Quantum Operators in the Fock Space and Wave Function Languages

A quantum operator acting on identical bosons can be described in terms of N–particle wave functions (the *first-quantized* formalism) or in terms of the creation and annihilation operators in the Fock space (the *second-quantized* formalism). In these notes I explain how to translate between the two formalisms.

The Fock space formalism is explained in my notes on free fields, harmonic oscillators, and identical bosons. On pages 8–12 of those notes, I define the bosonic Fock space as the Hilbert space of states containing arbitrary numbers of identical bosons,

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{H}(N \text{ identical bosons}), \tag{1}$$

then, starting with an arbitrary basis of one-particle states $|\alpha\rangle$ I build the occupation-number basis $|\{n_\alpha\}\rangle$ for the whole Fock space, and eventually define the creation operators and the annihilation operators in terms of that occupation number basis,

$$\begin{aligned} \hat{a}^\dagger_\alpha \left|\{n_\beta\}\right\rangle &\stackrel{\text{def}}{=} \sqrt{n_\alpha + 1}\,\left|\{n'_\beta = n_\beta + \delta_{\alpha\beta}\}\right\rangle, \\ \hat{a}_\alpha \left|\{n_\beta\}\right\rangle &\stackrel{\text{def}}{=} \begin{cases} \sqrt{n_\alpha}\,\left|\{n'_\beta = n_\beta - \delta_{\alpha\beta}\}\right\rangle & \text{for } n_\alpha > 0, \\ 0 & \text{for } n_\alpha = 0. \end{cases} \end{aligned} \tag{2}$$

In the present notes, I shall start by translating these definition to the language of N–boson wave function. And then I shall use the wave-function definitions of the $\hat{a}^\dagger_\alpha$ and $\hat{a}_\alpha$ operators to translate the more complicated one-body, two-body, *etc.*, operators between the Fock-space and the wave-function languages.

Creation and Annihilation Operators in the Wave Function Language

First, a quick note on multi-boson wave functions. A wave function of an N–particle state depends on all N particles' positions, $\psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$, where by abuse of notations each $\mathbf{x}_i$ includes all the independent degrees of freedom of the i^{th} particle,

$$\mathbf{x}_i \;=\; (x_i, y_i, z_i, \text{spin}_i, \text{isospin}_i, \ldots).$$

Moreover, the wave function must be totally symmetric WRT any permutations of the identical bosons,

$$\psi(\text{any permutation of the } \mathbf{x}_1, \ldots, \mathbf{x}_N) \;=\; \psi(\mathbf{x}_1, \ldots, \mathbf{x}_N). \tag{3}$$

This Bose symmetry plays essential role in the wave-function-language action of the creation and annihilation operators.

Definitions: Let the $\phi_\alpha(\mathbf{x})$ be the wave function of the one-particle states α which we want to be created by the $\hat{a}^\dagger_\alpha$ operators and annihilated by the $\hat{a}_\alpha$ operators. Then, *given an N–boson state $|N, \psi\rangle$ with a totally symmetric wave function $\psi(\mathbf{x}_1, \ldots, \mathbf{x}_1)$, we construct the totally symmetric wave functions $\psi'(\mathbf{x}_1, \ldots, \mathbf{x}_{N+1})$ and $\psi''(\mathbf{x}_1, \ldots, \mathbf{x}_{N-1})$ of the $(N+1)$–boson state $|N+1, \psi'\rangle = \hat{a}^\dagger_\alpha |N, \psi\rangle$ and the $(N-1)$–boson state $|N-1, \psi''\rangle = \hat{a}_\alpha |N, \psi\rangle$ according to:*

$$\psi'(\mathbf{x}_1, \ldots, \mathbf{x}_{N+1}) \;=\; \frac{1}{\sqrt{N+1}} \sum_{i=1}^{N+1} \phi_\alpha(\mathbf{x}_i) \times \psi(\mathbf{x}_1, \ldots, \cancel{\mathbf{x}_i}, \ldots, \mathbf{x}_{N+1}), \tag{4}$$

$$\psi''(\mathbf{x}_1, \ldots, \mathbf{x}_{N-1}) \;=\; \sqrt{N} \int d^3\mathbf{x}_N \, \phi^*_\alpha(\mathbf{x}_N) \times \psi(\mathbf{x}_1, \ldots, \mathbf{x}_{N-1}, \mathbf{x}_N). \tag{5}$$

In particular, for $N = 0$ the state $\hat{a}^\dagger_\alpha |0\rangle$ has $\psi'(x_1) = \phi_\alpha(x_1)$, while for $N = 1$ the state $\hat{a}_\alpha |\beta\rangle$ has $\psi''(\text{no arguments}) = \langle \phi_\alpha | \psi \rangle$. Also, for $N = 0$ we simply define $\hat{a}_\alpha |0\rangle \stackrel{\text{def}}{=} 0$.

Let me use eqs. (4) and (5) as *definitions* of the creation operators $\hat{a}^\dagger_\alpha$ and the annihilation operators $\hat{a}_\alpha$. To verify that these definitions are completely equivalent to the definitions (2) in terms of the occupation-number basis, I am going to prove the following lemmas:

Lemma 1: The creation operators $\hat{a}^\dagger_\alpha$ defined according to eq. (4) are indeed the hermitian conjugates of the operators $\hat{a}_\alpha$ defined according to eq. (5).

Lemma 2: The operators (4) and (5) obey the bosonic commutation relations

$$[\hat{a}_\alpha, \hat{a}_\beta] \;=\; 0, \qquad [\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta] \;=\; 0, \qquad [\hat{a}_\alpha, \hat{a}^\dagger_\beta] \;=\; \delta_{\alpha\beta}\,. \tag{6}$$

Lemma 3: Let $\phi_{\alpha\beta\cdots\omega}(\mathbf{x}_1, \mathbf{x}_2 \ldots, \mathbf{x}_N)$ be the N–boson wave function of the state

$$|\alpha, \beta, \cdots, \omega\rangle \;=\; \frac{1}{\sqrt{T}}\, \hat{a}^\dagger_\omega \cdots \hat{a}^\dagger_\beta \hat{a}^\dagger_\alpha\, |0\rangle \tag{7}$$

where the creation operators $\hat{a}^\dagger_\alpha$ act according to eq. (4) while T is the number of trivial permutations between *coincident* entries of the list $(\alpha, \beta, \ldots, \omega)$ (for example, $\alpha \leftrightarrow \beta$ when α and β happen to be equal). In terms of the occupation numbers n_γ, $T = \prod_\gamma n_\gamma!$. Then

$$\begin{aligned}
\phi_{\alpha\beta\cdots\omega}(\mathbf{x}_1, \mathbf{x}_2 \ldots, \mathbf{x}_N) \;&=\; \frac{1}{\sqrt{D}} \sum_{(\tilde{\alpha},\tilde{\beta},\ldots,\tilde{\omega})}^{\substack{\text{distinct permutations}\\ \text{of } (\alpha,\beta,\ldots,\omega)}} \phi_{\tilde{\alpha}}(\mathbf{x}_1) \times \phi_{\tilde{\beta}}(\mathbf{x}_2) \times \cdots \times \phi_{\tilde{\omega}}(\mathbf{x}_N) \\
&=\; \frac{1}{\sqrt{T \times N!}} \sum_{(\tilde{\alpha},\tilde{\beta},\ldots,\tilde{\omega})}^{\substack{\text{all } N! \text{ permutations}\\ \text{of } (\alpha,\beta,\ldots,\omega)}} \phi_{\tilde{\alpha}}(\mathbf{x}_1) \times \phi_{\tilde{\beta}}(\mathbf{x}_2) \times \cdots \times \phi_{\tilde{\omega}}(\mathbf{x}_N),
\end{aligned} \tag{8}$$

where $D = N!/T$ is the number of *distinct permutations*. In other words, the state (7) is precisely the symmetrized state of N bosons in individual states $|\alpha\rangle\,,\ |\beta\rangle\,,\ \ldots,\ |\omega\rangle$.

