Second Quantization of Identical Bosons

Quantum Mechanics of many identical bosons can be done in the wave-function formalism, but it's often convenient to use the formalism of the creation and annihilation operators in the Fock space. For historical reasons, this formalism is called the *"second quantization"*, but this name is misleading: There is no new quantization, just the same old quantum mechanics re-written in a new language. In these notes I shall develop the second quantization formalism for any kind of identical bosons — they can be relativistic particles, or non-relativistic particles (for example helium atoms), or even quasiparticles like phonons.

At the core of the second quantized formalism are the particle-creation and particleannihilation operators. For the relativistic particles these operators can be assembled into quantum fields; this procedure is the exact reversal of what we did in an earlier set of notes on the spectrum of a free scalar field. For the non-relativistic particles we may also construct the non-relativistic quantum fields, and I shall do it later in these notes.

THE FOCK SPACE AND ITS BASIS

The Fock space is the Hilbert space of an arbitrary number of identical bosons,

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

and our first task is to construct the basis of this space which may be interpreted in terms of occupation numbers n_{α} . Here α 's should label 1-particle quantum states, so we start with the single-particle Hilbert space \mathcal{H}_1 and build some kind of a complete orthonormal basis of states $|\alpha\rangle$ with wave-functions $\phi_{\alpha}(\mathbf{x})$.^{*} I assume $|\alpha\rangle$ to be eigenstates of some kind of a 1-particle Hamiltonian, $\hat{H}_1 |\alpha\rangle = \epsilon_{\alpha} |\alpha\rangle$, but the specific form of the operator \hat{H}_1 is not important for our purposes. For simplicity, I also assume the spectrum of α to be discrete.[†]

^{*} By abuse of notations, I include spin, isospin, and any other discrete quantum numbers a particle may have with the $\mathbf{x} = (x, y, z, \text{spin}, etc.)$.

[†] A continuum spectrum would lead to the same physics, but we would need more complicated formulae to handle states with occupation numbers $n_{\alpha} > 1$ for continuous α .

Given a one-particle basis $\{|\alpha\rangle\}$, we may construct a complete basis of the two-particle Hilbert space \mathcal{H}_2 using eigenstates of the operator $\hat{H}_2 = \hat{H}_1(1^{st}) + \hat{H}_1(2^{nd})$. Naively, this operator has eigenstates $|\alpha\rangle\otimes|\beta\rangle$ with energies $\epsilon_{\alpha}+\epsilon_{\beta}$ and wave functions $\phi_{\alpha}(\mathbf{x}_1)\times\phi_{\beta}(\mathbf{x}_2)$. However, two identical bosons must have a symmetric wave function $\phi_{\alpha\beta}(\mathbf{x}_1,\mathbf{x}_2) = \phi_{\alpha\beta}(\mathbf{x}_2,\mathbf{x}_1)$. Consequently, we must symmetrize:

$$|\alpha,\beta\rangle = |\beta,\alpha\rangle = \begin{cases} \frac{|\alpha\rangle \otimes |\beta\rangle + |\beta\rangle \otimes |\alpha\rangle}{\sqrt{2}} & \text{for } \beta \neq \alpha, \\ |\alpha\rangle \otimes |\alpha\rangle & \text{for } \beta = \alpha, \end{cases}$$
(2)

or in the wave-function Language

$$\phi_{\alpha\beta}(\mathbf{x}_1, \mathbf{x}_2) = \phi_{\beta\alpha}(\mathbf{x}_1, \mathbf{x}_2) = \begin{cases} \frac{\phi_{\alpha}(\mathbf{x}_1)\phi_{\beta}(\mathbf{x}_2) + \phi_{\beta}(\mathbf{x}_1)\phi_{\alpha}(\mathbf{x}_2)}{\sqrt{2}} & \text{for } \beta \neq \alpha, \\ \phi_{\alpha}(\mathbf{x}_1)\phi_{\alpha}(\mathbf{x}_2) & \text{for } \beta = \alpha, \end{cases}$$
(3)

Similarly, wave functions of N identical bosons must be totally symmetric,

 $\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \psi(\text{any permutation of the } \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N).$ (4)

To construct a complete basis of such N-particle wave functions, we use eigenstates of the

$$\hat{H}_N = \sum_{i=1}^N \hat{H}_1(i^{\text{th}} \text{ particle}).$$
(5)

Without the symmetry requirement (4), all eigenstates of this Hamiltonian would be of the form $|\alpha\rangle \otimes |\beta\rangle \otimes \cdots \otimes |\omega\rangle$, with energies $\epsilon_{\alpha} + \epsilon_{\beta} + \cdots + \epsilon_{\omega}$, but because we are in the Hilbert space of N identical bosons, we must symmetrize such states according to

$$|\alpha, \beta, \dots, \omega\rangle = \frac{|\alpha\rangle \otimes |\beta\rangle \otimes \dots \otimes |\omega\rangle + \text{ all distinct permutations of } \alpha, \beta, \dots, \omega}{\sqrt{\# \text{ of distinct permutations}}},$$

$$\phi_{\alpha\beta\cdots\omega}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \frac{\phi_{\alpha}(\mathbf{x}_1)\phi_{\beta}(\mathbf{x}_2)\cdots\phi_{\omega}(\mathbf{x}_N) + \text{ all distinct permutations of } \alpha, \beta, \dots, \omega}{\sqrt{\# \text{ of distinct permutations}}}$$
(6)

Consequently, the order of the N single-particle labels $\alpha, \beta, \ldots, \omega$ of a state (6) does not

matter,

$$|\alpha, \beta, \dots, \omega\rangle = |\text{any permutation of the } \alpha, \beta, \dots, \omega\rangle,$$
 (7)

which means that we may uniquely specify such a state in terms of its occupations numbers n_{β} that count how many times each β appears in the list $\alpha, \beta, \ldots, \omega$. For example,

$$\left|\alpha, \alpha, \alpha, \beta, \beta, \gamma, \gamma, \delta, \epsilon\right\rangle = \left|3_{\alpha}, 2_{\beta}, 2_{\gamma}, 1_{\delta}, 1_{\epsilon}, 0_{\text{all others}}\right\rangle.$$
(8)

Formally,

$$|\alpha_1 \dots, \alpha_N\rangle = |\{n_\beta\}\rangle$$
 where $n_\beta = \sum_{i=1}^N \delta_{\alpha_i,\beta}$. (9)

Note that $\sum_{\beta} n_{\beta} = N$, so all but a finite number of the occupations numbers must vanish.

The states (6) are eigenstates of the Hamiltonian (5) in the N-boson Hilbert space \mathcal{H}_N , so together they form a complete orthonormal basis of the \mathcal{H}_N . In terms of the occupation numbers, this basis comprises states $|\{n_\beta\}\rangle$ where n_β are non-negative integers which total up to N, $\sum_{\beta} n_\beta = N$. Removing the latter constraint, we construct a bigger Hilbert space which spans $|\{n_\beta\}\rangle$ with all values of the $N = \sum_{\beta} n_\beta$. Physically, this space is the Fock space

$$\mathcal{F} = |\text{vacuum}\rangle \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3 \oplus \cdots = \bigoplus_{N=0}^{\infty} \mathcal{H}_N$$
 (10)

of the quantum theory of an arbitrary number N = 0, 1, 2, 3, ... of identical bosons.

In other words, what we have done thus far is to construct a basis of the entire Fock space comprising states $|\{n_{\beta}\}\rangle$ with definite occupation numbers. We can think of this basis as a common eigenbasis of a family of commuting hermitian operators \hat{n}_{β} with eigenvalues $n_{\beta} = 0, 1, 2, \ldots$ Such operators are very useful for extending additive operators such as (5) to the whole Fock space and for writing them in compact form

$$\hat{H}\Big|_{\text{whole }\mathcal{F}} = \sum_{\beta} \epsilon_{\beta} \hat{n}_{\beta} \,. \tag{11}$$

Indeed, the operators (5) and (11) have the same eigenstates $|\alpha_1, \dots, \alpha_N\rangle$ and the same eigenvalues $\sum_{\beta} \epsilon_{\beta} n_{\beta} = \epsilon_{\alpha_1} + \dots + \epsilon_{\alpha_N}$.

For example, consider the free non-relativistic spinless particles (in a big box). The single-particle Hamiltonian is $\hat{H}_1 = \frac{1}{2m} \hat{\mathbf{P}}^2$, so we may identify $|\alpha\rangle$ as $|\mathbf{p}\rangle$. Consequently, the Fock-space Hamiltonian

$$\hat{H}_{\text{tot}} = \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} \times \hat{n}_{\mathbf{p}}$$
(12)

comprises all the net Hamiltonians $\hat{H}_N = \sum \frac{1}{2m} \hat{\mathbf{P}}^2(i^{\underline{\text{th}}})$ for any number N of the particles. Likewise, the Fock-space net momentum operator

$$\hat{\mathbf{P}}_{\text{tot}} = \sum_{\mathbf{p}} \mathbf{p} \times \hat{n}_{\mathbf{p}}$$
(13)

comprises the net momentum operators $\hat{\mathbf{P}}_N = \sum_i \hat{\mathbf{P}}(i^{\text{th}})$ of N particle systems for any N.

