S04E01 Second quantization

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1 The many-particle Hilbert space

$$\mathcal{F} = \mathcal{H}^0 \oplus \mathcal{H}^1 \oplus \mathcal{H}^2 \oplus \mathcal{H}^3 \oplus \cdots$$

We have

$$\begin{aligned}
\Psi &= \Psi^0 + \Psi^1 + \Psi^2 + \Psi^3 + \cdots \\
&= \Psi^0 + C_i|\psi_i\rangle + C_{ij}|\psi_i\rangle|\psi_j\rangle + C_{ijk}|\psi_i\rangle|\psi_j\rangle|\psi_k\rangle + \cdots
\end{aligned}$$

and

$$\begin{aligned}
\mathcal{P}_{12} C_{ij\cdots}|\psi_i\rangle|\psi_j\rangle\cdots &= C_{ij\cdots}|\psi_j\rangle|\psi_i\rangle\cdots \\
&= C_{ji\cdots}|\psi_i\rangle|\psi_j\rangle\cdots
\end{aligned}$$

which means that

$$C_{ji\cdots} = \zeta C_{ij\cdots}$$

Therefore, we define

$$|\psi_i\psi_j\cdots\rangle = \frac{1}{\sqrt{n!}}\sum_{\mathcal{P}} \zeta_{\mathcal{P}}|\psi_{\mathcal{P}i}\rangle|\psi_{\mathcal{P}j}\rangle\cdots$$

which is an over-complete basis of the n-particle Hilbert space.

$$\begin{aligned}
\langle\phi_i\phi_j\cdots|\psi_k\psi_l\cdots\rangle &= \frac{1}{n!}\sum_{\mathcal{P}}\sum_{\mathcal{Q}} \zeta_{\mathcal{P}}\zeta_{\mathcal{Q}}\langle\phi_{\mathcal{P}i}|\psi_{\mathcal{Q}k}\rangle\langle\phi_{\mathcal{P}j}|\psi_{\mathcal{Q}l}\rangle\cdots \\
&= \sum_{\mathcal{R}} \zeta_{\mathcal{R}}\langle\phi_i|\psi_{\mathcal{R}k}\rangle\langle\phi_j|\psi_{\mathcal{R}l}\rangle\cdots \qquad \mathcal{Q} = \mathcal{R}\mathcal{P} \\
&= \det\begin{pmatrix} \langle\phi_i|\psi_k\rangle & \langle\phi_i|\psi_l\rangle & \cdots \\ \langle\phi_j|\psi_k\rangle & \langle\phi_j|\psi_l\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}
\end{aligned}$$

In particular, this means that

$$\langle \psi_i \psi_i \cdots \psi_i \psi_j \psi_j \cdots \psi_j \cdots | \psi_i \psi_i \cdots \psi_i \psi_j \psi_j \cdots \psi_j \cdots \rangle = n_i! n_j! \cdots$$

A natural complete orthonormal basis of the n-particle subspace $\mathcal{H}^n$ is the occupation number basis

$$|n_i n_j \cdots\rangle = \frac{|\psi_i \psi_i \cdots \psi_i \psi_j \psi_j \cdots \psi_j \cdots\rangle}{\sqrt{n_i! n_j! \cdots}}$$

2   Creation and annihilation operators

We define

$$a^\dagger(\psi)|\psi_i \psi_j \cdots\rangle = |\psi \psi_i \psi_j \cdots\rangle$$

such that using

$$\begin{aligned}
\langle \phi_i \phi_j \cdots | a(\psi) | \psi_k \psi_l \cdots\rangle &= \langle \psi_k \psi_l \cdots | a^\dagger(\psi) | \phi_i \phi_j \cdots\rangle^* \\
&= \langle \psi_k \psi_l \cdots | \psi \phi_i \phi_j \cdots\rangle^* \\
&= \langle \psi \phi_i \phi_j \cdots | \psi_k \psi_l \cdots\rangle
\end{aligned}$$

one can prove that

$$a^\dagger(\phi)\, a^\dagger(\psi) - \zeta a^\dagger(\psi)\, a^\dagger(\phi) = 0$$

and its conjugate, as well as

$$a(\phi)\, a^\dagger(\psi) - \zeta a(\psi)\, a^\dagger(\phi) = \langle \phi | \psi \rangle$$

3   Second quantized operators

In the Fock space, n-body operators $\widetilde{\mathcal{O}}_n$ lifted from $\mathcal{O}_n : \mathcal{H}^n \to \mathcal{H}^n$ take the form

$$\widetilde{\mathcal{O}}_n = \widetilde{\mathcal{O}}_n|_{\mathcal{H}^0} \oplus \widetilde{\mathcal{O}}_n|_{\mathcal{H}^1} \oplus \widetilde{\mathcal{O}}_n|_{\mathcal{H}^2} \oplus \widetilde{\mathcal{O}}_n|_{\mathcal{H}^3} \oplus \cdots$$

3.1   One-body operators

are familiar: $\widetilde{\mathcal{O}}_1|_{\mathcal{H}^n}$ is like the total angular momentum of n particles

$$\widetilde{\mathcal{O}}_1|_{\mathcal{H}^n} = \left(\mathcal{O}_1 \otimes 1 \otimes \cdots \otimes 1\right) + \left(1 \otimes \mathcal{O}_1 \otimes \cdots \otimes 1\right) + \cdots + \left(1 \otimes 1 \otimes \cdots \otimes \mathcal{O}_1\right)$$