Together, the lemmas 1–3 establish that the definitions (4) and (5) of the creation and annihilation operators completely agree with the definitions (2)of the same operators in terms of the occupation number basis.

Proof of Lemma 1: To prove that the operators $\hat{a}^\dagger_\alpha$ and $\hat{a}_\alpha$ are hermitian conjugates of each other, we need to compare their matrix elements and verify that for any two states $|N,\psi\rangle$ and $|\widetilde{N},\widetilde{\psi}\rangle$ in the Fock space we have

$$\langle\widetilde{N},\widetilde{\psi}|\,\hat{a}_\alpha\,|N,\psi\rangle \;=\; \langle N,\psi|\,\hat{a}^\dagger_\alpha\,|\widetilde{N},\widetilde{\psi}\rangle^*. \tag{9}$$

Since the $\hat{a}_\alpha$ always lowers the number of particles by 1 while the $\hat{a}^\dagger_\alpha$ always raises it by 1, it is enough to check this equation for $\widetilde{N}=N-1$ — otherwise, we get automatic zero on both sides of this equation.

Let $\psi''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})$ be the wave function of the state $|N-1,\psi''\rangle=\hat{a}_\alpha\,|N,\Psi\rangle$ according to eq. (5). Then, on the LHS of eq. (9) we have

$$\begin{aligned}
\langle N-1,\widetilde{\psi}|\,\hat{a}_\alpha\,|N,\psi\rangle \;&=\; \big\langle N-1,\widetilde{\psi}\big|N-1,\psi''\big\rangle\\
&= \int\! d^3\mathbf{x}_1\;\cdots\int\! d^3\mathbf{x}_{N-1}\,\widetilde{\psi}^*(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\times\psi''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\\
&= \int\! d^3\mathbf{x}_1\;\cdots\int\! d^3\mathbf{x}_{N-1}\,\widetilde{\psi}^*(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\times\\
&\qquad\qquad\times\sqrt{N}\int\! d^3\mathbf{x}_N\,\phi^*_\alpha\times\psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)\\
&=\; \sqrt{N}\!\int\! d^3\mathbf{x}_1\;\cdots\int\! d^3\mathbf{x}_N\,\widetilde{\psi}^*(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\times\phi^*_\alpha(\mathbf{x}_N)\times\psi(\mathbf{x}_1,\ldots,\mathbf{x}_N).
\end{aligned}\tag{10}$$

Likewise, let $\widetilde{\psi}'(\mathbf{x}_1,\ldots,\mathbf{x}_N)$ be the wave function of the state $\big|N,\widetilde{\psi}'\big\rangle=\hat{a}^\dagger_\alpha\,|N-1,\widetilde{\psi}\rangle$ according to eq. (4). Then the matrix element on the RHS of eq. (9) becomes

$$\begin{aligned}
\langle N,\psi|\,\hat{a}^\dagger_\alpha\,|N-1,\widetilde{\psi}\rangle \;&=\int\! d^3\mathbf{x}_1\;\cdots\int\! d^3\mathbf{x}_N\,\psi^*(\mathbf{x}_1,\ldots,\mathbf{x}_N)\times\widetilde{\psi}'(\mathbf{x}_1,\ldots,\mathbf{x}_N)\\
&=\int\! d^3\mathbf{x}_1\;\cdots\int\! d^3\mathbf{x}_N\,\psi^*(\mathbf{x}_1,\ldots,\mathbf{x}_N)\times\\
&\qquad\qquad\times\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\phi_\alpha(\mathbf{x}_i)\times\widetilde{\psi}(\mathbf{x}_1,\ldots\,\cancel{\mathbf{x}_i},\ldots,\mathbf{x}_N)\\
&=\;\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\int\! d^3\mathbf{x}_1\;\cdots\int\! d^3\mathbf{x}_N\,\psi^*(\mathbf{x}_1,\ldots,\mathbf{x}_N)\times\\
&\qquad\qquad\times\phi_\alpha(\mathbf{x}_i)\times\widetilde{\psi}(\mathbf{x}_1,\ldots\,\cancel{\mathbf{x}_i},\ldots,\mathbf{x}_N).
\end{aligned}\tag{11}$$

By bosonic symmetry of the wavefunctions ψ and $\widetilde{\psi}$, all terms in the sum on the RHS are equal to each other. So, we may replace the summation with a single term — say, for $i = N$ — and multiply by N, thus

$$\langle N, \psi | \, \hat{a}^\dagger_\alpha \, | N-1, \widetilde{\psi} \rangle \;=\; \frac{N}{\sqrt{N}} \times \int d^3\mathbf{x}_1 \, \cdots \int d^3\mathbf{x}_N \, \psi^*(\mathbf{x}_1, \ldots, \mathbf{x}_N) \times \phi_\alpha(\mathbf{x}_N) \times \widetilde{\psi}(\mathbf{x}_1, \ldots \mathbf{x}_{N-1}). \tag{12}$$

By inspection, the RHS of eqs. (10) and (12) are complex conjugates of each other, thus

$$\langle N-1, \widetilde{\psi} | \, \hat{a}_\alpha \, | N, \psi \rangle \;=\; \langle N, \psi | \, \hat{a}^\dagger_\alpha \, | N-1, \widetilde{\psi} \rangle^* . \tag{9}$$

This completes the proof of Lemma 1.

Proof of Lemma 2: Let's start by verifying that the creation operators defined according to eq. (4) commute with each other. Pick any two such creation operators $\hat{a}^\dagger_\alpha$ and $\hat{a}^\dagger_\beta$, and pick any N-boson state $|N, \psi\rangle$. Consider the $(N+2)$-boson wavefunction $\psi'''(\mathbf{x}_1, \ldots, \mathbf{x}_{N+2})$ of the state $|N+2, \psi'''\rangle = \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \, |N, \psi\rangle$. Applying eq. (4) twice, we immediately obtain

$$\psi'''(\mathbf{x}_1, \ldots, \mathbf{x}_{N+2}) \;=\; \frac{1}{\sqrt{(N+1)(N+2)}} \sum_{\substack{i,j=1,\ldots,N+2 \\ i \neq j}} \begin{aligned} &\phi_\alpha(\mathbf{x}_i) \times \phi_\beta(\mathbf{x}_j) \times \\ &\qquad \times \psi(\mathbf{x}_1, \ldots, \mathbf{x}_{N+2} \text{ except } \mathbf{x}_i, \mathbf{x}_j). \end{aligned} \tag{13}$$

On the RHS of this formula, interchanging $\alpha \leftrightarrow \beta$ is equivalent to interchanging the summation indices $i \leftrightarrow j$ — which has no effect on the sum. Consequently, the states $\hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \, |N, \psi\rangle$ and $\hat{a}^\dagger_\beta \hat{a}^\dagger_\alpha \, |N, \psi\rangle$ have the same wavefunction (13), thus

$$\hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \, |N, \psi\rangle \;=\; \hat{a}^\dagger_\beta \hat{a}^\dagger_\alpha \, |N, \psi\rangle . \tag{14}$$

Since this is true for any N and any totally-symmetric wave function ψ, this means that the creation operators $\hat{a}^\dagger_\alpha$ and $\hat{a}^\dagger_\beta$ commute with each other.