CREATION AND ANNIHILATION OPERATORS

To construct more interesting operators in the Fock space we need the creation and the annihilation operators, so our next task is to construct the harmonic-oscillator-like $\hat{a}^{\dagger}_{\alpha}$ and \hat{a}_{α} . We begin this by noticing that in the Fock space, the occupation numbers n_{β} are completely independent from each other. That is, given any state $|\{n_{\beta}\}\rangle \in \mathcal{F}$, we may change one particular $n_{\alpha} \rightarrow n'_{\alpha} \pm 1$ while keeping all the other n_{β} unchanged, $n'_{\beta} = n_{\beta}$ for $\beta \neq \alpha$, and the state $|\{n'_{\beta}\}\rangle$ would be a valid state in the Fock space \mathcal{F} . This means that the Fock space is a direct product of single-mode Hilbert spaces,

$$\mathcal{F} = \bigotimes_{\beta} \mathcal{H}(\text{mode }\beta) \quad \text{where} \quad \mathcal{H}(\text{mode }\beta) \text{ spans } |n_{\beta}\rangle \text{ for } n_{\beta} = 0, 1, 2, 3, \dots$$
 (14)

The Hilbert space of a single mode looks like a Hilbert space of a Harmonic oscillator, so we may construct oscillator-like creation and annihilation operators according to

$$\hat{a}^{\dagger} |n\rangle \stackrel{\text{def}}{=} \sqrt{n+1} |n+1\rangle, \qquad \hat{a} |n\rangle \stackrel{\text{def}}{=} \begin{cases} \sqrt{n} |n-1\rangle & \text{for } n > 0, \\ 0 & \text{for } n = 0, \end{cases}$$
(15)

and hence $\hat{a}^{\dagger}\hat{a} = \hat{n}$ and $[\hat{a}, \hat{a}^{\dagger}] = 1$. Similarly, the direct product of single-mode Hilbert spaces in eq. (14) looks like a system of many harmonic oscillators, one oscillator for each

mode β . This allows us to construct a whole family of oscillator-like creation and annihilation operators in the Fock space, namely

$$\hat{a}^{\dagger}_{\alpha} |\{n_{\beta}\}\rangle \stackrel{\text{def}}{=} \sqrt{n_{\alpha} + 1} |\{n'_{\beta} = n_{\beta} + \delta_{\alpha\beta}\}\rangle,$$

$$\hat{a}_{\alpha} |\{n_{\beta}\}\rangle \stackrel{\text{def}}{=} \begin{cases} \sqrt{n_{\alpha}} |\{n'_{\beta} = n_{\beta} - \delta_{\alpha\beta}\}\rangle & \text{for } n_{\alpha} > 0, \\ 0 & \text{for } n_{\alpha} = 0, \end{cases}$$

$$\hat{n}_{\alpha} = \hat{a}^{\dagger}_{\alpha} \hat{a}_{\alpha}.$$
(16)

It is easy to see from these definitions that the operators $\hat{a}^{\dagger}_{\alpha}$, \hat{a}_{α} , and \hat{n}_{α} for different modes α commute with each other, but for the same mode $[\hat{a}_{\alpha}, \hat{a}^{\dagger}_{\alpha}] = 1$. Altogether, we have the bosonic commutation relations

$$[\hat{a}_{\alpha}, \hat{a}_{\beta}] = 0, \qquad [\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\beta}^{\dagger}] = 0, \qquad [\hat{a}_{\alpha}, \hat{a}_{\beta}^{\dagger}] = \delta_{\alpha\beta}.$$

$$(17)$$

The operators $\hat{a}^{\dagger}_{\alpha}$ and \hat{a}_{α} do not commute with the net particle number operator $\hat{N} = \sum_{\beta} \hat{n}_{\beta}$. Instead, $[\hat{N}, \hat{a}^{\dagger}_{\alpha}] = +\hat{a}^{\dagger}_{\alpha}$, $[\hat{N}, \hat{a}_{\alpha}] = -\hat{a}_{\alpha}$ and hence

$$\hat{N}\hat{a}^{\dagger}_{\alpha} = \hat{a}^{\dagger}_{\alpha}(\hat{N}+1) \quad \text{and} \quad \hat{N}\hat{a}_{\alpha} = \hat{a}_{\alpha}(\hat{N}-1), \tag{18}$$

an $\hat{a}^{\dagger}_{\alpha}$ operator creates a particle while an \hat{a}_{α} operator annihilates (destroys) a particle. That's why the $\hat{a}^{\dagger}_{\alpha}$ are called the *creation operators* and the \hat{a}_{α} are called the *annihilation operators*.

Now let's consider the action of the creation and annihilation operators in the wavefunction language.

Theorem: Let $|N,\psi\rangle$ be an N-boson quantum state with a most general — but totally symmetric — wave function $\psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)$. Let $\psi'(\mathbf{x}_1,\ldots,\mathbf{x}_{N+1})$ be the totally symmetric wave function of the (N+1) boson state $|N+1,\psi'\rangle = \hat{a}^{\dagger}_{\alpha} |N,\psi\rangle$ while $\psi''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})$ is the totally symmetric wave function of the (N-1) boson state $|N-1,\psi''\rangle = \hat{a}_{\alpha} |N,\psi\rangle$. Then:

$$\psi'(\mathbf{x}_1,\ldots,\mathbf{x}_{N+1}) = \frac{1}{\sqrt{N+1}} \sum_{i=1}^{N+1} \phi_\alpha(\mathbf{x}_i) \times \psi(\mathbf{x}_1,\ldots,\mathbf{x}_i,\ldots,\mathbf{x}_{N+1}),$$
(19)

$$\psi''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1}) = \sqrt{N} \int d^3 \mathbf{x}_N \,\phi^*_\alpha(\mathbf{x}_N) \times \psi(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1},\mathbf{x}_N).$$
(20)

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 momentarily use eqs. (19) and (20) as *definitions* of the creation operators $\hat{a}^{\dagger}_{\alpha}$ and the annihilation operators \hat{a}_{α} . To verify that these definitions are completely equivalent to the definitions (16) 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. (19) are indeed the hermitian conjugates of the operators \hat{a}_{α} defined according to eq. (20).

Lemma 2: The operators (19) and (20) obey the bosonic commutation relations

$$[\hat{a}_{\alpha}, \hat{a}_{\beta}] = 0, \qquad [\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\beta}^{\dagger}] = 0, \qquad [\hat{a}_{\alpha}, \hat{a}_{\beta}^{\dagger}] = \delta_{\alpha\beta}.$$

$$(21)$$

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

$$|\alpha, \beta, \cdots, \omega\rangle = \frac{1}{\sqrt{T}} \hat{a}^{\dagger}_{\omega} \cdots \hat{a}^{\dagger}_{\beta} \hat{a}^{\dagger}_{\alpha} |0\rangle$$
(22)

where the creation operators $\hat{a}^{\dagger}_{\alpha}$ act according to eq. (19) 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

$$\phi_{\alpha\beta\cdots\omega}(\mathbf{x}_{1},\mathbf{x}_{2}\ldots,\mathbf{x}_{N}) = \frac{1}{\sqrt{D}} \sum_{\substack{(\tilde{\alpha},\tilde{\beta},\ldots,\tilde{\omega})\\(\tilde{\alpha},\tilde{\beta},\ldots,\tilde{\omega})}}^{\text{distinct permutations}} \phi_{\tilde{\alpha}}(\mathbf{x}_{1}) \times \phi_{\tilde{\beta}}(\mathbf{x}_{2}) \times \cdots \times \phi_{\tilde{\omega}}(\mathbf{x}_{N})$$

$$= \frac{1}{\sqrt{T \times N!}} \sum_{\substack{(\tilde{\alpha},\tilde{\beta},\ldots,\tilde{\omega})\\(\tilde{\alpha},\tilde{\beta},\ldots,\tilde{\omega})}}^{\text{distinct permutations}} \phi_{\tilde{\alpha}}(\mathbf{x}_{1}) \times \phi_{\tilde{\beta}}(\mathbf{x}_{2}) \times \cdots \times \phi_{\tilde{\omega}}(\mathbf{x}_{N}),$$
(23)

where D = N!/T is the number of *distinct permutations*. In other words, the state (22) is precisely the symmetrized state of N bosons in individual states $|\alpha\rangle$, $|\beta\rangle$, ..., $|\omega\rangle$.

I shall prove the Lemmas 1–3 in the Appendix at the end of these notes. For the moment let me simply state that these three Lemmas that the definitions (19) and (20) of the creation and annihilation operators in the wave-function language indeed completely agree with the definitions (16) of the same operators in terms of the occupation number basis.

ONE-BODY AND TWO-BODY OPERATORS IN THE WAVE FUNCTION AND THE FOCK SPACE LANGUAGES

Of particular interest to QM of many-particle systems are operator products $\hat{a}^{\dagger}_{\alpha}\hat{a}^{\dagger}_{\beta}$, $\hat{a}^{\dagger}_{\alpha}\hat{a}^{\dagger}_{\beta}\hat{a}_{\gamma}\hat{a}_{\delta}$, etc., containing equal numbers of creation and annihilation operators. Such products — and their sums — commute with \hat{N} and may be used to construct physically interesting operators for systems where the particles are never created or destroyed. For example, for the free non-relativistic particles (in a big box)

$$\widehat{H}_{\text{tot}} = \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} \hat{a}_{\mathbf{p}}^{\dagger} \hat{a}_{\mathbf{p}}, \qquad \widehat{\mathbf{P}}_{\text{tot}} = \sum_{\mathbf{p}} \mathbf{p} \, \hat{a}_{\mathbf{p}}^{\dagger} \hat{a}_{\mathbf{p}}, \qquad (24)$$

cf. eqs. (12) and (13).

The operators (18) are examples of net one-body operators, *i.e.*, additive operators which act on one particle at a time In the wave-function language (AKA, the first-quantized formalism), such operators act on N-particle states according to

$$\hat{A}_{\text{net}}^{(\text{wf})} = \sum_{i=1}^{N} \hat{A}(i^{\text{th}} \text{ particle})$$
(25)

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

the net momentum operator
$$\hat{\mathbf{P}}_{\text{net}}^{(\text{wf})} = \sum_{i=1}^{N} \hat{\mathbf{p}}_{i},$$
 (26)

the net kinetic energy operator
$$\hat{K}_{\text{net}}^{(\text{wf})} = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_{i}^{2}}{2m},$$
 (27)

the net potential energy operator
$$\hat{V}_{\text{net}}^{(\text{wf})} = \sum_{i=1}^{N} V(\hat{\mathbf{x}}_i).$$
 (28)

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

$$\hat{A}_{\text{net}}^{(\text{fs})} = \sum_{\alpha,\beta} \langle \alpha | \hat{A} | \beta \rangle \times \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}$$
(29)

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

Lemma 4: Although eqs. (25) and (29) look very different from each other, they describe exactly the same net one-body operator.

At this point, it should be obvious to you why and how the lemma works when A has only diagonal matrix elements in the basis $\{|\alpha\rangle\}$, for example the energy and the momentum of a free particle in the momentum basis in eqs. (24). The general case with off-diagonal matrix elements is not so obvious, but you can find the proof in the Appendix to theses notes.

Lemma 5: Let \hat{A} , \hat{B} , and \hat{C} be some one-particle operators, and let $\hat{A}_{net}^{(fs)}$, $\hat{B}_{net}^{(fs)}$, and $\hat{C}_{net}^{(fs)}$ be the corresponding net one-body operators in the fock space according to eq. (29).

if
$$[\hat{A}, \hat{B}] = \hat{C}$$
 then $\left[\hat{A}_{\text{net}}^{(\text{fs})}, \hat{B}_{\text{net}}^{(\text{fs})}\right] = \hat{C}_{\text{net}}^{(\text{fs})}$. (30)

For example, consider a gas of free atoms with nonzero integer spin s = 1, 2, ... In terms of the creation and annihilation operators, the net spin operator for the whole gas becomes

$$\widehat{\mathbf{S}}_{\text{net}} = \sum_{\mathbf{p}} \sum_{m_s, m'_s} \langle s, m_s | \, \widehat{\mathbf{S}}_1 \, \left| s, m'_s \right\rangle \times \hat{a}^{\dagger}_{\mathbf{p}, m_s} \hat{a}_{\mathbf{p}, m'_s} \,, \tag{31}$$

and since the single atom's spin operator obeys the angular momentum commutation relations $[\hat{S}_1^i, \hat{S}_1^j] = i\epsilon^{ijk}\hat{S}_1^k$, the net spin operator satisfies the same relations $[\hat{S}_{net}^i, \hat{S}_{net}^j] = i\epsilon^{ijk}\hat{S}_{net}^k$.

