

s04E01 Second quantization

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1 The many-particle Hilbert space

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

We have

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

and

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

which means that

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

Therefore, we define

$$|\psi_i \psi_j \dots\rangle = \frac{1}{\sqrt{n!}} \sum_{\mathcal{P}} \zeta_{\mathcal{P}} |\psi_{\mathcal{P}_i}\rangle |\psi_{\mathcal{P}_j}\rangle \dots$$

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

$$\begin{aligned}\langle \phi_i \phi_j \dots | \psi_k \psi_l \dots \rangle &= \frac{1}{n!} \sum_{\mathcal{P}} \sum_{\mathcal{Q}} \zeta_{\mathcal{P}} \zeta_{\mathcal{Q}} \langle \phi_{\mathcal{P}_i} | \psi_{\mathcal{Q}_k} \rangle \langle \phi_{\mathcal{P}_j} | \psi_{\mathcal{Q}_l} \rangle \dots \\ &= \sum_{\mathcal{R}} \zeta_{\mathcal{R}} \langle \phi_i | \psi_{\mathcal{R}_k} \rangle \langle \phi_j | \psi_{\mathcal{R}_l} \rangle \dots \quad \mathcal{Q} = \mathcal{RP} \\ &= \det \begin{pmatrix} \langle \phi_i | \psi_k \rangle & \langle \phi_i | \psi_l \rangle & \dots \\ \langle \phi_j | \psi_k \rangle & \langle \phi_j | \psi_l \rangle & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}\end{aligned}$$

In particular, we have

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

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

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

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 $\tilde{\mathcal{O}}_n$ lifted from $\mathcal{O}_n : \mathcal{H}^n \rightarrow \mathcal{H}^n$ take the form

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

3.1 One-body operators

are familiar: their restrictions are like the total angular momentum operator of n particles, namely

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

It is then easy to verify that

$$\begin{aligned}
\tilde{\mathcal{O}}_1 &= \mathcal{O}_{1i} a^\dagger(\psi_i) a(\psi_i) \\
&= \mathcal{O}_{1i} \langle \phi_j | \psi_i \rangle \langle \psi_i | \phi_k \rangle a^\dagger(\phi_j) a(\phi_k) \\
&= \langle \phi_j | \mathcal{O}_1 | \phi_k \rangle a^\dagger(\phi_j) a(\phi_k)
\end{aligned}$$

3.2 Two-body operators

Notice that we may always write

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

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

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

$$\begin{aligned}
\tilde{\mathcal{O}}_2|_{\mathcal{H}_3} &= C_{IJ} [(\mathcal{O}_{1I} \otimes \mathcal{O}_{1J} \otimes 1) + (\mathcal{O}_{1I} \otimes 1 \otimes \mathcal{O}_{1J}) + (1 \otimes \mathcal{O}_{1I} \otimes \mathcal{O}_{1J})] \\
&\quad + C_{IJ} [(\mathcal{O}_{1J} \otimes \mathcal{O}_{1I} \otimes 1) + (\mathcal{O}_{1J} \otimes 1 \otimes \mathcal{O}_{1I}) + (1 \otimes \mathcal{O}_{1J} \otimes \mathcal{O}_{1I})]
\end{aligned}$$

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

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

where

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

The two-body operator can now be written as

$$\begin{aligned}
\tilde{\mathcal{O}}_2 &= C_{IJ} \langle \phi_i | \mathcal{O}_{1I} | \phi_j \rangle \langle \phi_k | \mathcal{O}_{1J} | \phi_l \rangle a^\dagger(\phi_i) a(\phi_j) a^\dagger(\phi_k) a(\phi_l) \\
&\quad - C_{IJ} \langle \phi_i | \mathcal{O}_{1I} \mathcal{O}_{1J} | \phi_l \rangle a^\dagger(\phi_i) a(\phi_l) \\
&= C_{IJ} \langle \phi_i | \mathcal{O}_{1I} | \phi_j \rangle \langle \phi_k | \mathcal{O}_{1J} | \phi_l \rangle a^\dagger(\phi_i) a(\phi_j) a^\dagger(\phi_k) a(\phi_l) \\
&\quad - C_{IJ} \langle \phi_i | \mathcal{O}_{1I} | \phi_j \rangle \langle \phi_k | \mathcal{O}_{1J} | \phi_l \rangle a^\dagger(\phi_i) a(\phi_l) \delta_{jk} \\
&= C_{IJ} \langle \phi_i | \mathcal{O}_{1I} | \phi_j \rangle \langle \phi_k | \mathcal{O}_{1J} | \phi_l \rangle a^\dagger(\phi_i) a^\dagger(\phi_k) a(\phi_l) a(\phi_j) \quad \text{or} \\
&= C_{IJ} \langle \phi_k | \mathcal{O}_{1J} | \phi_l \rangle \langle \phi_i | \mathcal{O}_{1I} | \phi_j \rangle a^\dagger(\phi_k) a^\dagger(\phi_i) a(\phi_j) a(\phi_l) \quad \text{as well}
\end{aligned}$$

and we finally conclude that

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

4 The number operator

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

5 Quantum statistical mechanics

is governed by

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