{\sum_{j=1}^{i-1}n_j}\hat{a}_i\left|0,\ldots,n_i,n_{i+1}\ldots\right\rangle\\ &= (-1)^{\sum_{j=1}^{i-1}n_j}\sqrt{n_i}\left|n_1,\ldots,n_i-1,n_{i+1}\ldots\right\rangle,\end{aligned}$$

$$\hat{a}_i^+\left|n_1,\ldots,n_i,\ldots\right\rangle = (-1)^{\sum_{j=1}^{i-1}n_j}\sqrt{n_i+1}\left|n_1,\ldots,n_i+1,n_{i+1}\ldots\right\rangle.$$

无论是玻色子还是费米子，都有

$$\hat{n}_i\left|n_1,\ldots,n_i,\ldots\right\rangle=\hat{a}_i^+\hat{a}_i\left|n_1,\ldots,n_i,\ldots\right\rangle=n_i\left|n_1,\ldots,n_i,\ldots\right\rangle$$ 。

2. 用产生消灭算符表示力学量

如何用厄米算符 $\hat{n}_i=\hat{a}_i^+\hat{a}_i$ 表示体系的力学量。

1) 可加性单粒子力学量

体系的力学量是每个粒子的力学量之和，例如动能算符。

对于单粒子力学量 $\hat{A}$，

$$\hat{A}\left|a_i\right\rangle=a_i\left|a_i\right\rangle,$$

若选取表象 A， $\hat{A}$ 有确定值。在按照 a_i 分布的 Fock 空间 $\left|n_1,\ldots,n_i,\ldots\right\rangle$，与 $\hat{A}$ 对应的体系力学量算符

$$\hat{\mathrm{A}}=\sum_i a_i\hat{n}_i=\sum_i a_i\hat{a}_i^+\hat{a}_i$$ 。

若选取表象 B， $\hat{A}$ 没有确定值，由表象变换，在按照 b_i 分布的 Fock 空间 $\left|\tilde{n}_1,\ldots\tilde{n}_i\ ,..\right\rangle$,

$$\begin{aligned}\hat{\mathrm{A}}&=\sum_i a_i\hat{a}_i^+\hat{a}_i\\&=\sum_{ijk}a_iS_{ji}S_{ik}^+\hat{b}_j^+\hat{b}_k\\&=\sum_{jk}\hat{b}_j^+\hat{b}_k\sum_i a_i\left\langle b_j\middle|a_i\right\rangle\left\langle a_i\middle|b_k\right\rangle\\&=\sum_{jk}\hat{b}_j^+\hat{b}_k\sum_i\left\langle b_j\middle|\hat{A}\middle|a_i\right\rangle\left\langle a_i\middle|b_k\right\rangle\text{。}\\&=\sum_{jk}\hat{b}_j^+\hat{b}_k\left\langle b_j\middle|\hat{A}\middle|b_k\right\rangle\end{aligned}$$

表明可加性力学量在单粒子算符自身表象是对角矩阵,在任意表象有非对角元。

应用：对于粒子间有相互作用的真实多粒子体系，其它所有粒子对某个粒子的作用可近似处理为一个平均势场。这就是平均场近似。这时，体系的力学量就是可加性单粒子算符，是所有(在势场中运动的)准粒子的贡献之和。

2) 可加性两粒子力学量

单粒子算符 $\hat{A}$ 的本征态 $\hat{A}\left|a_i\right\rangle = a_i\left|a_i\right\rangle$。在 A 表象，设两粒子态 $\left|a_i\right\rangle\left|a_j\right\rangle$ 是两粒子力学量 $\hat{V}$ 的本征态，

$$\hat{V}\left|a_i\right\rangle\left|a_j\right\rangle = V_{ij}\left|a_i\right\rangle\left|a_j\right\rangle,$$