Again, the proof of Lemma 5 is in the Appendix to these notes.

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Interactions between particles are described by operators involving two or more particles at the same time. For example, a two-body potential $V_2(\mathbf{x}_i - \mathbf{x}_j)$ gives rise to the net potential operator which acts on a wave functions of N particles as

$$\hat{V}_{\text{net}}\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \frac{1}{2} \sum_{i\neq j}^{i,j=1,\ldots,N} V_2(\mathbf{x}_i-\mathbf{x}_j)\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N).$$
(32)

In the Fock-space formalism, this operator becomes

$$\widehat{V}_{\text{net}} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha,\beta,\gamma,\delta} \times \hat{a}^{\dagger}_{\alpha} \hat{a}^{\dagger}_{\beta} \hat{a}_{\delta} \hat{a}_{\gamma}$$
(33)

where $V_{\alpha,\beta,\gamma,\delta}$ are the matrix elements

$$V_{\alpha,\beta,\gamma,\delta} = \int d\mathbf{x}_1 \int d\mathbf{x}_2 \,\phi^*_{\alpha}(\mathbf{x}_1) \phi^*_{\beta}(\mathbf{x}_2) \times V_2(\mathbf{x}_1 - \mathbf{x}_2) \times \phi_{\gamma}(\mathbf{x}_1) \phi_{\delta}(\mathbf{x}_2). \tag{34}$$

In particular, in the momentum basis $|\mathbf{p}\rangle$,

$$V_{\mathbf{p}_{1}',\mathbf{p}_{2}',\mathbf{p}_{1},\mathbf{p}_{2}} = L^{-3}\delta_{\mathbf{p}_{1}'+\mathbf{p}_{2}',\mathbf{p}_{1}+\mathbf{p}_{2}} \times W(\mathbf{q})$$

where $\mathbf{q} = \mathbf{p}_{1}' - \mathbf{p}_{1} = \mathbf{p}_{2} - \mathbf{p}_{2}'$ and $W(\mathbf{q}) = \int d\mathbf{x} \, e^{-i\mathbf{q}\mathbf{x}} \, V_{2}(\mathbf{x}),$ (35)

hence

$$\widehat{V}_{\text{net}} = \frac{1}{2} L^{-3} \sum_{\mathbf{q}} W(\mathbf{q}) \sum_{\mathbf{p}_1, \mathbf{p}_2} \hat{a}^{\dagger}_{\mathbf{p}_1 + \mathbf{q}} \hat{a}^{\dagger}_{\mathbf{p}_2 - \mathbf{q}} \hat{a}_{\mathbf{p}_2} \hat{a}_{\mathbf{p}_1} \,.$$
(36)

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

$$\hat{B}_{\text{net}}^{(\text{wf})} = \frac{1}{2} \sum_{i \neq j}^{i,j=1,\dots,N} \hat{B}(i^{\text{th}} \text{ and } j^{\text{th}} \text{ particles}).$$
(37)

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

$$\hat{B}_{\text{net}}^{(\text{fs})} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \left(\langle \alpha | \otimes \langle \beta | \rangle \hat{B}(|\gamma\rangle \otimes |\delta\rangle) \, \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}^{\dagger} \hat{a}_{\delta} \hat{a}_{\gamma} \,.$$
(38)

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 $\hat{B}_{net}^{(fs)}$, 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} .

Lemma 6: For any two-particle operator \hat{B} eqs. (37) and (38) define exactly the same net operator \hat{B}_{net} . Similar to the other lemmas, the proof of this Lemma 6 is in the Appendix to these notes.

The two-body operators in the Fock space obey the same kind of commutation relations as the corresponding two-particle operators. For example:

Lemma 7: Let \hat{A} be a one-particle operator while \hat{B} and \hat{C} are two-particle operators. Let $\hat{A}_{net}^{(fs)}$, $\hat{B}_{net}^{(fs)}$, and $\hat{C}_{net}^{(fs)}$ be the corresponding net operators in the Fock space according to eqs. (29) and (38).

$$\mathbf{if} \quad \left[\left(\hat{A}(1^{\mathrm{st}}) + \hat{A}(2^{\mathrm{nd}}) \right), \hat{B} \right] = \hat{C} \quad \mathbf{then} \quad \left[\hat{A}_{\mathrm{net}}^{(\mathrm{fs})}, \hat{B}_{\mathrm{net}}^{(\mathrm{fs})} \right] = \hat{C}_{\mathrm{net}}^{(\mathrm{fs})}. \tag{39}$$

Again, the proof of this Lemma is in the Appendix.

Generalization of the Fock-space formalism to operators involving more than two particles at the same time is straightforward. Three-body additive operators become sums of $\hat{a}^{\dagger}_{\alpha}\hat{a}^{\dagger}_{\beta}\hat{a}^{\dagger}_{\gamma}a_{\zeta}\hat{a}_{\epsilon}\hat{a}_{\delta}$ with appropriate matrix-element coefficients, four-body operators involve products $\hat{a}^{\dagger}\hat{a}^{\dagger}\hat{a}^{\dagger}\hat{a}^{\dagger}\hat{a}\hat{a}\hat{a}\hat{a}$ of four creation and four annihilation operators, *etc.*, *etc.*

NON-RELATIVISTIC QUANTUM FIELDS

In the previous section, we defined the creation and the annihilation operators in terms of a particular basis of single-particle states $|\alpha\rangle$. Changing to a new basis $\{|\mu\rangle\}$ involves a linear transform $|\mu\rangle = \sum_{\alpha} |\alpha\rangle \times \langle \alpha |\mu\rangle$ and hence a similar linear transform of the creation / annihilation operators from $\hat{a}^{\dagger}_{\alpha}$ and \hat{a}_{α} to \hat{a}^{\dagger}_{μ} and \hat{a}_{μ} , namely

$$\hat{a}^{\dagger}_{\mu} = \sum_{\alpha} \hat{a}^{\dagger}_{\alpha} \times \langle \alpha | \mu \rangle, \qquad \hat{a}_{\mu} = \sum_{\alpha} \hat{a}_{\alpha} \times \langle \mu | \alpha \rangle.$$
(40)

Indeed, in the Fock space $|\alpha\rangle = \hat{a}^{\dagger}_{\alpha} |0\rangle$ while $|\mu\rangle = \hat{a}^{\dagger}_{\mu} |0\rangle$, so the creation operators transform exactly like Dirac kets; by Hermitian conjugation, the annihilation operators transform like Dirac bras. And thanks to unitarity of this transform, the \hat{a}_{μ} and the \hat{a}^{\dagger}_{μ} obey the same bosonic commutation relations (17) as the \hat{a}_{α} and the $\hat{a}^{\dagger}_{\alpha}$.

Of particular importance is the coordinate basis in which the \mathbf{x} -labeled operators become quantum fields. Specifically, the *creation field*

$$\widehat{\Psi}^{\dagger}(\mathbf{x}) \equiv \widehat{a}_{\mathbf{x}}^{\dagger} = \sum_{\alpha} \widehat{a}_{\alpha}^{\dagger} \times \phi_{\alpha}(\mathbf{x})$$
(41)

which creates a particle at point \mathbf{x} , and the annihilation field

$$\widehat{\Psi}(\mathbf{x}) \equiv \widehat{a}_{\mathbf{x}} = \sum_{\alpha} \widehat{a}_{\alpha} \times \phi_{\alpha}^{*}(\mathbf{x})$$
(42)

which annihilates a particle at point \mathbf{x} . These fields obey the continuous version of the bosonic commutation relations (17), namely

$$\left[\widehat{\Psi}(\mathbf{x}), \widehat{\Psi}(\mathbf{x}')\right] = 0, \qquad \left[\widehat{\Psi}^{\dagger}(\mathbf{x}), \widehat{\Psi}^{\dagger}(\mathbf{x}')\right] = 0, \qquad \left[\widehat{\Psi}(\mathbf{x}), \widehat{\Psi}^{\dagger}(\mathbf{x}')\right] = \delta^{(3)}(\mathbf{x} - \mathbf{x}').$$
(43)

In the non-relativistic many-particle theory, many operators may be expressed in terms of the creation and annihilation fields as $\int d^3 \mathbf{x}$ (something local). For example, the net particle

number operator \hat{N} becomes

$$\hat{N} = \sum_{\alpha} \hat{a}^{\dagger}_{\alpha} \hat{a}_{\alpha} = \int d^3 \mathbf{x} \,\widehat{\Psi}^{\dagger}(\mathbf{x}) \widehat{\Psi}(\mathbf{x}), \qquad (44)$$

which tells us that $\hat{n}(\mathbf{x}) = \widehat{\Psi}^{\dagger}(\mathbf{x})\widehat{\Psi}(\mathbf{x})$ is the local particle density operator. Consequently, the potential energy operator for particles interacting with an external potential $V_e(\mathbf{x})$ is

$$\hat{V}_{\text{net}} = \int d^3 \mathbf{x} \, V_e(\mathbf{x}) \times \hat{n}(\mathbf{x}) = \int d^3 \mathbf{x} \, V_e(\mathbf{x}) \times \widehat{\Psi}^{\dagger}(\mathbf{x}) \widehat{\Psi}(\mathbf{x}).$$
(45)

Similarly, the net momentum operator is

$$\widehat{\mathbf{P}}_{\text{net}} = \sum_{\mathbf{p}} \mathbf{p} \, \hat{a}_{\mathbf{p}}^{\dagger} \hat{a}_{\mathbf{p}} = \int d^3 \mathbf{x} \, \widehat{\Psi}^{\dagger}(\mathbf{x}) \left(-i \nabla \widehat{\Psi}(\mathbf{x}) \right), \tag{46}$$

and the net non-relativistic kinetic energy operator is

$$\hat{H}_{\text{net}}^{\text{kin}} = \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} \hat{a}_{\mathbf{p}}^{\dagger} \hat{a}_{\mathbf{p}} = \int d^3 \mathbf{x} \,\widehat{\Psi}^{\dagger}(\mathbf{x}) \left(\frac{-\nabla^2}{2m} \,\widehat{\Psi}(\mathbf{x})\right) = +\frac{1}{2m} \int d^3 \mathbf{x} \,\nabla \widehat{\Psi}^{\dagger}(\mathbf{x}) \cdot \nabla \widehat{\Psi}(\mathbf{x}).$$
(47)