Next, let's pick any two annihilation operators $\hat{a}_\alpha$ and $\hat{a}_\beta$ *defined according to eq.* (5) and show that they commute with each other. Again, let $|N, \psi\rangle$ be an arbitrary N-boson state . For $N < 2$ we have

$$\hat{a}_\alpha \hat{a}_\beta \left|N, \psi\right\rangle \;=\; 0 \;=\; \hat{a}_\beta \hat{a}_\alpha^\dagger \left|N, \psi\right\rangle , \tag{15}$$

so let's focus on the non-trivial case of $N \geq 2$ and consider the $(N-2)$-boson wavefunction ψ'''' of the state $|N-2, \psi''''\rangle = \hat{a}_\alpha \hat{a}_\beta \left|N, \psi\right\rangle$. Applying eq. (5) twice, we obtain

$$\psi''''(\mathbf{x}_1, \ldots, \mathbf{x}_{N-2}) \;=\; \sqrt{N(N-1)} \int\! d^3\mathbf{x}_N \int\! d^3\mathbf{x}_{N-1} \begin{array}{l} \phi^*_\alpha(\mathbf{x}_N) \times \phi^*_\beta(\mathbf{x}_{N-1}) \times \\ \qquad\qquad \times\, \psi(\mathbf{x}_1, \ldots, \mathbf{x}_{N-2}, \mathbf{x}_{N-1}, \mathbf{x}_N). \end{array} \tag{16}$$

On the RHS of this formula, interchanging $\alpha \leftrightarrow \beta$ is equivalent to interchanging the integrated-over positions of the N^{th} and the $(N-1)^{\text{th}}$ boson in the original state $|N, \psi\rangle$. Thanks to bosonic symmetry of the wave-function ψ, this interchange has no effect, thus

$$\hat{a}_\alpha \hat{a}_\beta \left|N, \psi\right\rangle \;=\; \hat{a}_\beta \hat{a}_\alpha \left|N, \psi\right\rangle . \tag{17}$$

Therefore, when the annihilation operators defined according to eq. (5) act on the totally-symmetric wave functions of identical bosons, they commute with each other.

Finally, let's pick a creation operator $\hat{a}^\dagger_\beta$ and an annihilation operator $\hat{a}_\alpha$, pick an arbitrary N-boson state $|N, \psi\rangle$, and consider the difference between the states

$$\left|N, \psi^5\right\rangle \;=\; \hat{a}^\dagger_\beta \hat{a}_\alpha \left|N, \psi\right\rangle \quad \text{and} \quad \left|N, \psi^6\right\rangle \;=\; \hat{a}_\alpha \hat{a}^\dagger_\beta \left|N, \psi\right\rangle . \tag{18}$$

Suppose $N > 0$. Applying eq. (5) to the wave function ψ and then applying eq. (4) to the result, we obtain

$$\begin{aligned} \psi^5(\mathbf{x}_1, \ldots, \mathbf{x}_N) \;&=\; \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \phi_\beta(\mathbf{x}_i) \times \psi''(\mathbf{x}_1, \ldots, \cancel{\mathbf{x}_i}, \ldots, \mathbf{x}_N) \\ &=\; \sum_{i=1}^{N} \phi_\beta(\mathbf{x}_i) \times \int\! d^3\mathbf{x}_{N+1}\, \phi^*_\alpha(\mathbf{x}_{N+1}) \times \psi(\mathbf{x}_1, \ldots, \cancel{\mathbf{x}_i}, \ldots, \mathbf{x}_N, \mathbf{x}_{N+1}). \end{aligned} \tag{19}$$

On the other hand, applying first eq. (4) and then eq. (5), we arrive at

$$\begin{aligned}
\psi^6(\mathbf{x}_1,\ldots,\mathbf{x}_N) \;&=\; \sqrt{N+1}\int\! d^3\mathbf{x}_{N+1}\,\phi^*_\alpha(\mathbf{x}_{N+1})\times\psi'(\mathbf{x}_1,\ldots,\mathbf{x}_N,\mathbf{x}_{N+1})\\
&=\int\! d^3\mathbf{x}_{N+1}\,\phi^*_\alpha(\mathbf{x}_{N+1})\times\sum_{i=1}^{N+1}\phi_\beta(\mathbf{x}_i)\times\psi(\mathbf{x}_1,\ldots,\cancel{\mathbf{x}_i},\ldots,\mathbf{x}_{N+1})\\
&=\int\! d^3\mathbf{x}_{N+1}\,\phi^*_\alpha(\mathbf{x}_{N+1})\times\left(\begin{array}{l}\displaystyle\sum_{i=1}^{N}\phi_\beta(\mathbf{x}_i)\times\psi(\mathbf{x}_1,\ldots,\cancel{\mathbf{x}_i},\ldots,\mathbf{x}_N,\mathbf{x}_{N+1})\\ \qquad+\;\phi_\beta(\mathbf{x}_{N+1})\times\psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)\end{array}\right)\\
&=\sum_{i=1}^{N}\phi_\beta(\mathbf{x}_i)\times\int\! d^3\mathbf{x}_{N+1}\,\phi^*_\alpha(\mathbf{x}_{N+1})\times\psi(\mathbf{x}_1,\ldots,\cancel{\mathbf{x}_i},\ldots,\mathbf{x}_N,\mathbf{x}_{N+1})\\
&\qquad+\;\psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)\times\int\! d^3\mathbf{x}_{N+1}\,\phi^*_\alpha(\mathbf{x}_{N+1})\times\phi_\beta(\mathbf{x}_{N+1})\\
&=\;\psi^5(\mathbf{x}_1,\ldots,\mathbf{x}_N)\qquad\langle\!\langle\,\text{compare to eq. (19)}\,\rangle\!\rangle\\
&\qquad+\;\psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)\times\big\langle\phi_\alpha\big|\phi_\beta\big\rangle\,.
\end{aligned}\tag{20}$$

Comparing eqs. (19) and (20), we see that

$$\psi^6(\mathbf{x}_1,\ldots,\mathbf{x}_N)-\psi^5(\mathbf{x}_1,\ldots,\mathbf{x}_N)\;=\;\psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)\times\big\langle\phi_\alpha\big|\phi_\beta\big\rangle\;=\;\psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)\times\delta_{\alpha\beta}\,,\tag{21}$$

where $\big\langle\phi_\alpha\big|\phi_\beta\big\rangle=\delta_{\alpha\beta}$ by orthonormality of the 1-particle basis $\{\phi_\gamma(\mathbf{x})\}_\gamma$. In Dirac notations, eq. (21) amounts to

$$\big(\hat a_\alpha\hat a^\dagger_\beta-\hat a^\dagger_\beta\hat a_\alpha\big)\,|N,\psi\rangle\;=\;|N,\psi\rangle\times\delta_{\alpha\beta}\,.\tag{22}$$

Thus far, we have checked this formula for all bosonic states $|N,\psi\rangle$ except for the vacuum $|0\rangle$. To complete the proof, note that

$$\hat a_\alpha\,|0\rangle\;=\;0\quad\Longrightarrow\quad\hat a^\dagger_\beta\hat a_\alpha\,|0\rangle\;=\;0,\tag{23}$$

while

$$\hat a_\alpha\hat a^\dagger_\beta\,|0\rangle\;=\;\hat a_\alpha\,\big|1,\phi_\beta\big\rangle\;=\;\big\langle\phi_\alpha\big|\phi_\beta\big\rangle\times|0\rangle\;=\;\delta_{\alpha\beta}\times|0\rangle\,,\tag{24}$$

hence

$$\left(\hat{a}_\alpha \hat{a}^\dagger_\beta - \hat{a}^\dagger_\beta \hat{a}_\alpha\right)|0\rangle \;=\; \delta_{\alpha\beta} \times |0\rangle\,. \tag{25}$$

Altogether, eqs. (22) and (25) verify that

$$[\hat{a}_\alpha, \hat{a}^\dagger_\beta]\,|\Psi\rangle \;=\; \delta_{\alpha\beta}\Psi \tag{26}$$

for any state Ψ in the bosonic Fock space, hence the operators $\hat{a}_\alpha$ and $\hat{a}^\dagger_\beta$ defined according to eqs. (4) and (5) indeed obey the commutation relation $[\hat{a}_\alpha, \hat{a}^\dagger_\beta] = \delta_{\alpha,\beta}$.

This completes the proof of Lemma 2.