显然，有 $V_{ij} = V_{ji}$。在 Fock 空间 $\left|n_1,\ldots,n_i,\ldots\right\rangle$，考虑到两粒子可处于不同单粒子态，也可处于同一态，与 $\hat{V}$ 对应的体系力学量算符

$$\begin{aligned}\hat{\mathrm{V}} &= \frac{1}{2}\sum_{i\neq j}\hat{n}_i\hat{n}_j V_{ij} + \frac{1}{2}\sum_i \hat{n}_i(\hat{n}_i - 1)V_{ii} \\ &= \frac{1}{2}\sum_{ij}(\hat{n}_i\hat{n}_j - \hat{n}_j\delta_{ij})V_{ij}\end{aligned}$$

由对易反对易关系，$i\neq j$ 时，有

$$\hat{n}_i\hat{n}_j - \hat{n}_j\delta_{ij} = \hat{n}_i\hat{n}_j = \hat{a}_i^+\hat{a}_i\hat{a}_j^+\hat{a}_j = \pm\hat{a}_i^+\hat{a}_j^+\hat{a}_i\hat{a}_j = \hat{a}_i^+\hat{a}_j^+\hat{a}_j\hat{a}_i$$

$i = j$ 时，有

$$\begin{aligned}\hat{n}_i\hat{n}_j - \hat{n}_j\delta_{ij} &= \hat{n}_i\hat{n}_i - \hat{n}_i = \hat{a}_i^+\hat{a}_i\hat{a}_i^+\hat{a}_i - \hat{a}_i^+\hat{a}_i \\ &= \hat{a}_i^+\left(1\pm\hat{a}_i^+\hat{a}_i\right)\hat{a}_i - \hat{a}_i^+\hat{a}_i \\ &= \pm\hat{a}_i^+\hat{a}_i^+\hat{a}_i\hat{a}_i = \hat{a}_i^+\hat{a}_i^+\hat{a}_i\hat{a}_i\end{aligned}$$

最后一步把两个消灭算符进行了对易。

结合$i \neq j$和$i = j$两种情况，都有

$$\hat{n}_i \hat{n}_j - \hat{n}_j \delta_{ij} = \hat{a}_i^+ \hat{a}_j^+ \hat{a}_j \hat{a}_i$$

故有

$$\hat{\mathrm{V}} = \frac{1}{2} \sum_{ij} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_j \hat{a}_i V_{ij} \text{。}$$

在B表象，由单粒子算符$\hat{B}$定义的两粒子态$\left|b_i\right\rangle\left|b_j\right\rangle$不是$\hat{V}$的本征态。由表象变换，在按照$b_i$分布的 Fock 态$\left|\tilde{n}_1, \ldots, \tilde{n}_i, \ldots\right\rangle$，

$$\begin{aligned}
\hat{\mathrm{V}} &= \frac{1}{2} \sum_{ij} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_j \hat{a}_i V_{ij} \\
&= \frac{1}{2} \sum_{ijklmn} \hat{b}_k^+ \hat{b}_l^+ \hat{b}_m \hat{b}_n S_{ki} S_{lj} S_{jm}^+ S_{in}^+ V_{ij} \\
&= \frac{1}{2} \sum_{ijklmn} \hat{b}_k^+ \hat{b}_l^+ \hat{b}_m \hat{b}_n \left\langle b_k \middle| a_i \right\rangle \left\langle b_l \middle| a_j \right\rangle \left\langle a_j \middle| b_m \right\rangle \left\langle a_i \middle| b_n \right\rangle V_{ij} \\
&= \frac{1}{2} \sum_{klmn} \hat{b}_k^+ \hat{b}_l^+ \hat{b}_m \hat{b}_n \sum_{ij} \left\langle b_k \right| \left\langle b_l \right| \hat{V} \left| a_j \right\rangle \left| a_i \right\rangle \left\langle a_i \middle| b_n \right\rangle \left\langle a_j \middle| b_m \right\rangle \\
&= \frac{1}{2} \sum_{klmn} \hat{b}_k^+ \hat{b}_l^+ \hat{b}_m \hat{b}_n \sum_{j} \left\langle b_k \right| \left\langle b_l \right| \hat{V} \left| a_j \right\rangle \left\langle a_j \middle| b_m \right\rangle \left| b_n \right\rangle \\
&= \frac{1}{2} \sum_{klmn} \hat{b}_k^+ \hat{b}_l^+ \hat{b}_m \hat{b}_n \left\langle b_k \right| \left\langle b_l \right| \hat{V} \left| b_m \right\rangle \left| b_n \right\rangle
\end{aligned}$$