Thus, the non-relativistic particles in an external potential $V_e(\mathbf{x})$ but not interacting with each other have the Fock-space Hamiltonian of the form

$$\hat{H} = \hat{H}_{\text{net}}^{\text{kin}} + \hat{V}_{\text{net}} = \int d^3 \mathbf{x} \left(\frac{1}{2m} \nabla \widehat{\Psi}^{\dagger}(\mathbf{x}) \cdot \nabla \widehat{\Psi}(\mathbf{x}) + V_e(\mathbf{x}) \widehat{\Psi}^{\dagger}(\mathbf{x}) \widehat{\Psi}(\mathbf{x}) \right)
= \int d^3 \mathbf{x} \, \widehat{\Psi}^{\dagger}(\mathbf{x}) \left(-\frac{\nabla^2}{2m} + V_e(\mathbf{x}) \right) \widehat{\Psi}(\mathbf{x}).$$
(48)

For this Hamiltonian, the Heisenberg equations for the quantum fields become similar to the ordinary Schrödinger equations for single-particle wave functions. Indeed, in the Heisenberg picture of QM, the time-dependent quantum fields satisfy

$$i\frac{\partial}{\partial t}\widehat{\Psi}(\mathbf{x},t) = \left[\widehat{\Psi}(\mathbf{x},t),\widehat{H}\right] = \left(-\frac{\nabla^2}{2m} + V_e(\mathbf{x})\right)\widehat{\Psi}(\mathbf{x},t),$$

$$-i\frac{\partial}{\partial t}\widehat{\Psi}^{\dagger}(\mathbf{x},t) = \left[\widehat{H},\widehat{\Psi}(\mathbf{x},t)\right] = \left(-\frac{\nabla^2}{2m} + V_e(\mathbf{x})\right)\widehat{\Psi}^{\dagger}(\mathbf{x},t).$$
(49)

Despite the similarity, these are not the true Schrödinger equations of the many-particle system because: (1) They apply in the wrong picture of QM (Heisenberg instead of Schrödinger).

(2) The true wave-function $\psi(\mathbf{x}_1, \ldots, \mathbf{x}_N; t)$ of N particles depends on all of their coordinates $\mathbf{x}_1, \ldots, \mathbf{x}_N$, unlike the quantum field $\widehat{\Psi}(\mathbf{x}, t)$ which depends on a single \mathbf{x} regardless of how many particles we have (or rather had since $\widehat{\Psi}$ does not preserve N). (3) Adding interactions to the Hamiltonian (48) would make eqs. (49) non-linear, while the true Schrödinger equations are always linear, no matter what.

Indeed, let the particles have a two-body interaction potential (32). In terms of the quantum creation and annihilation fields, the Fock-space two-body potential becomes

$$\widehat{V}_{\text{int}} = \frac{1}{2} \int d^3 \mathbf{x}_1 \int d^3 \mathbf{x}_2 \, V_2(\mathbf{x}_1 - \mathbf{x}_2) \times \widehat{\Psi}^{\dagger}(\mathbf{x}_1) \widehat{\Psi}^{\dagger}(\mathbf{x}_2) \widehat{\Psi}(\mathbf{x}_2) \widehat{\Psi}(\mathbf{x}_1).$$
(50)

Adding this interaction to the free Hamiltonian (48) makes the Heisenberg equations for the quantum fields nonlinear (and non-local), namely:

$$i\frac{\partial}{\partial t}\widehat{\Psi}(\mathbf{x},t) = \left[\widehat{\Psi}(\mathbf{x},t),\widehat{H}\right] = \left(-\frac{\nabla^2}{2m} + V_e(\mathbf{x})\right)\widehat{\Psi}(\mathbf{x},t) + \int d^3\mathbf{x}' V_2(\mathbf{x}'-\mathbf{x})\widehat{\Psi}^{\dagger}(\mathbf{x}')\widehat{\Psi}(\mathbf{x}') \times \widehat{\Psi}(\mathbf{x}), -i\frac{\partial}{\partial t}\widehat{\Psi}^{\dagger}(\mathbf{x},t) = -\left[\widehat{\Psi}^{\dagger}(\mathbf{x},t),\widehat{H}\right] = \left(-\frac{\nabla^2}{2m} + V_e(\mathbf{x})\right)\widehat{\Psi}^{\dagger}(\mathbf{x},t) + \widehat{\Psi}^{\dagger}(\mathbf{x}) \times \int d^3\mathbf{x}' V_2(\mathbf{x}'-\mathbf{x})\widehat{\Psi}^{\dagger}(\mathbf{x}')\widehat{\Psi}(\mathbf{x}').$$
(51)

However, without the two-body (or multi-body) interactions between the particles, the Heisenberg equations (49) are linear and look just like Schrödinger equation for a singleparticle wave function. This similarity suggest that the quantum fields $\widehat{\Psi}(\mathbf{x}, t)$ and $\widehat{\Psi}^{\dagger}(\mathbf{x}, t)$ may be obtained via the *second quantization*, which works like this: First, one quantizes a single particle and writes the Schrödinger equation for its wave function. Second, one re-interprets this wave function as a *classical field* $\psi(\mathbf{x}, t)$ and the the Schrödinger equation becomes an Euler-Lagrange field equation which follows from the Lagrangian density

$$\mathcal{L}_{\text{Schr}} = -\hbar \operatorname{Im}(\psi^* \dot{\psi}) - \frac{\hbar^2}{2m} \nabla \psi^* \nabla \psi - V_e(\mathbf{x}) \times \psi^* \psi.$$
(52)

(Note, $-\hbar \operatorname{Im}(\psi^* \dot{\psi}) = i\hbar \psi^* \dot{\psi} + a$ total derivative.) Third, one switches to the Hamiltonian formalism where the canonical conjugate field for $\psi(\mathbf{x})$ is $\varpi(\mathbf{x}) = i\hbar\psi^*(\mathbf{x})$ and the classical

Hamiltonian is

$$H = \int d^3 \mathbf{x} \left(i\hbar \psi^* \times \dot{\psi} - \mathcal{L} \right) = \int d^3 \mathbf{x} \left(\frac{\hbar^2}{2m} \nabla \psi^* \nabla \psi + V_e(\mathbf{x}) \times \psi^* \psi \right).$$
(53)

Finally, one quantizes the fields $\psi(\mathbf{x})$ and $\psi^*(\mathbf{x})$, hence the name "second quantization" as the "first quantization" was writing down the single-particle Schrödinger equation in the first place. Consequently, $\psi(\mathbf{x})$ and $\psi^*(\mathbf{x})$ become quantum fields $\widehat{\Psi}(\mathbf{x})$ and $\widehat{\Psi}^{\dagger}(\mathbf{x})$ obeying the commutation relations (43) (which follow from the $i\hbar\psi^*(\mathbf{x})$ being the canonical conjugate of $\psi(\mathbf{x})$), and the classical Hamiltonian (53) becomes the Hamiltonian operator (48).

Historically, the second quantization was used as a *heuristic* for deriving the non-relativistic quantum field theory. Some people tried to take the second quantization literally and got into all kinds of trouble because it does not make physical sense: A wave function is not a classical field, and it should not be quantized again. Instead, one should not take the intermediate steps of the second quantization seriously but focus on the end result — which is a perfectly good quantum field theory. However, the physical content of this theory is not a single particle but an arbitrary number of identical bosons, and the $\widehat{\Psi}(\mathbf{x})$ and $\widehat{\Psi}^{\dagger}(\mathbf{x})$ are not quantized-again wave functions but quantum fields which destroy and create particles in the Fock space. And of course, physically there is only one quantization.

The physically correct way to derive the non-relativistic QFT is the way we did it in this note, the second quantization is only an old heuristic. Today, when one talks about a second-quantized theory, it is simply a name for a quantum theory of an arbitrary number of particles, usually formulated in terms of creation and annihilation operators in the Fock space.

Appendix: Proofs of the Lemmas

Lemma 1: The creation operators $\hat{a}^{\dagger}_{\alpha}$ defined according to eq. (19) are indeed the hermitian conjugates of the operators \hat{a}_{α} defined according to eq. (20).

Reminder: the equations (19) and (20) spell out the wavefunctions $\psi'(\mathbf{x}_1, \ldots, \mathbf{x}_{N+1})$ and $\psi''(\mathbf{x}, \ldots, \mathbf{x}_{N-1})$ of the states $|N+1, \psi'\rangle = \hat{a}^{\dagger}_{\alpha} |N, \psi\rangle$ and $|N-1, \psi''\rangle = \hat{a}_{\alpha} |N, psi\rangle$ in terms

of the (totally symmetric) wave function $\psi(\mathbf{x}_1, \ldots, \mathbf{x}_N)$ of the *N*-boson state $|N, \psi\rangle$. Specifically,

$$\psi'(\mathbf{x}_1,\ldots,\mathbf{x}_{N+1}) = \frac{1}{\sqrt{N+1}} \sum_{i=1}^{N+1} \phi_\alpha(\mathbf{x}_i) \times \psi(\mathbf{x}_1,\ldots,\mathbf{x}_i,\ldots,\mathbf{x}_{N+1}),$$
(19)

$$\psi''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1}) = \sqrt{N} \int d^3 \mathbf{x}_N \,\phi^*_\alpha(\mathbf{x}_N) \times \psi(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1},\mathbf{x}_N).$$
(20)

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

$$\langle \widetilde{N}, \widetilde{\psi} | \hat{a}_{\alpha} | N, \psi \rangle = \langle N, \psi | \hat{a}_{\alpha}^{\dagger} | \widetilde{N}, \widetilde{\psi} \rangle^{*}.$$
(54)