Proof of Lemma 3: Let me start with a note on the normalization factor $1/\sqrt{T}$ in eq. (7). We need this factor to properly normalize the multi-boson states in which some bosons may be in the same 1-particle mode. For example, for the two particle states,

$$|\alpha,\beta\rangle \;=\; \hat{a}^\dagger_\beta \hat{a}^\dagger_\alpha\,|0\rangle \quad \text{when } \alpha \neq \beta, \quad \text{but} \quad |\alpha,\alpha\rangle \;=\; \frac{1}{\sqrt{2}}\,\hat{a}^\dagger_\alpha \hat{a}^\dagger_\alpha\,|0\rangle\,. \tag{27}$$

In terms of the occupation numbers, the properly normalized states are

$$|\{n_\alpha\}_\alpha\rangle \;=\; \bigotimes_\alpha \left(|n_\alpha\rangle \;=\; \frac{\left(\hat{a}^\dagger_\alpha\right)^{n_\alpha}}{\sqrt{n_\alpha!}}\,|0\rangle\right)_{\text{mode }\alpha} \;=\; \left(\prod_\alpha \frac{\left(\hat{a}^\dagger_\alpha\right)^{n_\alpha}}{\sqrt{n_\alpha!}}\right)|\text{vacuum}\rangle\,. \tag{28}$$

hence the factor $1/\sqrt{T}$ in eq. (7).

Now let's work out the wave functions of the states (7) by successively applying the creation operators according to eq. (4):

1. For $N = 1$, states $|\alpha\rangle = \hat{a}^\dagger_\alpha\,|0\rangle$ have wave functions $\phi_\alpha(\mathbf{x})$.
2. For $N = 2$, states $\sqrt{T}\,|\alpha,\beta\rangle = \hat{a}^\dagger_\beta \hat{a}^\dagger_\alpha\,|0\rangle$ have wavefunctions

$$\sqrt{T} \times \phi_{\alpha\beta}(\mathbf{x}_1,\mathbf{x}_2) \;=\; \frac{1}{\sqrt{2}}\Big(\phi_\beta(\mathbf{x}_1)\phi_\alpha(\mathbf{x}_2) \;+\; \phi_\beta(\mathbf{x}_2)\phi_\alpha(\mathbf{x}_1)\Big). \tag{29}$$

3. For $N = 3$, states $\sqrt{T}\,|\alpha,\beta,\gamma\rangle = \hat{a}^\dagger_\gamma \hat{a}^\dagger_\beta \hat{a}^\dagger_\alpha\,|0\rangle$ have

$$\begin{aligned}
\sqrt{T} \times \phi_{\alpha\beta\gamma}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3) \;&=\; \frac{1}{\sqrt{3}} \begin{pmatrix} \phi_\gamma(\mathbf{x}_1) \times \frac{1}{\sqrt{2}}\big(\phi_\beta(\mathbf{x}_2)\phi_\alpha(\mathbf{x}_3) - \phi_\beta(\mathbf{x}_3)\phi_\alpha(\mathbf{x}_2)\big) \\ +\ \phi_\gamma(\mathbf{x}_2) \times \frac{1}{\sqrt{2}}\big(\phi_\beta(\mathbf{x}_1)\phi_\alpha(\mathbf{x}_3) - \phi_\beta(\mathbf{x}_3)\phi_\alpha(\mathbf{x}_1)\big) \\ +\ \phi_\gamma(\mathbf{x}_3) \times \frac{1}{\sqrt{2}}\big(\phi_\beta(\mathbf{x}_1)\phi_\alpha(\mathbf{x}_2) - \phi_\beta(\mathbf{x}_2)\phi_\alpha(\mathbf{x}_1)\big) \end{pmatrix} \\
&=\; \frac{1}{\sqrt{3!}} \sum_{(\tilde{\mathbf{x}}_1,\tilde{\mathbf{x}}_2,\tilde{\mathbf{x}}_3)}^{\substack{\text{6 permutations}\\ \text{of } (\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)}} \phi_\gamma(\tilde{\mathbf{x}}_1)\phi_\beta(\tilde{\mathbf{x}}_2)\phi_\alpha(\tilde{\mathbf{x}}_3) \\
&=\; \frac{1}{\sqrt{3!}} \sum_{(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})}^{\substack{\text{6 permutations}\\ \text{of } (\alpha,\beta,\gamma)}} \phi_{\tilde{\alpha}}(\mathbf{x}_1)\phi_{\tilde{\beta}}(\mathbf{x}_2)\phi_{\tilde{\gamma}}(\mathbf{x}_3).
\end{aligned} \tag{30}$$

Proceeding in this fashion, acting with a product of N creation operators on the vacuum we obtain a totally symmetrized product of the 1-particle wave functions $\phi_\alpha(\mathbf{x})$ through $\phi_\omega(\mathbf{x})$. Extrapolating from eq.(30), the N-particle state $\sqrt{T}\,|\alpha,\ldots,\omega\rangle = \hat{a}^\dagger_\omega \cdots \hat{a}^\dagger_\alpha\,|0\rangle$, has the totally-symmetrized wave function

$$\sqrt{T} \times \phi_{\alpha\cdots\omega}(\mathbf{x}_1,\ldots,\mathbf{x}_N) \;=\; \frac{1}{\sqrt{N!}} \sum_{(\tilde{\alpha},\ldots,\tilde{\omega})}^{\substack{\text{all permutations}\\ \text{of } (\alpha,\ldots,\omega)}} \phi_{\tilde{\alpha}}(\mathbf{x}_1) \times \cdots \times \phi_{\tilde{\omega}}(\mathbf{x}_N). \tag{31}$$

Dividing both sides of this formula by the $\sqrt{T}$ factor, we immediately arrive at the second line of eq. (8).

Finally, the top line of eq. (8) obtains from the bottom line by adding up coincident terms. Indeed, if some one-particle states appear multiple times in the list $(\alpha,\ldots,\omega)$, then permuting coincident entries of this list has no effect. Altogether, there T such trivial permutations. By group theory, this means that out of $N!$ possible permutations of the list, there are only $D = N!/T$ *distinct* permutations. But for each distinct permutations, there are T coincident terms in the sum on the bottom line of eq. (8). Adding them up gives us the top line of eq. (8).

This completes the proof of Lemma 3.

Altogether, the three lemmas verify that the operators $\hat{a}_\alpha^\dagger$ and $\hat{a}_\alpha$ defined according to eqs. (4) and (5) are indeed the creation and the annihilation operators in the bosonic Fock space.

One-body and Two-body Operators in the Wave Function and the Fock Space Languages

The one-body operators are the additive operators acting on one particle at a time, for example the net momentum or net kinetic energy of several bosons. In the wave-function language (AKA, the first-quantized formalism), such operators act on N–particle states according to

$$\hat{A}_{\rm net}^{(1)} = \sum_{i=1}^{N} \hat{A}(i^{\rm th}\,\text{particle}) \tag{32}$$

where $\hat{A}$ is some kind of a single-particle operator. For example,

$$\text{the net momentum operator} \quad \hat{\mathbf{P}}_{\rm net}^{(1)} = \sum_{i=1}^{N} \hat{\mathbf{p}}_i\,, \tag{33}$$

$$\text{the net kinetic energy operator} \quad \hat{K}_{\rm net}^{(1)} = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m}\,, \tag{34}$$

$$\text{the net potential energy operator} \quad \hat{V}_{\rm net}^{(1)} = \sum_{i=1}^{N} V(\hat{\mathbf{x}}_i). \tag{35}$$

In the Fock space language (AKA, the second-quantized formalism), such net one-body operators take form

$$\hat{A}_{\rm net}^{(2)} = \sum_{\alpha,\beta} \langle\alpha|\,\hat{A}\,|\beta\rangle \times \hat{a}_\alpha^\dagger \hat{a}_\beta \tag{36}$$

where the matrix elements $A_{\alpha,\beta} = \langle\alpha|\,\hat{A}\,|\beta\rangle$ are taken in the one-particle Hilbert space.