用到了完备性条件

$$\sum_{ij} \left| a_i \right\rangle \left| a_j \right\rangle \left\langle a_j \right| \left\langle a_i \right| = \sum_i \left| a_i \right\rangle \left\langle a_i \right| = 1 \text{。}$$

表明可加性两粒子算符在两粒子算符的自身表象是二阶张量，在任意表象是四

阶张量。

应用：超出平均场近似，考虑两粒子关联，例如配对相互作用。

3) 单粒子连续谱情形

对于有分离谱的单粒子力学量，$\hat{A}|a_i\rangle = a_i|a_i\rangle$，正交归一和完备性条件为

$$\langle a_i|a_j\rangle = \delta_{ij}, \qquad \sum_i |a_i\rangle\langle a_i| = 1 \ ,$$

产生和消灭算符 $\hat{a}_i, \hat{a}_i^+$ 满足

$$\begin{cases} \left[\hat{a}_i,\ \hat{a}_j\right] = 0 \\ \left[\hat{a}_i^+,\ \hat{a}_j^+\right] = 0 \\ \left[\hat{a}_i,\ \hat{a}_j^+\right] = \delta_{ij} \end{cases} \quad \begin{cases} \left\{\hat{a}_i,\ \hat{a}_j\right\} = 0 \\ \left\{\hat{a}_i^+\ \ \hat{a}_j^+\right\} = \\ \left\{\hat{a}_i,\ \hat{a}_j^+\right\} = \delta_{ij} \end{cases} ,$$

粒子数算符定义为 $\hat{n}_i = \hat{a}_i^+\hat{a}_i$。

对于坐标与自旋的单粒子力学量组 $\left(\hat{\vec{r}},\hat{\sigma}\right)$，本征态 $|\vec{r},\sigma\rangle$ 满足

$$\begin{aligned} &\hat{\vec{r}}|\vec{r},\sigma\rangle = \vec{r}|\vec{r},\sigma\rangle, \qquad \hat{\sigma}|\vec{r},\sigma\rangle = \sigma|\vec{r},\sigma\rangle, \\ &\langle \vec{r}\,',\sigma'|\vec{r}\,'',\sigma''\rangle = \delta\left(\vec{r}\,'-\vec{r}\,''\right)\delta_{\sigma'\sigma''}, \\ &\int d^3\vec{r}\sum_\sigma |\vec{r},\sigma\rangle\langle\vec{r},\sigma| = 1 \end{aligned}$$

消灭产生算符 $\hat{\psi}_\sigma\left(\vec{r}\right)$，$\hat{\psi}_\sigma^+\left(\vec{r}\right)$ 和粒子数算符，

$$\hat{N} = \int d^3\vec{r}\sum_\sigma \hat{n}_\sigma(\vec{r}), \qquad \hat{n}_\sigma(\vec{r}) = \hat{\psi}_\sigma^+(\vec{r})\hat{\psi}_\sigma(\vec{r}) \ ,$$

满足对易关系

$$\begin{cases} \left[\hat{\psi}_{\sigma'}(\vec{r}\,'),\ \hat{\psi}_{\sigma''}(\vec{r}\,'')\right] = 0 \\ \left[\hat{\psi}_{\sigma'}^+(\vec{r}\,'),\ \hat{\psi}_{\sigma''}^+(\vec{r}\,'')\right] = 0 \\ \left[\hat{\psi}_{\sigma'}(\vec{r}\,'),\ \hat{\psi}_{\sigma''}^+(\vec{r}\,'')\right] = \delta\left(\vec{r}\,'-\vec{r}\,''\right)\delta_{\sigma'\sigma''} \end{cases} \quad \begin{cases} \left\{\hat{\psi}_{\sigma'}(\vec{r}\,'),\ \hat{\psi}_{\sigma''}(\vec{r}\,'')\right\} = 0 \\ \left\{\hat{\psi}_{\sigma'}^+(\vec{r}\,'),\ \hat{\psi}_{\sigma''}^+(\vec{r}\,'')\right\} = 0 \\ \left\{\hat{\psi}_{\sigma'}(\vec{r}\,'),\ \hat{\psi}_{\sigma''}^+(\vec{r}\,'')\right\} = \delta\left(\vec{r}\,'-\vec{r}\,''\right)\delta_{\sigma'\sigma''} \end{cases} 。$$