Since the \hat{a}_{α} always lowers the number of particles by 1 while the $\hat{a}_{\alpha}^{\dagger}$ always raises it by 1, it is enough to check this equation for $\tilde{N} = N - 1$ — 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. (20). Then, on the LHS of eq. (54) we have

$$\langle N-1, \widetilde{\psi} | \hat{a}_{\alpha} | N, \psi \rangle = \langle N-1, \widetilde{\psi} | N-1, \psi'' \rangle$$

$$= \int d^{3} \mathbf{x}_{1} \cdots \int d^{3} \mathbf{x}_{N-1} \widetilde{\psi}^{*}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N-1}) \times \psi''(\mathbf{x}_{1}, \dots, \mathbf{x}_{N-1})$$

$$= \int d^{3} \mathbf{x}_{1} \cdots \int d^{3} \mathbf{x}_{N-1} \widetilde{\psi}^{*}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N-1}) \times$$

$$\times \sqrt{N} \int d^{3} \mathbf{x}_{N} \phi_{\alpha}^{*} \times \psi(\mathbf{x}_{1}, \dots, \mathbf{x}_{N})$$

$$= \sqrt{N} \int d^{3} \mathbf{x}_{1} \cdots \int d^{3} \mathbf{x}_{N} \widetilde{\psi}^{*}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N-1}) \times \phi_{\alpha}^{*}(\mathbf{x}_{N}) \times \psi(\mathbf{x}_{1}, \dots, \mathbf{x}_{N}).$$

$$(55)$$

Likewise, let $\widetilde{\psi}'(\mathbf{x}_1,\ldots,\mathbf{x}_N)$ be the wave function of the state $|N,\widetilde{\psi}'\rangle = \hat{a}^{\dagger}_{\alpha}|N-1,\widetilde{\psi}\rangle$ ac-

cording to eq. (19). Then the matrix element on the RHS of eq. (54) becomes

$$\langle N, \psi | \, \hat{a}^{\dagger}_{\alpha} \, | N - 1, \widetilde{\psi} \rangle = \int d^{3} \mathbf{x}_{1} \, \cdots \int d^{3} \mathbf{x}_{N} \, \psi^{*}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N}) \times \widetilde{\psi}'(\mathbf{x}_{1}, \dots, \mathbf{x}_{N}) \\ = \int d^{3} \mathbf{x}_{1} \, \cdots \int d^{3} \mathbf{x}_{N} \, \psi^{*}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N}) \times \\ \times \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \phi_{\alpha}(\mathbf{x}_{i}) \times \widetilde{\psi}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N}) \\ = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \int d^{3} \mathbf{x}_{1} \, \cdots \int d^{3} \mathbf{x}_{N} \, \psi^{*}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N}) \times \\ \times \phi_{\alpha}(\mathbf{x}_{i}) \times \widetilde{\psi}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N}).$$

$$(56)$$

By bosonic symmetry of the wavefunctions ψ and $\tilde{\psi}$, 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

$$\langle N, \psi | \hat{a}^{\dagger}_{\alpha} | N - 1, \widetilde{\psi} \rangle = \frac{N}{\sqrt{N}} \times \int d^{3} \mathbf{x}_{1} \cdots \int d^{3} \mathbf{x}_{N} \psi^{*}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N}) \times \phi_{\alpha}(\mathbf{x}_{N}) \times \widetilde{\psi}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N-1}).$$
(57)

By inspection, the RHS of eqs. (55) and (57) are complex conjugates of each other, thus

$$\langle N-1, \widetilde{\psi} | \hat{a}_{\alpha} | N, \psi \rangle = \langle N, \psi | \hat{a}_{\alpha}^{\dagger} | N-1, \widetilde{\psi} \rangle^{*}.$$
(54)

This completes the proof of Lemma 1.

Lemma 2: The operators (19) and (20) obey the bosonic commutation relations

$$[\hat{a}_{\alpha}, \hat{a}_{\beta}] = 0, \qquad [\hat{a}_{\alpha}^{\dagger}, \hat{a}_{\beta}^{\dagger}] = 0, \qquad [\hat{a}_{\alpha}, \hat{a}_{\beta}^{\dagger}] = \delta_{\alpha\beta}.$$

$$(58)$$

Proof: Let's start by verifying that the creation operators defined according to eq. (19) 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. (19) twice, we immediately obtain

$$\psi^{\prime\prime\prime}(\mathbf{x}_{1},\ldots,\mathbf{x}_{N+2}) = \frac{1}{\sqrt{(N+1)(N+2)}} \sum_{\substack{i,j=1,\ldots,N+2\\i\neq j}} \phi_{\alpha}(\mathbf{x}_{i}) \times \phi_{\beta}(\mathbf{x}_{j}) \times \\ \times \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{N+2} \text{ except } \mathbf{x}_{i},\mathbf{x}_{j}).$$
(59)

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 (59), thus

$$\hat{a}^{\dagger}_{\alpha}\hat{a}^{\dagger}_{\beta}|N,\psi\rangle = \hat{a}^{\dagger}_{\beta}\hat{a}^{\dagger}_{\alpha}|N,\psi\rangle.$$
(60)

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}_{α} and \hat{a}_{β} defined according to eq. (20) and show that they commute with each other. Again, let $|N,\psi\rangle$ be an arbitrary N-boson state . For N < 2 we have

$$\hat{a}_{\alpha}\hat{a}_{\beta}|N,\psi\rangle = 0 = \hat{a}_{\beta}\hat{a}_{\alpha}^{\dagger}|N,\psi\rangle, \qquad (61)$$

so let's focus on the non-trivial case of $N \ge 2$ and consider the (N-2)-boson wavefunction ψ'''' of the state $|N-2,\psi''''\rangle = \hat{a}_{\alpha}\hat{a}_{\beta} |N,\psi\rangle$. Applying eq. (20) twice, we obtain

$$\psi^{\prime\prime\prime\prime}(\mathbf{x}_{1},\ldots,\mathbf{x}_{N-2}) = \sqrt{N(N-1)} \int d^{3}\mathbf{x}_{N} \int d^{3}\mathbf{x}_{N-1} \ \phi^{*}_{\alpha}(\mathbf{x}_{N}) \times \phi^{*}_{\beta}(\mathbf{x}_{N-1}) \times \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{N-2},\mathbf{x}_{N-1},\mathbf{x}_{N}).$$
(62)

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

$$\hat{a}_{\alpha}\hat{a}_{\beta}|N,\psi\rangle = \hat{a}_{\beta}\hat{a}_{\alpha}|N,\psi\rangle.$$
(63)

Therefore, when the annihilation operators defined according to eq. (20) act on the totallysymmetric 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}_{α} , pick an arbitrary N-boson state $|N,\psi\rangle$, and consider the difference between the states

$$|N,\psi^5\rangle = \hat{a}^{\dagger}_{\beta}\hat{a}_{\alpha}|N,\psi\rangle \text{ and } |N,\psi^6\rangle = \hat{a}_{\alpha}\hat{a}^{\dagger}_{\beta}|N,\psi\rangle.$$
 (64)

Suppose N > 0. Applying eq. (20) to the wave function ψ and then applying eq. (19) to the result, we obtain

$$\psi^{5}(\mathbf{x}_{1},\ldots,\mathbf{x}_{N}) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \phi_{\beta}(\mathbf{x}_{i}) \times \psi''(\mathbf{x}_{1},\ldots,\mathbf{x}_{i},\ldots,\mathbf{x}_{N})$$

$$= \sum_{i=1}^{N} \phi_{\beta}(\mathbf{x}_{i}) \times \int d^{3}\mathbf{x}_{N+1} \phi_{\alpha}^{*}(\mathbf{x}_{N+1}) \times \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{i},\ldots,\mathbf{x}_{N},\mathbf{x}_{N+1}).$$
(65)

On the other hand, applying first eq. (19) and then eq. (20), we arrive at

$$\begin{split} \psi^{6}(\mathbf{x}_{1},\ldots,\mathbf{x}_{N}) &= \sqrt{N+1} \int d^{3}\mathbf{x}_{N+1} \phi_{\alpha}^{*}(\mathbf{x}_{N+1}) \times \psi'(\mathbf{x}_{1},\ldots,\mathbf{x}_{N},\mathbf{x}_{N+1}) \\ &= \int d^{3}\mathbf{x}_{N+1} \phi_{\alpha}^{*}(\mathbf{x}_{N+1}) \times \sum_{i=1}^{N+1} \phi_{\beta}(\mathbf{x}_{i}) \times \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{i},\ldots,\mathbf{x}_{N+1}) \\ &= \int d^{3}\mathbf{x}_{N+1} \phi_{\alpha}^{*}(\mathbf{x}_{N+1}) \times \left(\sum_{i=1}^{N} \phi_{\beta}(\mathbf{x}_{i}) \times \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{N},\mathbf{x}_{N+1}) \right) \\ &+ \phi_{\beta}(\mathbf{x}_{N+1}) \times \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{N}) \\ &= \sum_{i=1}^{N} \phi_{\beta}(\mathbf{x}_{i}) \times \int d^{3}\mathbf{x}_{N+1} \phi_{\alpha}^{*}(\mathbf{x}_{N+1}) \times \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{N},\mathbf{x}_{N+1}) \\ &+ \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{N}) \times \int d^{3}\mathbf{x}_{N+1} \phi_{\alpha}^{*}(\mathbf{x}_{N+1}) \times \phi_{\beta}(\mathbf{x}_{N+1}) \\ &= \psi^{5}(\mathbf{x}_{1},\ldots,\mathbf{x}_{N}) \quad \langle\langle \text{ compare to eq. (65) } \rangle\rangle \\ &+ \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{N}) \times \langle\phi_{\alpha}|\phi_{\beta}\rangle \,. \end{split}$$
(66)

Comparing eqs. (65) and (66), we see that

$$\psi^{6}(\mathbf{x}_{1},\ldots,\mathbf{x}_{N})-\psi^{5}(\mathbf{x}_{1},\ldots,\mathbf{x}_{N}) = \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{N})\times\left\langle\phi_{\alpha}|\phi_{\beta}\right\rangle = \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{N})\times\delta_{\alpha\beta}, \quad (67)$$

where $\langle \phi_{\alpha} | \phi_{\beta} \rangle = \delta_{\alpha\beta}$ by orthonormality of the 1-particle basis $\{\phi_{\gamma}(\mathbf{x})\}_{\gamma}$. In Dirac notations, eq. (67) amounts to

$$\left(\hat{a}_{\alpha}\hat{a}_{\beta}^{\dagger}-\hat{a}_{\beta}^{\dagger}\hat{a}_{\alpha}\right)|N,\psi\rangle = |N,\psi\rangle \times \delta_{\alpha\beta}.$$
(68)

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

$$\hat{a}_{\alpha} |0\rangle = 0 \implies \hat{a}_{\beta}^{\dagger} \hat{a}_{\alpha} |0\rangle = 0,$$
 (69)

while

$$\hat{a}_{\alpha}\hat{a}^{\dagger}_{\beta}|0\rangle = \hat{a}_{\alpha}|1,\phi_{\beta}\rangle = \langle\phi_{\alpha}|\phi_{\beta}\rangle \times |0\rangle = \delta_{\alpha\beta} \times |0\rangle, \qquad (70)$$

hence

$$\left(\hat{a}_{\alpha}\hat{a}_{\beta}^{\dagger}-\hat{a}_{\beta}^{\dagger}\hat{a}_{\alpha}\right)\left|0\right\rangle = \delta_{\alpha\beta}\times\left|0\right\rangle.$$

$$(71)$$

Altogether, eqs. (68) and (71) verify that

$$[\hat{a}_{\alpha}, \hat{a}_{\beta}^{\dagger}] |\Psi\rangle = \delta_{\alpha\beta}\Psi \tag{72}$$

for any state Ψ in the bosonic Fock space, hence the operators \hat{a}_{α} and $\hat{a}_{\beta}^{\dagger}$ defined according to eqs. (19) and (20) indeed obey the commutation relation $[\hat{a}_{\alpha}, \hat{a}_{\beta}^{\dagger}] = \delta_{\alpha,\beta}$.