Theorem 1: *Although eqs.* (32) *and* (36) *look very different from each other, they describe exactly the same net one-body operator.*

Proof: To establish the equality between the operators (32) and (36), we are going to verify that they have exactly the same matrix elements between any N–boson states $\langle N, \widetilde{\psi}|$ and $|N, \psi\rangle$,

$$\langle N, \widetilde{\psi}|\, \hat{A}^{(1)}_{\text{net}}\, |N, \psi\rangle \;=\; \langle N, \widetilde{\psi}|\, \hat{A}^{(2)}_{\text{net}}\, |N, \psi\rangle\,. \tag{37}$$

Let's start by relating the matrix elements on the LHS of this formula to the $A_{\alpha,\beta} = \langle\alpha|\, \hat{A}\, |\beta\rangle$. For $N = 1$ the relation is very simple: Since the states $|\alpha\rangle$ make a complete basis of the 1-particle Hilbert space, for any 1-particle states $\langle\widetilde{\psi}|$ and $|\psi\rangle$

$$\langle\widetilde{\psi}|\, \hat{A}\, |\psi\rangle \;=\; \sum_{\alpha,\beta} \langle\widetilde{\psi}|\alpha\rangle \times \langle\alpha|\, \hat{A}\, |\beta\rangle \times \langle\beta|\psi\rangle \;=\; \sum_{\alpha,\beta} A_{\alpha\beta} \times \int d^3\tilde{\mathbf{x}}\, \widetilde{\psi}^*(\tilde{\mathbf{x}})\phi_\alpha(\tilde{\mathbf{x}}) \times \int d^3\mathbf{x}\, \phi^*_\beta(\mathbf{x})\psi(\mathbf{x}). \tag{38}$$

This is undergraduate-level QM.

In the N–particle Hilbert space we have a similar formula for the matrix elements of the $\hat{A}$ acting on particle $\#i$, the only modification being integrals over the coordinates of the other particles,

$$\begin{aligned}
&\langle N, \widetilde{\psi}|\, \hat{A}_1(i^{\text{th}})\, |N, \psi\rangle \;= \\
&\quad = \int\!\cdots\!\int d^3\mathbf{x}_1 \cdots \cancel{d^3\mathbf{x}_i} \cdots d^3\mathbf{x}_N \sum_{\alpha,\beta} A_{\alpha\beta} \times \left(\int d^3\tilde{\mathbf{x}}_i\, \widetilde{\psi}^*(\mathbf{x}_1, \ldots, \tilde{\mathbf{x}}_i, \ldots, \mathbf{x}_N)\phi_\alpha(\tilde{\mathbf{x}}_i)\right) \\
&\qquad\qquad \times \left(\int d^3\mathbf{x}_i\, \phi^*_\beta(\mathbf{x}_i)\psi(\mathbf{x}_1, \ldots, \mathbf{x}_i, \ldots, \mathbf{x}_N)\right) \\
&\quad = \sum_{\alpha,\beta} A_{\alpha\beta} \times \int\!\cdots\!\int d^3\mathbf{x}_1 \cdots d^3\mathbf{x}_N\, d^3\tilde{\mathbf{x}}_i\, \widetilde{\psi}^*(\mathbf{x}_1, \ldots, \tilde{\mathbf{x}}_i, \ldots, \mathbf{x}_N) \times \phi_\alpha(\tilde{\mathbf{x}}_i) \\
&\qquad\qquad \times \phi^*_\beta(\mathbf{x}_i) \times \psi(\mathbf{x}_1, \ldots, \mathbf{x}_i, \ldots, \mathbf{x}_N).
\end{aligned} \tag{39}$$

For symmetric wave-functions of identical bosons, we get the same matrix element regardless of which particle $\#i$ we are acting on with the operator $\hat{A}$, hence for the *net* A operator (32),

$$\begin{aligned}
\langle N, \widetilde{\psi}|\, \hat{A}^{(1)}_{\text{net}}\, |N, \psi\rangle \;=\; N \times \sum_{\alpha,\beta} A_{\alpha\beta} \times \int\!\cdots\!\int & d^3\mathbf{x}_1 \cdots d^3\mathbf{x}_{N-1}\, d^3\mathbf{x}_N d^3\tilde{\mathbf{x}}_N \\
& \widetilde{\psi}^*(\mathbf{x}_1, \ldots, \mathbf{x}_{N-1}, \tilde{\mathbf{x}}_N) \times \phi_\alpha(\tilde{\mathbf{x}}_N) \\
& \times \phi^*_\beta(\mathbf{x}_N) \times \psi(\mathbf{x}_1, \ldots, \mathbf{x}_{N-1}, \mathbf{x}_N).
\end{aligned} \tag{40}$$

Now consider matrix elements of the Fock-space operator (36). In light of eq. (5), the state $|N-1,\psi''\rangle = \hat{a}_\beta\,|N,\psi\rangle$ has wave-function

$$\psi''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1}) \;=\; \sqrt{N}\int\! d^3\mathbf{x}_N\,\phi^*_\beta(\mathbf{x}_N)\times\psi(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1},\mathbf{x}_N). \tag{41}$$

Likewise, the state $\left|N-1,\widetilde{\psi}''\right\rangle = \hat{a}_\alpha\,|N,\widetilde{\psi}\rangle$ has wave-function

$$\widetilde{\psi}''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1}) \;=\; \sqrt{N}\int\! d^3\tilde{\mathbf{x}}_N\,\phi^*_\alpha(\tilde{\mathbf{x}}_N)\times\widetilde{\psi}(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1},\tilde{\mathbf{x}}_N). \tag{42}$$

Consequently,

$$\begin{aligned}
\langle N,\widetilde{\psi}|\,\hat{a}^\dagger_\alpha\hat{a}_\beta\,|N,\psi\rangle \;&=\; \left\langle N-1,\widetilde{\psi}''\right|\left|N-1,\psi''\right\rangle\\
&= \int\!\cdots\!\int\! d^3\mathbf{x}_1\cdots\mathbf{x}_{N-1}\,\widetilde{\psi}''^*(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\times\psi''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\\
&= \int\!\cdots\!\int\! d^3\mathbf{x}_1\cdots\mathbf{x}_{N-1}\,\sqrt{N}\int\! d^3\tilde{\mathbf{x}}_N\,\phi_\alpha(\tilde{\mathbf{x}}_N)\times\widetilde{\psi}^*(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1},\tilde{\mathbf{x}}_N)\times\\
&\qquad\qquad\times\sqrt{N}\int\! d^3\mathbf{x}_N\,\phi^*_\beta(\mathbf{x}_N)\times\psi(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1},\mathbf{x}_N).
\end{aligned} \tag{43}$$

Comparing this formula to the integrals in eq. (40), we see that

$$\langle N,\widetilde{\psi}|\,\hat{A}^{(1)}_{\rm net}\,|N,\psi\rangle \;=\; \sum_{\alpha,\beta} A_{\alpha\beta}\times\langle N,\widetilde{\psi}|\,\hat{a}^\dagger_\alpha\hat{a}_\beta\,|N,\psi\rangle \;=\; \langle N,\widetilde{\psi}|\,\hat{A}^{(2)}_{\rm net}\,|N,\psi\rangle\,. \tag{44}$$

Quod erat demonstrandum.