可加性单粒子算符的形式

$$\hat{A} = \sum_{j,k} \hat{b}_j^+ \hat{b}_k \left\langle b_j \middle| \hat{A} \middle| b_k \right\rangle$$

$$\Rightarrow \sum_{\sigma'\sigma''} \int d^3\vec{r}\,' d^3\vec{r}\,'' \hat{\psi}_{\sigma'}^+(\vec{r}\,')\hat{\psi}_{\sigma''}(\vec{r}\,'')\left\langle \vec{r}\,',\sigma' \middle| \hat{A} \middle| \vec{r}\,'',\sigma'' \right\rangle ,$$

可加性两粒子算符（两粒子势）的形式

$$\hat{V} = \frac{1}{2}\sum_{klmn} \hat{b}_k^+ \hat{b}_l^+ \hat{b}_m \hat{b}_n \left\langle b_k \right| \left\langle b_l \middle| \hat{V} \middle| b_m \right\rangle \left| b_n \right\rangle$$

$$\Rightarrow \frac{1}{2}\sum_{\sigma_1\sigma_2\sigma_3\sigma_4} \int d^3\vec{r}_1 d^3\vec{r}_2 d^3\vec{r}_3 d^3\vec{r}_4 \hat{\psi}_{\sigma_1}^+(\vec{r}_1)\hat{\psi}_{\sigma_2}^+(\vec{r}_2)\hat{\psi}_{\sigma_3}(\vec{r}_3)\hat{\psi}_{\sigma_4}(\vec{r}_4)$$

$$\times \left\langle \vec{r}_1,\sigma_1 \right| \left\langle \vec{r}_2,\sigma_2 \middle| \hat{V} \middle| \vec{r}_3,\sigma_3 \right\rangle \left| \vec{r}_4,\sigma_4 \right\rangle$$

3.量子动力学与二次量子化

在 Heisenberg 绘景讨论消灭算符的运动方程

$$i\hbar \frac{d\hat{a}_i}{dt} = \left[\hat{a}_i,\ \hat{H} \right] 。$$

忽略三体和三体以上相互作用，只考虑单粒子与两粒子相互作用，在任意的分离单粒子表象 A，

$$\hat{H} = \hat{H}_0 + \hat{V}$$

$$= \sum_{k,l} \hat{a}_k^+ \hat{a}_l \left\langle a_k \middle| \hat{H}_0 \middle| a_l \right\rangle + \frac{1}{2}\sum_{klmn} \hat{a}_k^+ \hat{a}_l^+ \hat{a}_m \hat{a}_n \left\langle a_k \right| \left\langle a_l \middle| \hat{V} \middle| a_m \right\rangle \left| a_n \right\rangle ,$$

其中 $\hat{H}_0$ 包含了单粒子的动能和在外场中的势能。

$$\left[\hat{a}_i,\ \hat{a}_k^+ \hat{a}_l \right] = \hat{a}_i \hat{a}_k^+ \hat{a}_l - \hat{a}_k^+ \hat{a}_l \hat{a}_i = \hat{a}_i \hat{a}_k^+ \hat{a}_l \mp \hat{a}_k^+ \hat{a}_i \hat{a}_l$$

$$= \hat{a}_i \hat{a}_k^+ \hat{a}_l - \left(\hat{a}_i \hat{a}_k^+ - \delta_{ik} \right) \hat{a}_l = \hat{a}_l \delta_{ik} ,$$

$$\left[\hat{a}_i,\ \hat{a}_k^+\hat{a}_l^+\hat{a}_m\hat{a}_n\right]=\hat{a}_l^+\hat{a}_m\hat{a}_n\delta_{ik}+\hat{a}_k^+\hat{a}_n\hat{a}_m\delta_{il},$$