This completes the proof of Lemma 2.

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

$$|\alpha, \beta, \cdots, \omega\rangle = \frac{1}{\sqrt{T}} \hat{a}^{\dagger}_{\omega} \cdots \hat{a}^{\dagger}_{\beta} \hat{a}^{\dagger}_{\alpha} |0\rangle$$
(73)

where the creation operators $\hat{a}^{\dagger}_{\alpha}$ act according to eq. (19) 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

$$\phi_{\alpha\beta\cdots\omega}(\mathbf{x}_{1},\mathbf{x}_{2}\ldots,\mathbf{x}_{N}) = \frac{1}{\sqrt{D}} \sum_{(\tilde{\alpha},\tilde{\beta},\ldots,\tilde{\omega})}^{\text{distinct permutations}} \phi_{\tilde{\alpha}}(\mathbf{x}_{1}) \times \phi_{\tilde{\beta}}(\mathbf{x}_{2}) \times \cdots \times \phi_{\tilde{\omega}}(\mathbf{x}_{N})$$

$$= \frac{1}{\sqrt{T \times N!}} \sum_{(\tilde{\alpha},\tilde{\beta},\ldots,\tilde{\omega})}^{\text{all }N! \text{ permutations}} \phi_{\tilde{\alpha}}(\mathbf{x}_{1}) \times \phi_{\tilde{\beta}}(\mathbf{x}_{2}) \times \cdots \times \phi_{\tilde{\omega}}(\mathbf{x}_{N}),$$
(74)

where D = N!/T is the number of *distinct permutations*. In other words, the state (73) is precisely the symmetrized state of N bosons in individual states $|\alpha\rangle$, $|\beta\rangle$, ..., $|\omega\rangle$.

Proof: Let me start with a note on the normalization factor $1/\sqrt{T}$ in eq. (73). 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,

$$|\alpha,\beta\rangle = \hat{a}^{\dagger}_{\beta}\hat{a}^{\dagger}_{\alpha}|0\rangle \quad \text{when } \alpha \neq \beta, \quad \text{but} \quad |\alpha,\alpha\rangle = \frac{1}{\sqrt{2}}\hat{a}^{\dagger}_{\alpha}\hat{a}^{\dagger}_{\alpha}|0\rangle.$$
 (75)

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

$$|\{n_{\alpha}\}_{\alpha}\rangle = \bigotimes_{\alpha} \left(|n_{\alpha}\rangle = \frac{\left(\hat{a}_{\alpha}^{\dagger}\right)^{n_{\alpha}}}{\sqrt{n_{\alpha}!}} |0\rangle\right)_{\text{mode }\alpha} = \left(\prod_{\alpha} \frac{\left(\hat{a}_{\alpha}^{\dagger}\right)^{n_{\alpha}}}{\sqrt{n_{\alpha}!}}\right) |\text{vacuum}\rangle.$$
(76)

hence the factor $1/\sqrt{T}$ in eq. (73).

Now let's work out the wave functions of the states (73) by successively applying the creation operators according to eq. (19):

- 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

$$\sqrt{T} \times \phi_{\alpha\beta}(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{\sqrt{2}} \Big(\phi_\beta(\mathbf{x}_1) \phi_\alpha(\mathbf{x}_2) + \phi_\beta(\mathbf{x}_2) \phi_\alpha(\mathbf{x}_1) \Big).$$
(77)

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

$$\sqrt{T} \times \phi_{\alpha\beta\gamma}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \frac{1}{\sqrt{3}} \begin{pmatrix} \phi_{\gamma}(\mathbf{x}_1) \times \frac{1}{\sqrt{2}} (\phi_{\beta}(\mathbf{x}_2)\phi_{\alpha}(\mathbf{x}_3) + \phi_{\beta}(\mathbf{x}_3)\phi_{\alpha}(\mathbf{x}_2)) \\ + \phi_{\gamma}(\mathbf{x}_2) \times \frac{1}{\sqrt{2}} (\phi_{\beta}(\mathbf{x}_1)\phi_{\alpha}(\mathbf{x}_3) + \phi_{\beta}(\mathbf{x}_3)\phi_{\alpha}(\mathbf{x}_1)) \\ + \phi_{\gamma}(\mathbf{x}_3) \times \frac{1}{\sqrt{2}} (\phi_{\beta}(\mathbf{x}_1)\phi_{\alpha}(\mathbf{x}_2) + \phi_{\beta}(\mathbf{x}_2)\phi_{\alpha}(\mathbf{x}_1)) \end{pmatrix}$$

$$= \frac{1}{\sqrt{3!}} \sum_{(\tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}_2, \tilde{\mathbf{x}}_3)}^{6 \text{ permutations}} \phi_{\gamma}(\tilde{\mathbf{x}}_1) \phi_{\beta}(\tilde{\mathbf{x}}_2) \phi_{\alpha}(\tilde{\mathbf{x}}_3)$$

$$= \frac{1}{\sqrt{3!}} \sum_{(\tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}_2, \tilde{\mathbf{x}}_3)}^{6 \text{ permutations}} \phi_{\gamma}(\tilde{\mathbf{x}}_1) \phi_{\beta}(\tilde{\mathbf{x}}_2) \phi_{\alpha}(\tilde{\mathbf{x}}_3)$$

$$= \frac{1}{\sqrt{3!}} \sum_{(\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma})}^{\text{of } (\alpha, \beta, \gamma)} \phi_{\tilde{\alpha}}(\mathbf{x}_1) \phi_{\tilde{\beta}}(\mathbf{x}_2) \phi_{\tilde{\gamma}}(\mathbf{x}_3).$$
(78)

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.(78), the *N*-particle state $\sqrt{T} |\alpha, \ldots, \omega\rangle = \hat{a}_{\omega}^{\dagger} \cdots \hat{a}_{\alpha}^{\dagger} |0\rangle$, has the totally-symmetrized wave function

$$\sqrt{T} \times \phi_{\alpha \cdots \omega}(\mathbf{x}_1, \dots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \sum_{(\tilde{\alpha}, \dots, \tilde{\omega})}^{\text{all permutations}} \phi_{\tilde{\alpha}}(\mathbf{x}_1) \times \dots \times \phi_{\tilde{\omega}}(\mathbf{x}_N).$$
(79)

Dividing both sides of this formula by the \sqrt{T} factor, we immediately arrive at the second line of eq. (74).

Finally, the top line of eq. (74) obtains from the bottom line by adding up coincident terms. Indeed, if some one-particle states appear multiple times in the list (α, \ldots, ω) , 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. (74). Adding them up gives us the top line of eq. (74). This completes the proof of Lemma 3.

Lemma 4: For any one-particle operator \hat{A} , the wave-function-language equation

$$\hat{A}_{\text{net}}^{(\text{wf})} = \sum_{i=1}^{N} \hat{A}(i^{\text{th}} \text{ particle})$$
(25)

and the Fock-space-language equation

$$\hat{A}_{\text{net}}^{(\text{fs})} = \sum_{\alpha,\beta} \langle \alpha | \hat{A} | \beta \rangle \times \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}$$
(80)

define exactly the same one-body additive operator \hat{A}_{net} .

Proof: To establish the equality between the operators (25) and (80), we are going to verify that they have exactly the same matrix elements between any N-boson states $\langle N, \tilde{\psi} |$ and $|N, \psi \rangle$,

$$\langle N, \widetilde{\psi} | \hat{A}_{\text{net}}^{(\text{wf})} | N, \psi \rangle = \langle N, \widetilde{\psi} | \hat{A}_{\text{net}}^{(\text{fs})} | N, \psi \rangle.$$
(81)

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 $\langle \tilde{\psi} |$ and $|\psi\rangle$

$$\langle \widetilde{\psi} | \hat{A} | \psi \rangle = \sum_{\alpha, \beta} \langle \widetilde{\psi} | \alpha \rangle \times \langle \alpha | \hat{A} | \beta \rangle \times \langle \beta | \psi \rangle = \sum_{\alpha, \beta} A_{\alpha\beta} \times \int d^3 \tilde{\mathbf{x}} \, \widetilde{\psi}^*(\tilde{\mathbf{x}}) \phi_\alpha(\tilde{\mathbf{x}}) \times \int d^3 \mathbf{x} \, \phi_\beta^*(\mathbf{x}) \psi(\mathbf{x}).$$
(82)

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,

$$\langle N, \widetilde{\psi} | \hat{A}_{1}(i^{\text{th}}) | N, \psi \rangle =$$

$$= \int \cdots \int d^{3}\mathbf{x}_{1} \cdots d^{3}\mathbf{x}_{N} \sum_{\alpha,\beta} A_{\alpha\beta} \times \left(\int d^{3}\widetilde{\mathbf{x}}_{i} \,\widetilde{\psi}^{*}(\mathbf{x}_{1}, \dots, \widetilde{\mathbf{x}}_{i}, \dots, \mathbf{x}_{N}) \phi_{\alpha}(\widetilde{\mathbf{x}}_{i}) \right)$$

$$\times \left(\int d^{3}\mathbf{x}_{i} \,\phi_{\beta}^{*}(\mathbf{x}_{i}) \psi(\mathbf{x}_{1}, \dots, \mathbf{x}_{i}, \dots, \mathbf{x}_{N}) \right)$$

$$= \sum_{\alpha,\beta} A_{\alpha\beta} \times \int \cdots \int d^{3}\mathbf{x}_{1} \cdots d^{3}\mathbf{x}_{N} \, d^{3}\widetilde{\mathbf{x}}_{i} \,\widetilde{\psi}^{*}(\mathbf{x}_{1}, \dots, \widetilde{\mathbf{x}}_{i}, \dots, \mathbf{x}_{N}) \times \phi_{\alpha}(\widetilde{\mathbf{x}}_{i})$$

$$\times \phi_{\beta}^{*}(\mathbf{x}_{i}) \times \psi(\mathbf{x}_{1}, \dots, \mathbf{x}_{i}, \dots, \mathbf{x}_{N}).$$

$$(83)$$

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 (25),

Now consider matrix elements of the Fock-space operator (80). In light of eq. (20), the state $|N - 1, \psi''\rangle = \hat{a}_{\beta} |N, \psi\rangle$ has wave-function

$$\psi''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1}) = \sqrt{N} \int d^3 \mathbf{x}_N \,\phi^*_\beta(\mathbf{x}_N) \times \psi(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1},\mathbf{x}_N). \tag{85}$$

