Free Fields, Harmonic Oscillators, and Identical Bosons

A free quantum field and its canonical conjugate are equivalent to a family of harmonic oscillators (one oscillator for each plane wave), which is in turn equivalent to a quantum theory of free identical bosons. In this note, I will show how all of this works for the relativistic scalar field $\hat{\varphi}(x)$ and its conjugate $\hat{\pi}(x)$. And then I will turn around and show that a quantum theory of any kind of identical bosons is equivalent to a family of oscillators. (Harmonic for the free particles, non-harmonic if the particles interact with each other.) Moreover, for the non-relativistic particles, the oscillator family is in turn equivalent to a non-relativistic quantum field theory.

In this note we shall work in the Schrödinger picture of Quantum Mechanics because it's more convenient for dealing with the eigenstates and the eigenvalues. Consequently, all operators — including the quantum fields such as $\hat{\varphi}(\mathbf{x})$ — are time-independent.

From Relativistic Fields to Harmonic Oscillators

Let us start with the relativistic scalar field $\hat{\varphi}(\mathbf{x})$ and its conjugate $\hat{\pi}(\mathbf{x})$; they obey the canonical commutation relations

$$[\hat{\varphi}(\mathbf{x}),\hat{\varphi}(\mathbf{x}')]\;=\;0,\quad [\hat{\pi}(\mathbf{x}),\hat{\pi}(\mathbf{x}')]\;=\;0,\quad [\hat{\varphi}(\mathbf{x}),\hat{\pi}(\mathbf{x}')]\;=\;i\delta^{(3)}(\mathbf{x}-\mathbf{x}') \tag{1}$$

and are governed by the Hamiltonian

$$\hat{H}\;=\;\int\!d^3\mathbf{x}\left(\tfrac{1}{2}\hat{\pi}^2(\mathbf{x})\;+\;\tfrac{1}{2}(\nabla\hat{\varphi}(\mathbf{x}))^2\;+\;\tfrac{1}{2}m^2\hat{\varphi}^2(\mathbf{x})\right). \tag{2}$$

We want to expand the fields into plane-wave modes $\hat{\varphi}_{\mathbf{k}}$ and $\hat{\pi}_{\mathbf{k}}$, and to avoid technical difficulties with the oscillators and their eigenstates, we want discrete modes. Therefore, we replace the infinite $\mathbf{x}$ space with a finite but very large box of size $L\times L\times L$, and impose periodic boundary conditions — $\hat{\varphi}(x+L,y,z)=\hat{\varphi}(x,y+L,z)=\hat{\varphi}(x,y,z+L)=\hat{\varphi}(x,y,z)$, *etc.*, *etc.* For large L, the specific boundary conditions are unimportant, so I have chosen the periodic conditions since they give us particularly simple plane-wave modes

$$\psi_{\mathbf{k}}(\mathbf{x}) \;=\; L^{-3/2}e^{i\mathbf{k}\mathbf{x}} \qquad \text{where} \quad k_x, k_y, k_z \;=\; \frac{2\pi}{L} \times \text{an integer.} \tag{3}$$

Expanding the quantum fields into such modes, we get

$$\begin{aligned} \hat{\varphi}(\mathbf{x}) \;&=\; \sum_{\mathbf{k}} L^{-3/2}e^{i\mathbf{k}\mathbf{x}} \times \hat{\varphi}_{\mathbf{k}}, \qquad & \hat{\varphi}_{\mathbf{k}} \;&=\; \int d^3\mathbf{x}\, L^{-3/2}e^{-i\mathbf{k}\mathbf{x}} \times \hat{\varphi}(\mathbf{x}), \\ \hat{\pi}(\mathbf{x}) \;&=\; \sum_{\mathbf{k}} L^{-3/2}e^{i\mathbf{k}\mathbf{x}} \times \hat{\pi}_{\mathbf{k}}, \qquad & \hat{\pi}_{\mathbf{k}} \;&=\; \int d^3\mathbf{x}\, L^{-3/2}e^{-i\mathbf{k}\mathbf{x}} \times \hat{\pi}(\mathbf{x}). \end{aligned} \tag{4}$$

A note on hermiticity: The classical fields $\varphi(\mathbf{x})$ and $\pi(\mathbf{x})$ are real (*i.e.*, their values are real numbers), so the corresponding quantum fields are hermitian, $\hat{\varphi}^\dagger(\mathbf{x}) = \hat{\varphi}(\mathbf{x})$ and $\hat{\pi}^\dagger(\mathbf{x}) = \hat{\pi}(\mathbf{x})$. However, the mode operators $\hat{\varphi}_{\mathbf{k}}$ and $\hat{\pi}_{\mathbf{k}}$ are not hermitian; instead, eqs. (4) give us $\hat{\varphi}^\dagger_{\mathbf{k}} = \hat{\varphi}_{-\mathbf{k}}$ and $\hat{\pi}^\dagger_{\mathbf{k}} = \hat{\pi}_{-\mathbf{k}}$.