故

$$i\hbar\frac{d\hat{a}_i}{dt}=\left[\hat{a}_i,\ \hat{\mathrm{H}}\right]$$
$$=\sum_l\hat{a}_l\left\langle a_i\right|\hat{H}_0\left|a_l\right\rangle+\sum_{lmn}\hat{a}_l^+\hat{a}_m\hat{a}_n\left\langle a_i\right|\left\langle a_l\right|\hat{V}\left|a_m\right\rangle\left|a_n\right\rangle\ 。$$

如果选择 A 为 $\hat{V}$ 有确定值的表象，即

$$\hat{V}\left|a_m\right\rangle\left|a_n\right\rangle=V_{mn}\left|a_m\right\rangle\left|a_n\right\rangle\ ,$$

由 $\left|a_i\right\rangle$ 的正交归一化，有

$$i\hbar\frac{d\hat{a}_i}{dt}=\sum_l\left\langle a_i\right|\hat{H}_0\left|a_l\right\rangle\hat{a}_l+\sum_l V_{il}\hat{a}_l^+\hat{a}_l\hat{a}_i\ 。$$

如果表象 A 为连续的坐标自旋表象，有

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}_\sigma(\vec{r},t)=\sum_{\sigma'}\int d^3\vec{r}\,'\left\langle\vec{r},\sigma\right|\hat{H}_0\left|\vec{r}\,',\sigma'\right\rangle\hat{\psi}_{\sigma'}(\vec{r}\,',t)$$
$$+\sum_{\sigma'}\int d^3\vec{r}\,'V(\vec{r},\vec{r}\,')\hat{\psi}_{\sigma'}^+(\vec{r}\,',t)\hat{\psi}_{\sigma'}(\vec{r}\,',t)\hat{\psi}_\sigma(\vec{r},t)\ 。$$

如果 $\hat{H}_0$ 只是坐标和动量的函数，与自旋无关，

$$\left\langle\vec{r},\sigma\right|\hat{H}_0\left|\vec{r}\,',\sigma'\right\rangle=\hat{H}_0\left(\vec{r},-i\hbar\vec{\nabla}\right)\delta\left(\vec{r}-\vec{r}\,'\right)\delta_{\sigma\sigma'}\ ,$$

有

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}_\sigma(\vec{r},t)=\hat{H}_0\left(\vec{r},-i\hbar\vec{\nabla}\right)\hat{\psi}_\sigma(\vec{r},t)$$
$$+\sum_{\sigma'}\int d^3\vec{r}\,'\hat{\psi}_{\sigma'}^+(\vec{r}\,',t)\hat{\psi}_{\sigma'}(\vec{r}\,',t)\hat{\psi}_\sigma(\vec{r},t)V(\vec{r},\vec{r}\,')\ 。$$

$\hat{V}=0$ 时，Heisenberg 绘景中平均场近似下多粒子体系的消灭算符 $\hat{\psi}_\sigma(\vec{r},t)$ 满足的运动方程

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}_\sigma(\vec{r},t)=\hat{H}_0\left(\vec{r},-i\hbar\vec{\nabla}\right)\hat{\psi}_\sigma(\vec{r},t)$$

与 Schroedinger 绘景中单粒子波函数 $\psi_\sigma(\vec{r},t)$ 满足的波动方程

$$i\hbar\frac{\partial}{\partial t}\psi_\sigma(\vec{r},t)=\hat{H}_0\left(\vec{r},-i\hbar\vec{\nabla}\right)\psi_\sigma(\vec{r},t)$$

一致。

可将上面引入 Fock 空间处理多体问题的步骤看成是二次量子化：量子力学将力学量量子化，变成算符，但波函数仍然是经典的函数，进入粒子数表象后，等价于把波函数也量子化了，也变成了算符。