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

$$\widetilde{\psi}''(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1}) = \sqrt{N} \int d^3 \widetilde{\mathbf{x}}_N \,\phi^*_\alpha(\widetilde{\mathbf{x}}_N) \times \widetilde{\psi}(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1},\widetilde{\mathbf{x}}_N).$$
(86)

Consequently,

$$\langle N, \widetilde{\psi} | \, \hat{a}^{\dagger}_{\alpha} \hat{a}_{\beta} \, | N, \psi \rangle = \langle N - 1, \widetilde{\psi}'' | \, | N - 1, \psi'' \rangle$$

$$= \int \cdots \int d^{3} \mathbf{x}_{1} \cdots \mathbf{x}_{N-1} \, \widetilde{\psi}''^{*}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N-1}) \times \psi''(\mathbf{x}_{1}, \dots, \mathbf{x}_{N-1})$$

$$= \int \cdots \int d^{3} \mathbf{x}_{1} \cdots \mathbf{x}_{N-1} \sqrt{N} \int d^{3} \widetilde{\mathbf{x}}_{N} \, \phi_{\alpha}(\widetilde{\mathbf{x}}_{N}) \times \widetilde{\psi}^{*}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N-1}, \widetilde{\mathbf{x}}_{N}) \times$$

$$\times \sqrt{N} \int d^{3} \mathbf{x}_{N} \, \phi_{\beta}^{*}(\mathbf{x}_{N}) \times \psi(\mathbf{x}_{1}, \dots, \mathbf{x}_{N-1}, \mathbf{x}_{N}).$$

$$(87)$$

Comparing this formula to the integrals in eq. (84), we see that

$$\langle N, \widetilde{\psi} | \hat{A}_{\text{net}}^{(\text{wf})} | N, \psi \rangle = \sum_{\alpha, \beta} A_{\alpha\beta} \times \langle N, \widetilde{\psi} | \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta} | N, \psi \rangle = \langle N, \widetilde{\psi} | \hat{A}_{\text{net}}^{(\text{fs})} | N, \psi \rangle.$$
(88)

This completes the proof of Lemma 4.

Lemma 5: Let \hat{A} , \hat{B} , and \hat{C} be some one-particle operators, and let $\hat{A}_{net}^{(fs)}$, $\hat{B}_{net}^{(fs)}$, and $\hat{C}_{net}^{(fs)}$ be the corresponding net one-body operators in the fock space according to eq. (80). For these operators,

if
$$[\hat{A}, \hat{B}] = \hat{C}$$
 then $\left[\hat{A}_{\text{net}}^{(\text{fs})}, \hat{B}_{\text{net}}^{(\text{fs})}\right] = \hat{C}_{\text{net}}^{(\text{fs})}$. (30)

Proof: The Lemma follows from the commutator

$$[\hat{a}^{\dagger}_{\alpha}\hat{a}_{\beta},\hat{a}^{\dagger}_{\gamma}\hat{a}_{\delta}] = \delta_{\beta,\gamma}\hat{a}^{\dagger}_{\alpha}\hat{a}_{\delta} - \delta_{\alpha,\delta}\hat{a}^{\dagger}_{\gamma}\hat{a}_{\beta}$$

$$\tag{89}$$

which you should have calculated in homework set #2, problem 4(a). Indeed, given

$$\hat{A}_{\text{tot}}^{\text{(fs)}} = \sum_{\alpha,\beta} \langle \alpha | \hat{A} | \beta \rangle \ \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}$$
(90)

and

$$\hat{B}_{\text{tot}}^{(\text{fs})} = \sum_{\gamma,\delta} \langle \gamma | \hat{B} | \delta \rangle \ \hat{a}_{\gamma}^{\dagger} \hat{a}_{\delta} , \qquad (91)$$

we immediately have

$$\begin{split} \left[\hat{A}_{\text{tot}}^{(\text{fs})}, \hat{B}_{\text{tot}}^{(\text{fs})}\right] &= \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha | \hat{A} | \beta \rangle \langle \gamma | \hat{B} | \delta \rangle \left[\hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}, \hat{a}_{\gamma}^{\dagger} \hat{a}_{\delta} \right] \\ &\quad \langle \langle \text{ using eq. (89) } \rangle \rangle \\ &= \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha | \hat{A} | \beta \rangle \langle \gamma | \hat{B} | \delta \rangle \left(\delta_{\beta,\gamma} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\delta} - \delta_{\alpha,\delta} \hat{a}_{\gamma}^{\dagger} \hat{a}_{\beta} \right) \\ &= \sum_{\alpha,\delta} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\delta} \times \sum_{\beta=\gamma} \langle \alpha | \hat{A} | \gamma \rangle \langle \gamma | \hat{B} | \delta \rangle - \sum_{\beta,\gamma} \hat{a}_{\gamma}^{\dagger} \hat{a}_{\beta} \times \sum_{\alpha=\delta} \langle \gamma | \hat{B} | \alpha \rangle \langle \alpha | \hat{A} | \beta \rangle \\ &= \sum_{\alpha,\delta} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\delta} \langle \alpha | \hat{A} \hat{B} | \delta \rangle - \sum_{\beta,\gamma} \hat{a}_{\gamma}^{\dagger} \hat{a}_{\beta} \langle \gamma | \hat{B} \hat{A} | \beta \rangle \\ &\quad \langle \langle \text{ renaming summation indices } \rangle \rangle \\ &= \sum_{\alpha,\beta} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta} \times \left(\langle \alpha | \hat{A} \hat{B} | \beta \rangle - \langle \alpha | \hat{B} \hat{A} | \beta \rangle \right) \\ &= \sum_{\alpha,\beta} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta} \times \langle \alpha | \left([\hat{A}, \hat{B}] = \hat{C} \right) | \beta \rangle \equiv \hat{C}_{\text{tot}}^{(\text{fs})}. \end{split}$$

This completes the proof of Lemma 5.

Lemma 6: For any two-particle operator \hat{B} , the wave-function-language equation

$$\hat{B}_{\text{net}}^{(\text{wf})} = \frac{1}{2} \sum_{i \neq j}^{i,j=1,\dots,N} \hat{B}(i^{\text{th}} \text{ and } j^{\text{th}} \text{ particles})$$
(37)

and the Fock-space-language equation

$$\hat{B}_{\text{net}}^{(\text{fs})} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} (\langle \alpha | \otimes \langle \beta |) \hat{B}(|\gamma\rangle \otimes |\delta\rangle) \, \hat{a}^{\dagger}_{\alpha} \hat{a}^{\dagger}_{\beta} \hat{a}_{\delta} \hat{a}_{\gamma} \,. \tag{38}$$

define exactly the same net operator \hat{B}_{net} . That is, for any two N-boson states

$$\langle N, \widetilde{\psi} | \hat{B}_{\text{net}}^{(\text{wf})} | N, \psi \rangle = \langle N, \widetilde{\psi} | \hat{B}_{\text{net}}^{(\text{fs})} | N, \psi \rangle \text{ for any states } \langle N, \widetilde{\psi} | \text{ and } | N, \psi \rangle.$$
 (93)

Proof: This works similarly to the Lemma 4, except for more integrals. Let

$$B_{\alpha\beta,\gamma\delta} = \left(\langle \alpha | \otimes \langle \beta | \right) \hat{B}_2 (|\gamma\rangle \otimes |\delta\rangle \right) \tag{94}$$

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

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

$$\langle N, \widetilde{\psi} | \hat{B}_{2}(i^{\text{th}}, j^{\text{th}}) | N, \psi \rangle =$$

$$= \sum_{\alpha, \beta, \gamma, \delta} B_{\alpha\beta, \gamma\delta} \times \int \cdots \int d^{3}\mathbf{x}_{1} \cdots d^{3}\boldsymbol{x}_{1} \cdots d^{3}\boldsymbol{x}_{N}$$

$$\int \int d^{3} \widetilde{\mathbf{x}}_{i} d^{3} \widetilde{\mathbf{x}}_{j} \widetilde{\psi}^{*}(\mathbf{x}_{1}, \dots, \widetilde{\mathbf{x}}_{i}, \dots, \widetilde{\mathbf{x}}_{j}, \dots, \mathbf{x}_{N}) \phi_{\alpha}(\widetilde{\mathbf{x}}_{i}) \phi_{\beta}(\widetilde{\mathbf{x}}_{j})$$

$$\times \int \int d^{3}\mathbf{x}_{i} d^{3}\mathbf{x}_{j} \phi^{*}_{\gamma}(\mathbf{x}_{i}) \phi^{*}_{\delta}(\mathbf{x}_{j}) \psi(\mathbf{x}_{1}, \dots, \mathbf{x}_{i}, \dots, \mathbf{x}_{j}, \dots, \mathbf{x}_{N})$$

$$(96)$$

For identical bosons — and hence totally symmetric wave-functions ψ and $\tilde{\psi}$ — 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

$$\langle N, \widetilde{\psi} | \hat{B}_{\text{net}}^{(\text{wf})} | N, \psi \rangle = \frac{N(N-1)}{2} \times \langle N, \widetilde{\psi} | \hat{B}_2(N-1,N) | N, \psi \rangle$$

$$= \frac{N(N-1)}{2} \times \sum_{\alpha,\beta,\gamma,\delta} B_{\alpha\beta,\gamma\delta} \times I_{\alpha\beta,\gamma\delta}$$
(97)

where

$$I_{\alpha\beta,\gamma\delta} = \int \cdots \int d^{3}\mathbf{x}_{1} \cdots d^{3}\mathbf{x}_{N-2}$$

$$\iint d^{3}\tilde{\mathbf{x}}_{N-1} d^{3}\tilde{\mathbf{x}}_{N} \widetilde{\psi}^{*}(\mathbf{x}_{1}, \dots, \mathbf{x}_{N-2}, \tilde{\mathbf{x}}_{N-1}, \tilde{\mathbf{x}}_{N}) \phi_{\alpha}(\tilde{\mathbf{x}}_{N-1}) \phi_{\beta}(\tilde{\mathbf{x}}_{N}) \qquad (98)$$

$$\times \iint d^{3}\mathbf{x}_{N-1} d^{3}\mathbf{x}_{N} \phi_{\gamma}^{*}(\mathbf{x}_{N-1}) \phi_{\delta}^{*}(\mathbf{x}_{N}) \psi(\mathbf{x}_{1}, \dots, \mathbf{x}_{N-2}, \mathbf{x}_{N-1}, \mathbf{x}_{N})$$