It is then easy to verify that

$$\widetilde{\mathcal{O}}_1 = \mathcal{O}_{1i} a^\dagger(\psi_i)\, a(\psi_i)$$
$$= \mathcal{O}_{1i} \langle \phi_j | \psi_i \rangle \langle \psi_i | \phi_k \rangle\, a^\dagger(\phi_j)\, a(\phi_k)$$
$$= \langle \phi_j | \mathcal{O}_1 | \phi_k \rangle\, a^\dagger(\phi_j)\, a(\phi_k)$$

3.2 Two-body operators

Notice that we may always write

$$\mathcal{O}_2 = \sum_{I \leq J} C_{IJ} \left[\left(\mathcal{O}_{1I} \otimes \mathcal{O}_{1J} \right) + \left(\mathcal{O}_{1J} \otimes \mathcal{O}_{1I} \right) \right]$$

since the original two-body operator is (always) symmetric under permutation.

For concreteness, take the three-particle Hilbert space as an example,

$$\widetilde{\mathcal{O}}_2|_{\mathcal{H}_3} = C_{IJ} \left[\left(\mathcal{O}_{1I} \otimes \mathcal{O}_{1J} \otimes 1 \right) + \left(\mathcal{O}_{1I} \otimes 1 \otimes \mathcal{O}_{1J} \right) + \left(1 \otimes \mathcal{O}_{1I} \otimes \mathcal{O}_{1J} \right) \right]$$
$$+ C_{IJ} \left[\left(\mathcal{O}_{1J} \otimes \mathcal{O}_{1I} \otimes 1 \right) + \left(\mathcal{O}_{1J} \otimes 1 \otimes \mathcal{O}_{1I} \right) + \left(1 \otimes \mathcal{O}_{1J} \otimes \mathcal{O}_{1I} \right) \right]$$

where we have suppressed the $\sum_{I \leq J}$ symbol. Notice that this can be written as

$$\widetilde{\mathcal{O}}_2|_{\mathcal{H}_3} = C_{IJ} \widetilde{\mathcal{O}}_{1I}|_{\mathcal{H}_3} \widetilde{\mathcal{O}}_{1J}|_{\mathcal{H}_3} - C_{IJ} \widetilde{\mathcal{O}}_{1I} \widetilde{\mathcal{O}}_{1J}|_{\mathcal{H}_3}$$

where

$$\widetilde{\mathcal{O}}_{1I} \widetilde{\mathcal{O}}_{1J}|_{\mathcal{H}_3} = \left(\mathcal{O}_{1I} \mathcal{O}_{1J} \otimes 1 \otimes 1 \right) + \left(1 \otimes \mathcal{O}_{1I} \mathcal{O}_{1J} \otimes 1 \right) + \left(1 \otimes 1 \otimes \mathcal{O}_{1I} \mathcal{O}_{1J} \right)$$

The two-body operator can now be written as

$$\widetilde{\mathcal{O}}_2 = C_{IJ} \langle \phi_i | \mathcal{O}_{1I} | \phi_j \rangle \langle \phi_k | \mathcal{O}_{1J} | \phi_l \rangle\, a^\dagger(\phi_i)\, a(\phi_j)\, a^\dagger(\phi_k)\, a(\phi_l)$$
$$- C_{IJ} \langle \phi_i | \mathcal{O}_{1I} \mathcal{O}_{1J} | \phi_l \rangle\, a^\dagger(\phi_i)\, a(\phi_l)$$
$$= C_{IJ} \langle \phi_i | \mathcal{O}_{1I} | \phi_j \rangle \langle \phi_k | \mathcal{O}_{1J} | \phi_l \rangle\, a^\dagger(\phi_i)\, a(\phi_j)\, a^\dagger(\phi_k)\, a(\phi_l)$$
$$- C_{IJ} \langle \phi_i | \mathcal{O}_{1I} | \phi_j \rangle \langle \phi_k | \mathcal{O}_{1J} | \phi_l \rangle\, a^\dagger(\phi_i)\, a(\phi_l)\, \delta_{jk}$$
$$= C_{IJ} \langle \phi_i | \mathcal{O}_{1I} | \phi_j \rangle \langle \phi_k | \mathcal{O}_{1J} | \phi_l \rangle\, a^\dagger(\phi_i)\, a^\dagger(\phi_k)\, a(\phi_l)\, a(\phi_j)$$
$$= C_{IJ} \langle \phi_k | \mathcal{O}_{1J} | \phi_l \rangle \langle \phi_i | \mathcal{O}_{1I} | \phi_j \rangle\, a^\dagger(\phi_k)\, a^\dagger(\phi_i)\, a(\phi_j)\, a(\phi_l) \qquad \text{as well}$$

and we finally conclude that

$$\widetilde{\mathcal{O}}_2 = \tfrac{1}{2} \langle \phi_i | \langle \phi_k | \mathcal{O}_2 | \phi_j \rangle | \phi_l \rangle\, a^\dagger(\phi_i)\, a^\dagger(\phi_k)\, a(\phi_l)\, a(\phi_j)$$

4 The number operator

is the identity operator $1 : \mathcal{H}^1 \to \mathcal{H}^1$ lifted to the Fock space: $\mathcal{N} = a^\dagger(\phi_i)\, a(\phi_i)$.

5 Quantum statistical mechanics

is governed by

$$\rho = Z^{-1} e^{-\beta \mathcal{H} + \beta \mu \mathcal{N}}$$