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Now consider the two-body operators — the additive operators acting on two particles at a time. For example, the net two-body potential

$$\hat{V}^{(1)}_{|rmnet} \;=\; \frac{1}{2}\sum_{i\neq j}^{i,j=1,\ldots,N} V(\hat{\mathbf{x}}_i-\hat{\mathbf{x}}_j). \tag{45}$$

More generally, in the wave-function language we start with some operator $\hat{B}$ in a two-particle Hilbert space, make it act on all (i,j) pairs of particles in the N-particle Hilbert space, and total up the pairs,

$$\hat{B}^{(1)}_{\rm net} \;=\; \frac{1}{2} \sum_{i\neq j}^{i,j=1,\ldots,N} \hat{B}(i^{\rm th} \text{ and } j^{\rm th} \text{ particles}). \tag{46}$$

In the Fock space language, such a two-body operator becomes

$$\hat{B}^{(2)}_{\rm net} \;=\; \tfrac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \left(\langle\alpha|\otimes\langle\beta|\right)\hat{B}\left(|\gamma\rangle\otimes|\delta\rangle\right)\hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_\delta \hat{a}_\gamma\,. \tag{47}$$

Note: in this formula, it is OK to use the un-symmetrized 2-particle states $\langle\alpha|\otimes\langle\beta|$ and $|\gamma\rangle\otimes|\delta\rangle$, and hence the un-symmetrized matrix elements of the $\hat{B}_2$. At the level of the second-quantized operator $\hat{B}^{(2)}_{\rm net}$, the Bose symmetry is automatically provided by $\hat{a}^\dagger_\alpha\hat{a}^\dagger_\beta = \hat{a}^\dagger_\beta\hat{a}^\dagger_\gamma$ and $\hat{a}_\delta\hat{a}_\gamma = \hat{a}_\gamma\hat{a}_\delta$, even for the un-symmetrized matrix elements of the two-particle operator $\hat{B}$.

For example, the two-body potential $V(\hat{\mathbf{x}}_1 - \hat{\mathbf{x}}_2)$ in the un-symmetrized momentum basis has matrix elements

$$\begin{aligned}
\left(\langle\mathbf{p}'_1|\otimes\langle\mathbf{p}'_2|\right)\hat{V}\left(|\mathbf{p}_1\rangle\otimes|\mathbf{p}_2\rangle\right) \;&=\; L^{-3}\delta_{\mathbf{p}'_1+\mathbf{p}'_2,\mathbf{p}_1+\mathbf{p}_2} \times W(\mathbf{q}) \\
\text{where}\quad \mathbf{q} = \mathbf{p}'_1 - \mathbf{p}_1 &= \mathbf{p}_2 - \mathbf{p}'_2 \\
\text{and}\quad W(\mathbf{q}) \;&=\; \int\! d\mathbf{x}\, e^{-i\mathbf{q}\mathbf{x}}\, V_2(\mathbf{x}),
\end{aligned} \tag{48}$$

hence

$$\hat{V}^{(2)}_{\rm net} \;=\; \tfrac{1}{2} L^{-3} \sum_{\mathbf{q}} W(\mathbf{q}) \sum_{\mathbf{p}_1,\mathbf{p}_2} \hat{a}^\dagger_{\mathbf{p}_1+\mathbf{q}} \hat{a}^\dagger_{\mathbf{p}_2-\mathbf{q}} \hat{a}_{\mathbf{p}_2} \hat{a}_{\mathbf{p}_1}\,. \tag{49}$$

Theorem: *Again, for any two-particle operator $\hat{B}$ eqs.* (46) *and* (47) *define exactly the same net operator $\hat{B}_{\rm net}$.* Indeed, the operators defined according to the two equations have the same matrix elements between any two N–boson states,

$$\langle N,\widetilde{\psi}|\,\hat{B}^{(1)}_{\rm net}\,|N,\psi\rangle \;=\; \langle N,\widetilde{\psi}|\,\hat{B}^{(2)}_{\rm net}\,|N,\psi\rangle \quad \text{for any states } \langle N,\widetilde{\psi}| \text{ and } |N,\psi\rangle\,. \tag{50}$$

Proof: This works similarly to the previous theorem, except for more integrals. Let

$$B_{\alpha\beta,\gamma\delta} \;=\; \bigl(\langle\alpha|\otimes\langle\beta|\bigr)\hat{B}_2\bigl(|\gamma\rangle\otimes|\delta\rangle\bigr) \tag{51}$$

be matrix elements of a two-body operator $\hat{B}_2$ between *un-symmetrized* two-particle states.

Then for generic two-particle states $\langle\widetilde{\psi}|$ and $|\psi\rangle$ — symmetric or not — we have

$$\begin{aligned}
\langle\widetilde{\psi}|\,\hat{B}_2\,|\psi\rangle \;&=\; \sum_{\alpha,\beta,\gamma,\delta} B_{\alpha\beta,\gamma\delta}\times\langle\widetilde{\psi}|\big(|\alpha\rangle\otimes|\beta\rangle\big)\times\big(\langle\gamma|\otimes\langle\delta|\big)|\psi\rangle\\
&=\; \sum_{\alpha,\beta,\gamma,\delta} B_{\alpha\beta,\gamma\delta}\times\iint d^3\tilde{\mathbf{x}}_1\,d^3\tilde{\mathbf{x}}_2\,\widetilde{\psi}^*(\tilde{\mathbf{x}}_1,\tilde{\mathbf{x}}_2)\phi_\alpha(\tilde{\mathbf{x}}_1)\phi_\beta(\tilde{\mathbf{x}}_2)\\
&\qquad\qquad\times\iint d^3\mathbf{x}_1\,d^3\mathbf{x}_2\,\phi^*_\gamma(\mathbf{x}_1)\phi^*_\delta(\mathbf{x}_2)\psi(\mathbf{x}_1,\mathbf{x}_2).
\end{aligned}\tag{52}$$

Similarly, in the Hilbert space of $N>2$ particles — identical bosons or not — the operator $\hat{B}_2$ acting on particles $\#i$ and $\#j$ has matrix elements

$$\begin{aligned}
&\langle N,\widetilde{\psi}|\,\hat{B}_2(i^{\mathrm{th}},j^{\mathrm{th}})\,|N,\psi\rangle \;=\\
&\quad=\sum_{\alpha,\beta,\gamma,\delta} B_{\alpha\beta,\gamma\delta}\times\int\!\cdots\!\int d^3\mathbf{x}_1\cdots\cancel{d^3\mathbf{x}_i}\cdots\cancel{d^3\mathbf{x}_j}\cdots d^3\mathbf{x}_N\\
&\qquad\qquad\iint d^3\tilde{\mathbf{x}}_i\,d^3\tilde{\mathbf{x}}_j\,\widetilde{\psi}^*(\mathbf{x}_1,\ldots,\tilde{\mathbf{x}}_i,\ldots,\tilde{\mathbf{x}}_j,\ldots,\mathbf{x}_N)\phi_\alpha(\tilde{\mathbf{x}}_i)\phi_\beta(\tilde{\mathbf{x}}_j)\\
&\qquad\qquad\times\iint d^3\mathbf{x}_i\,d^3\mathbf{x}_j\,\phi^*_\gamma(\mathbf{x}_i)\phi^*_\delta(\mathbf{x}_j)\psi(\mathbf{x}_1,\ldots,\mathbf{x}_i,\ldots,\mathbf{x}_j,\ldots,\mathbf{x}_N)
\end{aligned}\tag{53}$$

For identical bosons — and hence totally symmetric wave-functions ψ and $\widetilde{\psi}$ — such matrix elements do not depend on the choice of particles on which $\hat{B}_2$ acts, so we may just as well let $i=N-1$ and $j=N$. Consequently, the *net* $\hat{B}$ operator (21) has matrix elements

$$\begin{aligned}
\langle N,\widetilde{\psi}|\,\hat{B}^{(1)}_{\mathrm{net}}\,|N,\psi\rangle \;&=\; \frac{N(N-1)}{2}\times\langle N,\widetilde{\psi}|\,\hat{B}_2(N-1,N)\,|N,\psi\rangle\\
&=\; \frac{N(N-1)}{2}\times\sum_{\alpha,\beta,\gamma,\delta} B_{\alpha\beta,\gamma\delta}\times I_{\alpha\beta,\gamma\delta}
\end{aligned}\tag{54}$$

where

$$\begin{aligned}
I_{\alpha\beta,\gamma\delta} \;&=\int\!\cdots\!\int d^3\mathbf{x}_1\cdots d^3\mathbf{x}_{N-2}\\
&\qquad\iint d^3\tilde{\mathbf{x}}_{N-1}\,d^3\tilde{\mathbf{x}}_N\,\widetilde{\psi}^*(\mathbf{x}_1,\ldots,\mathbf{x}_{N-2},\tilde{\mathbf{x}}_{N-1},\tilde{\mathbf{x}}_N)\phi_\alpha(\tilde{\mathbf{x}}_{N-1})\phi_\beta(\tilde{\mathbf{x}}_N)\\
&\qquad\times\iint d^3\mathbf{x}_{N-1}\,d^3\mathbf{x}_N\,\phi^*_\gamma(\mathbf{x}_{N-1})\phi^*_\delta(\mathbf{x}_N)\psi(\mathbf{x}_1,\ldots,\mathbf{x}_{N-2},\mathbf{x}_{N-1},\mathbf{x}_N)
\end{aligned}\tag{55}$$