Now let's compare these formulae to the Fock space formalism. Applying eq. (20) twice,

we find that the (N-2)-particle state

$$\left|N-2,\psi'''\right\rangle = \hat{a}_{\delta}\hat{a}_{\gamma}\left|N,\psi\right\rangle \tag{99}$$

has wave function

$$\psi^{\prime\prime\prime}(\mathbf{x}_{1},\ldots,\mathbf{x}_{N-2}) = \sqrt{N(N-1)} \iint d^{3}\mathbf{x}_{N-1} d^{3}\mathbf{x}_{N} \phi^{*}_{\gamma}(\mathbf{x}_{N-1}) \phi^{*}_{\delta}(\mathbf{x}_{N}) \times \psi(\mathbf{x}_{1},\ldots,\mathbf{x}_{N-2},\mathbf{x}_{N-1},\mathbf{x}_{N}).$$
(100)

Likewise, the (N-2)–particle state

$$\left|N-2,\widetilde{\psi}^{\prime\prime\prime}\right\rangle = \hat{a}_{\beta}\hat{a}_{\alpha}\left|N,\widetilde{\psi}\right\rangle \tag{101}$$

has wave function

$$\widetilde{\psi}^{\prime\prime\prime\prime}(\mathbf{x}_{1},\ldots,\mathbf{x}_{N-2}) = \sqrt{N(N-1)} \iint d^{3}\mathbf{x}_{N-1} d^{3}\mathbf{x}_{N} \phi_{\beta}^{*}(\widetilde{\mathbf{x}}_{N-1})\phi_{\alpha}^{*}(\widetilde{\mathbf{x}}_{N}) \times \widetilde{\psi}(\mathbf{x}_{1},\ldots,\mathbf{x}_{N-2},\widetilde{\mathbf{x}}_{N-1},\widetilde{\mathbf{x}}_{N}).$$
(102)

Taking Dirac product of these two states, we obtain

$$\langle N, \widetilde{\psi} | \hat{a}^{\dagger}_{\alpha} \hat{a}^{\dagger}_{\beta} \hat{a}_{\delta} \hat{a}_{\gamma} | N, \psi \rangle = \langle N - 2, \widetilde{\psi}^{\prime \prime \prime} | | N - 2, \psi^{\prime \prime \prime} \rangle$$

$$= \int \cdots \int d^{3} \mathbf{x}_{1} \cdots d^{3} \mathbf{x}_{N-2} \widetilde{\psi}^{\prime \prime \prime \ast} (\mathbf{x}_{1}, \dots, \mathbf{x}_{N-2}) \times \psi^{\prime \prime \prime} (\mathbf{x}_{1}, \dots, \mathbf{x}_{N-2})$$

$$= N(N-1) \times I_{\alpha\beta,\gamma\delta}$$

$$(103)$$

where $I_{\alpha\beta,\gamma\delta}$ is exactly the same mega-integral as in eq. (98). Therefore,

$$\langle N, \widetilde{\psi} | \hat{B}_{\text{net}}^{(\text{wf})} | N, \psi \rangle = \frac{1}{2} \sum_{\alpha, \beta, \gamma, \delta} B_{\alpha\beta, \gamma\delta} \times \langle N, \widetilde{\psi} | \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}^{\dagger} \hat{a}_{\delta} \hat{a}_{\gamma} | N, \psi \rangle = \langle N, \widetilde{\psi} | \hat{B}_{\text{net}}^{(\text{fs})} | N, \psi \rangle$$
(104)

where the second equality follows directly from the eq. (38) for the $\hat{B}_{net}^{(fs)}$ operator.

This completes the proof of Lemma 6.

Lemma 7: Let \hat{A} be a one-particle operator while \hat{B} and \hat{C} are two-particle operators. Let $\hat{A}_{\text{net}}^{(\text{fs})}$, $\hat{B}_{\text{net}}^{(\text{fs})}$, and $\hat{C}_{\text{net}}^{(\text{fs})}$ be the corresponding net operators in the Fock space according to eqs. (80) and (38). For these operators,

if
$$\left[\left(\hat{A}(1^{\mathrm{st}}) + \hat{A}(2^{\mathrm{nd}})\right), \hat{B}\right] = \hat{C}$$
 then $\left[\hat{A}_{\mathrm{net}}^{(\mathrm{fs})}, \hat{B}_{\mathrm{net}}^{(\mathrm{fs})}\right] = \hat{C}_{\mathrm{net}}^{(\mathrm{fs})}$. (105)

Proof: Similarly to Lemma 5, this Lemma also follows from a commutator you should have calculated in homework set #2, problem 4(a), namely

$$[\hat{a}^{\dagger}_{\mu}\hat{a}_{\nu},\hat{a}^{\dagger}_{\alpha}\hat{a}^{\dagger}_{\beta}\hat{a}_{\gamma}\hat{a}_{\delta}] = \delta_{\nu\alpha}\hat{a}^{\dagger}_{\mu}\hat{a}^{\dagger}_{\beta}\hat{a}_{\gamma}\hat{a}_{\delta} + \delta_{\nu\beta}\hat{a}^{\dagger}_{\alpha}\hat{a}^{\dagger}_{\mu}\hat{a}_{\gamma}\hat{a}_{\delta} - \delta_{\mu\gamma}\hat{a}^{\dagger}_{\alpha}\hat{a}^{\dagger}_{\beta}\hat{a}_{\nu}\hat{a}_{\delta} - \delta_{\mu\delta}\hat{a}^{\dagger}_{\alpha}\hat{a}^{\dagger}_{\beta}\hat{a}_{\gamma}\hat{a}_{\nu}.$$
(106)

Indeed, in the Fock space

$$\hat{A}_{\text{tot}}^{(\text{fs})} = \sum_{\mu n u} \langle \mu | \hat{A} | \nu \rangle \ \hat{a}_{\mu}^{\dagger} \hat{a}_{\nu}$$
(80)

and

$$\hat{B}_{\text{tot}}^{(\text{fs})} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha \otimes \beta | \hat{B} | \gamma \otimes \delta \rangle \ \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}^{\dagger} \hat{a}_{\gamma} \hat{a}_{\delta} , \qquad (38)$$

so the commutator $\left[\hat{A}_{\text{net}}^{(\text{fs})}, \hat{B}_{\text{net}}^{(\text{fs})}\right]$ is a linear combination of the commutators (106). Specifically,

$$\begin{split} \left[\hat{A}_{\text{tot}}^{\text{(fs)}}, \hat{B}_{\text{tot}}^{\text{(fs)}}\right] &= \frac{1}{2} \sum_{\mu,\nu,\alpha,\beta,\gamma,\delta} \langle \mu | \hat{A} | \nu \rangle \langle \alpha \otimes \beta | \hat{B} | \gamma \otimes \delta \rangle \left[\hat{a}_{\mu}^{\dagger} \hat{a}_{\nu}, \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}^{\dagger} \hat{a}_{\gamma} \hat{a}_{\delta} \right] \\ &= \frac{1}{2} \sum_{\mu,\beta,\gamma,\delta} \hat{a}_{\mu}^{\dagger} \hat{a}_{\beta}^{\dagger} \hat{a}_{\gamma} \hat{a}_{\delta} \times \sum_{\nu} \langle \mu | \hat{A} | \nu \rangle \langle \nu \otimes \beta | \hat{B} | \gamma \otimes \delta \rangle \\ &+ \frac{1}{2} \sum_{\alpha,\mu,\gamma,\delta} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\mu}^{\dagger} \hat{a}_{\gamma} \hat{a}_{\delta} \times \sum_{\nu} \langle \mu | \hat{A} | \nu \rangle \langle \alpha \otimes \nu | \hat{B} | \gamma \otimes \delta \rangle \\ &- \frac{1}{2} \sum_{\alpha,\beta,\nu,\delta} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}^{\dagger} \hat{a}_{\nu} \hat{a}_{\delta} \times \sum_{\mu} \langle \alpha \otimes \beta | \hat{B} | \mu \otimes \delta \rangle \langle \mu | \hat{A} | \nu \rangle \\ &- \frac{1}{2} \sum_{\alpha,\beta,\gamma,\nu} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}^{\dagger} \hat{a}_{\gamma} \hat{a}_{\nu} \times \sum_{\mu} \langle \alpha \otimes \beta | \hat{B} | \gamma \otimes \mu \rangle \langle \mu | \hat{A} | \nu \rangle \\ &\langle \text{(renaming summation indices } \rangle \rangle \\ &= \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta}^{\dagger} \hat{a}_{\gamma} \hat{a}_{\delta} \times C_{\alpha,\beta,\gamma,\delta} \,, \end{split}$$

where

$$C_{\alpha,\beta,\gamma,\delta} = \sum_{\lambda} \langle \alpha | \hat{A} | \lambda \rangle \langle \lambda \otimes \beta | \hat{B} | \gamma \otimes \delta \rangle + \sum_{\lambda} \langle \beta | \hat{A} | \lambda \rangle \langle \alpha \otimes \lambda | \hat{B} | \gamma \otimes \delta \rangle$$
$$- \sum_{\lambda} \langle \alpha \otimes \beta | \hat{B} | \lambda \otimes \delta \rangle \langle \lambda | \hat{A} | \gamma \rangle - \sum_{\lambda} \langle \alpha \otimes \beta | \hat{B} | \gamma \otimes \lambda \rangle \langle \lambda | \hat{A} | \delta \rangle$$
$$= \langle \alpha \otimes \beta | \left(\hat{A}(1^{st}) \hat{B} + \hat{A}(2^{nd}) \hat{B} - \hat{B} \hat{A}(1^{st}) - \hat{B} \hat{A}(2^{nd}) \right) | \gamma \otimes \delta \rangle$$
$$= \langle \alpha \otimes \beta | \left[\left(\hat{A}(1^{st}) + \hat{A}(2^{nd}) \right), \hat{B} \right] | \gamma \otimes \delta \rangle \equiv \langle \alpha \otimes \beta | \hat{C} | \gamma \otimes \delta \rangle.$$
(108)

Consequently, $\left[\hat{A}_{\text{tot}}^{(\text{fs})}, \hat{B}_{\text{tot}}^{(\text{fs})}\right] = \hat{C}_{\text{tot}}^{(\text{fs})}.$

This completes the proof of Lemma 7