Now let's compare these formulae to the Fock space formalism. Applying eq. (5) *twice*, we find that the $(N-2)$–particle state

$$\left|N-2,\psi'''\right\rangle \;=\; \hat{a}_\delta\hat{a}_\gamma\left|N,\psi\right\rangle \tag{56}$$

has wave function

$$\begin{aligned}\psi'''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-2}) \;=\; \sqrt{N(N-1)}\iint & d^3\mathbf{x}_{N-1}\,d^3\mathbf{x}_N\,\phi^*_\gamma(\mathbf{x}_{N-1})\phi^*_\delta(\mathbf{x}_N)\\ &\times\psi(\mathbf{x}_1,\ldots,\mathbf{x}_{N-2},\mathbf{x}_{N-1},\mathbf{x}_N).\end{aligned} \tag{57}$$

Likewise, the $(N-2)$–particle state

$$\left|N-2,\widetilde{\psi}'''\right\rangle \;=\; \hat{a}_\beta\hat{a}_\alpha\left|N,\widetilde{\psi}\right\rangle \tag{58}$$

has wave function

$$\begin{aligned}\widetilde{\psi}'''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-2}) \;=\; \sqrt{N(N-1)}\iint & d^3\mathbf{x}_{N-1}\,d^3\mathbf{x}_N\,\phi^*_\beta(\tilde{\mathbf{x}}_{N-1})\phi^*_\alpha(\tilde{\mathbf{x}}_N)\\ &\times\widetilde{\psi}(\mathbf{x}_1,\ldots,\mathbf{x}_{N-2},\tilde{\mathbf{x}}_{N-1},\tilde{\mathbf{x}}_N).\end{aligned} \tag{59}$$

Taking Dirac product of these two states, we obtain

$$\begin{aligned}\langle N,\widetilde{\psi}|\,\hat{a}^\dagger_\alpha\hat{a}^\dagger_\beta\hat{a}_\delta\hat{a}_\gamma\,|N,\psi\rangle \;&=\; \left\langle N-2,\widetilde{\psi}'''\right|\left|N-2,\psi'''\right\rangle\\ &=\int\!\cdots\!\int d^3\mathbf{x}_1\cdots d^3\mathbf{x}_{N-2}\,\widetilde{\psi}'''^*(\mathbf{x}_1,\ldots,\mathbf{x}_{N-2})\times\psi'''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-2})\\ &=\; N(N-1)\times I_{\alpha\beta,\gamma\delta}\end{aligned} \tag{60}$$

where $I_{\alpha\beta,\gamma\delta}$ is exactly the same mega-integral as in eq. (55). Therefore,

$$\langle N,\widetilde{\psi}|\,\hat{B}^{(1)}_{\rm net}\,|N,\psi\rangle \;=\; \tfrac{1}{2}\sum_{\alpha,\beta,\gamma,\delta}B_{\alpha\beta,\gamma\delta}\times\langle N,\widetilde{\psi}|\,\hat{a}^\dagger_\alpha\hat{a}^\dagger_\beta\hat{a}_\delta\hat{a}_\gamma\,|N,\psi\rangle \;=\; \langle N,\widetilde{\psi}|\,\hat{B}^{(2)}_{\rm net}\,|N,\psi\rangle \tag{61}$$

where the second equality follows directly from the eq. (47) for the $\hat{B}^{(2)}_{\rm net}$ operator. *Quod erat demonstrandum.*

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I would like to conclude these notes with a couple of simple theorems about the commutators of the net one-body and two-body operators.

Theorem 1: *Let $\hat{A}$, $\hat{B}$, and $\hat{C}$ be some one-particle operators, and let $\hat{A}^{(2)}_{\rm net}$, $\hat{B}^{(2)}_{\rm net}$, and $\hat{C}^{(2)}_{\rm net}$ be the corresponding net one-body operators in the fock space according to eq.* (36)*.*

$$\textbf{if}\quad [\hat{A},\hat{B}]\;=\;\hat{C}\quad\textbf{then}\quad \left[\hat{A}^{(2)}_{\rm net},\hat{B}^{(2)}_{\rm net}\right]\;=\;\hat{C}^{(2)}_{\rm net}\,. \tag{62}$$

Theorem 2: *Now let $\hat{A}$ be a one-particle operator while $\hat{B}$ and $\hat{C}$ are two-particle operators. Let $\hat{A}^{(2)}_{\rm net}$, $\hat{B}^{(2)}_{\rm net}$, and $\hat{C}^{(2)}_{\rm net}$ be the corresponding net operators in the Fock space according to eqs.* (36) *and* (47)*.*

$$\textbf{if}\quad \left[\bigl(\hat{A}(1^{\rm st})+\hat{A}(2^{\rm nd})\bigr),\hat{B}\right]\;=\;\hat{C}\quad\textbf{then}\quad \left[\hat{A}^{(2)}_{\rm net},\hat{B}^{(2)}_{\rm net}\right]\;=\;\hat{C}^{(2)}_{\rm net}\,. \tag{63}$$

Proof of Theorem 1: The theorem follows from the commutator

$$[\hat{a}^\dagger_\alpha\hat{a}_\beta,\hat{a}^\dagger_\gamma\hat{a}_\delta]\;=\;\delta_{\beta,\gamma}\hat{a}^\dagger_\alpha\hat{a}_\delta\;-\;\delta_{\alpha,\delta}\hat{a}^\dagger_\gamma\hat{a}_\beta \tag{64}$$

which you should have calculated in homework set#3, problem 4(a). Indeed, given

$$\hat{A}^{(2)}_{\rm tot}\;=\sum_{\alpha,\beta}\langle\alpha|\,\hat{A}\,|\beta\rangle\;\hat{a}^\dagger_\alpha\hat{a}_\beta \tag{65}$$

and

$$\hat{B}^{(2)}_{\rm tot}\;=\sum_{\gamma,\delta}\langle\gamma|\,\hat{B}\,|\delta\rangle\;\hat{a}^\dagger_\gamma\hat{a}_\delta\,, \tag{66}$$

we immediately have

$$
\begin{aligned}
\left[\hat{A}^{(2)}_{\rm tot},\hat{B}^{(2)}_{\rm tot}\right] &= \sum_{\alpha,\beta,\gamma,\delta} \langle\alpha|\,\hat{A}\,|\beta\rangle\;\langle\gamma|\,\hat{B}\,|\delta\rangle\;[\hat{a}^\dagger_\alpha\hat{a}_\beta,\hat{a}^\dagger_\gamma\hat{a}_\delta] \\
&\qquad \langle\!\langle\,\text{using eq. (64)}\,\rangle\!\rangle \\
&= \sum_{\alpha,\beta,\gamma,\delta} \langle\alpha|\,\hat{A}\,|\beta\rangle\;\langle\gamma|\,\hat{B}\,|\delta\rangle\;\Big(\delta_{\beta,\gamma}\hat{a}^\dagger_\alpha\hat{a}_\delta\;-\;\delta_{\alpha,\delta}\hat{a}^\dagger_\gamma\hat{a}_\beta\Big) \\
&= \sum_{\alpha,\delta}\hat{a}^\dagger_\alpha\hat{a}_\delta\times\sum_{\beta=\gamma}\langle\alpha|\,\hat{A}\,|\gamma\rangle\,\langle\gamma|\,\hat{B}\,|\delta\rangle\;-\sum_{\beta,\gamma}\hat{a}^\dagger_\gamma\hat{a}_\beta\times\sum_{\alpha=\delta}\langle\gamma|\,\hat{B}\,|\alpha\rangle\,\langle\alpha|\,\hat{A}\,|\beta\rangle \\
&= \sum_{\alpha,\delta}\hat{a}^\dagger_\alpha\hat{a}_\delta\;\langle\alpha|\,\hat{A}\hat{B}\,|\delta\rangle\;-\sum_{\beta,\gamma}\hat{a}^\dagger_\gamma\hat{a}_\beta\;\langle\gamma|\,\hat{B}\hat{A}\,|\beta\rangle \\
&\qquad \langle\!\langle\,\text{renaming summation indices}\,\rangle\!\rangle \\
&= \sum_{\alpha,\beta}\hat{a}^\dagger_\alpha\hat{a}_\beta\times\Big(\langle\alpha|\,\hat{A}\hat{B}\,|\beta\rangle\;-\;\langle\alpha|\,\hat{B}\hat{A}\,|\beta\rangle\Big) \\
&= \sum_{\alpha,\beta}\hat{a}^\dagger_\alpha\hat{a}_\beta\times\langle\alpha|\,\Big([\hat{A},\hat{B}]=\hat{C}\Big)\,|\beta\rangle\;\equiv\;\hat{C}^{(2)}_{\rm tot}.
\end{aligned}
\tag{67}
$$

Quod erat demonstrandum.

Proof of Theorem 2: Similarly to the theorem 1, this theorem also follows from a commutator you should have calculated in homework set#3, problem 4(a), namely

$$
[\hat{a}^\dagger_\mu\hat{a}_\nu,\hat{a}^\dagger_\alpha\hat{a}^\dagger_\beta\hat{a}_\gamma\hat{a}_\delta]\;=\;\delta_{\nu\alpha}\hat{a}^\dagger_\mu\hat{a}^\dagger_\beta\hat{a}_\gamma\hat{a}_\delta+\delta_{\nu\beta}\hat{a}^\dagger_\alpha\hat{a}^\dagger_\mu\hat{a}_\gamma\hat{a}_\delta-\delta_{\mu\gamma}\hat{a}^\dagger_\alpha\hat{a}^\dagger_\beta\hat{a}_\nu\hat{a}_\delta-\delta_{\mu\delta}\hat{a}^\dagger_\alpha\hat{a}^\dagger_\beta\hat{a}_\gamma\hat{a}_\nu\,. \tag{68}
$$

Indeed, in the Fock space

$$
\hat{A}^{(2)}_{\rm tot}\;=\;\sum_{\mu\,nu}\langle\mu|\,\hat{A}\,|\nu\rangle\;\hat{a}^\dagger_\mu\hat{a}_\nu \tag{36}
$$

and

$$
\hat{B}^{(2)}_{\rm tot}\;=\;\tfrac{1}{2}\sum_{\alpha,\beta,\gamma,\delta}\langle\alpha\otimes\beta|\,\hat{B}\,|\gamma\otimes\delta\rangle\;\hat{a}^\dagger_\alpha\hat{a}^\dagger_\beta\hat{a}_\gamma\hat{a}_\delta\,, \tag{47}
$$

so the commutator $\left[\hat{A}^{(2)}_{\rm net}, \hat{B}^{(2)}_{\rm net}\right]$ is a linear combination of the commutators (68). Specifically,

$$
\begin{aligned}
[\hat{A}^{(2)}_{\rm tot}, \hat{B}^{(2)}_{\rm tot}] \;&=\; \tfrac{1}{2}\sum_{\mu,\nu,\alpha,\beta,\gamma,\delta} \langle\mu|\,\hat{A}\,|\nu\rangle\; \langle\alpha\otimes\beta|\,\hat{B}\,|\gamma\otimes\delta\rangle\; [\hat{a}^\dagger_\mu \hat{a}_\nu, \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_\gamma \hat{a}_\delta] \\
&\qquad \langle\!\langle \text{ using eq. (68) } \rangle\!\rangle \\
&=\; \tfrac{1}{2}\sum_{\mu,\beta,\gamma,\delta} \hat{a}^\dagger_\mu \hat{a}^\dagger_\beta \hat{a}_\gamma \hat{a}_\delta \times \sum_\nu \langle\mu|\,\hat{A}\,|\nu\rangle\, \langle\nu\otimes\beta|\,\hat{B}\,|\gamma\otimes\delta\rangle \\
&\qquad +\; \tfrac{1}{2}\sum_{\alpha,\mu,\gamma,\delta} \hat{a}^\dagger_\alpha \hat{a}^\dagger_\mu \hat{a}_\gamma \hat{a}_\delta \times \sum_\nu \langle\mu|\,\hat{A}\,|\nu\rangle\, \langle\alpha\otimes\nu|\,\hat{B}\,|\gamma\otimes\delta\rangle \\
&\qquad -\; \tfrac{1}{2}\sum_{\alpha,\beta,\nu,\delta} \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_\nu \hat{a}_\delta \times \sum_\mu \langle\alpha\otimes\beta|\,\hat{B}\,|\mu\otimes\delta\rangle\, \langle\mu|\,\hat{A}\,|\nu\rangle \\
&\qquad -\; \tfrac{1}{2}\sum_{\alpha,\beta,\gamma,\nu} \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_\gamma \hat{a}_\nu \times \sum_\mu \langle\alpha\otimes\beta|\,\hat{B}\,|\gamma\otimes\mu\rangle\, \langle\mu|\,\hat{A}\,|\nu\rangle \\
&\qquad \langle\!\langle \text{ renaming summation indices } \rangle\!\rangle \\
&=\; \tfrac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_\gamma \hat{a}_\delta \times C_{\alpha,\beta,\gamma,\delta}\,,
\end{aligned}
\tag{69}
$$

where

$$
\begin{aligned}
C_{\alpha,\beta,\gamma,\delta} \;&= \sum_\lambda \langle\alpha|\,\hat{A}\,|\lambda\rangle\, \langle\lambda\otimes\beta|\,\hat{B}\,|\gamma\otimes\delta\rangle \;+\; \sum_\lambda \langle\beta|\,\hat{A}\,|\lambda\rangle\, \langle\alpha\otimes\lambda|\,\hat{B}\,|\gamma\otimes\delta\rangle \\
&\qquad -\; \sum_\lambda \langle\alpha\otimes\beta|\,\hat{B}\,|\lambda\otimes\delta\rangle\;\; \langle\lambda|\,\hat{A}\,|\gamma\rangle \;-\; \sum_\lambda \langle\alpha\otimes\beta|\,\hat{B}\,|\gamma\otimes\lambda\rangle\;\; \langle\lambda|\,\hat{A}\,|\delta\rangle \\
&=\; \langle\alpha\otimes\beta|\,\Big(\hat{A}(1^{\rm st})\hat{B} \;+\; \hat{A}(2^{\rm nd})\hat{B} \;-\; \hat{B}\hat{A}(1^{\rm st}) \;-\; \hat{B}\hat{A}(2^{\rm nd})\Big)\,|\gamma\otimes\delta\rangle \\
&=\; \langle\alpha\otimes\beta|\,\Big[\Big(\hat{A}(1^{\rm st}) + \hat{A}(2^{\rm nd})\Big)\,,\hat{B}\Big]\,|\gamma\otimes\delta\rangle \;\equiv\; \langle\alpha\otimes\beta|\,\hat{C}\,|\gamma\otimes\delta\rangle\,.
\end{aligned}
\tag{70}
$$

Consequently, $\left[\hat{A}^{(2)}_{\rm tot}, \hat{B}^{(2)}_{\rm tot}\right] = \hat{C}^{(2)}_{\rm tot}$. *Quod erat demonstrandum.*