The commutation relations between the mode operators follow from eqs. (1), namely

$$[\hat{\varphi}_{\mathbf{k}}, \hat{\varphi}_{\mathbf{k}'}] \;=\; 0, \quad [\hat{\pi}_{\mathbf{k}}, \hat{\pi}_{\mathbf{k}'}] \;=\; 0, \quad [\hat{\varphi}_{\mathbf{k}}, \hat{\pi}_{\mathbf{k}'}] \;=\; i\,\delta_{\mathbf{k},-\mathbf{k}'}\,. \tag{5}$$

The first two relations here are obvious, but the third needs a bit of algebra:

$$\begin{aligned} [\hat{\varphi}_{\mathbf{k}}, \hat{\pi}_{\mathbf{k}'}] \;&=\; \int d^3\mathbf{x} \int d^3\mathbf{x}'\, L^{-3}e^{-i\mathbf{k}\mathbf{x}}e^{-i\mathbf{k}'\mathbf{x}'} \times [\hat{\varphi}(\mathbf{x}), \hat{\pi}(\mathbf{x}')] \\ &=\; \int d^3\mathbf{x} \int d^3\mathbf{x}'\, L^{-3}e^{-i\mathbf{k}\mathbf{x}}e^{-i\mathbf{k}'\mathbf{x}'} \times i\delta^{(3)}(\mathbf{x} - \mathbf{x}') \\ &=\; i\,L^{-3} \int\limits_{\text{box}} d^3\mathbf{x}\, e^{-i\mathbf{x}(\mathbf{k}+\mathbf{k}')} \\ &=\; i\,\delta_{\mathbf{k},-\mathbf{k}'}\,. \end{aligned} \tag{6}$$

Equivalently,

$$[\hat{\varphi}_{\mathbf{k}}, \hat{\pi}^\dagger_{\mathbf{k}'}] \;=\; [\hat{\varphi}^\dagger_{\mathbf{k}}, \hat{\pi}_{\mathbf{k}'}] \;=\; i\,\delta_{\mathbf{k},\mathbf{k}'}\,, \quad [\hat{\varphi}_{\mathbf{k}}, \hat{\pi}_{\mathbf{k}'}] \;=\; [\hat{\varphi}^\dagger_{\mathbf{k}}, \hat{\pi}^\dagger_{\mathbf{k}'}] \;=\; i\,\delta_{\mathbf{k}+\mathbf{k}',\mathbf{0}}\,. \tag{7}$$

Now let's express the Hamiltonian (2) in terms of the modes. For the first term, we have

$$\begin{aligned}
\int d^3\mathbf{x}\,\hat{\pi}^2(\mathbf{x}) \;&=\; \int d^3\mathbf{x}\,\hat{\pi}^\dagger(\mathbf{x})\hat{\pi}(\mathbf{x}) \;=\; \int d^3\mathbf{x}\,\sum_{\mathbf{k}}\sum_{\mathbf{k}'} L^{-3}e^{-i\mathbf{k}\mathbf{x}}e^{+i\mathbf{k}'\mathbf{x}}\times\hat{\pi}^\dagger_{\mathbf{k}}\hat{\pi}_{\mathbf{k}'}\\
&=\; \sum_{\mathbf{k},\mathbf{k}'}\hat{\pi}^\dagger_{\mathbf{k}}\hat{\pi}_{\mathbf{k}'}\times\left(L^{-3}\int\limits_{\text{box}} d^3\mathbf{x}\,e^{i\mathbf{x}(\mathbf{k}'-\mathbf{k})} \;=\; \delta_{\mathbf{k},\mathbf{k}'}\right)\\
&=\; \sum_{\mathbf{k}}\hat{\pi}^\dagger_{\mathbf{k}}\hat{\pi}_{\mathbf{k}}\,.
\end{aligned}\tag{8}$$

Similarly, the last term becomes

$$\int d^3\mathbf{x}\,\hat{\varphi}^2(\mathbf{x}) \;=\; \sum_{\mathbf{k}}\hat{\varphi}^\dagger_{\mathbf{k}}\hat{\varphi}_{\mathbf{k}}\,,\tag{9}$$

while in the second term

$$\nabla\hat{\varphi}(\mathbf{x}) \;=\; \sum_{\mathbf{k}} L^{-3/2}e^{i\mathbf{k}\mathbf{x}}\times i\mathbf{k}\,\hat{\varphi}_{\mathbf{k}} \;=\; \sum_{\mathbf{k}} L^{-3/2}e^{-i\mathbf{k}\mathbf{x}}\times -i\mathbf{k}\,\hat{\varphi}^\dagger_{\mathbf{k}}\,,\tag{10}$$

hence

$$\int d^3\mathbf{x}\,(\nabla\hat{\varphi}(\mathbf{x}))^2 \;=\; \sum_{\mathbf{k}}\mathbf{k}^2\,\hat{\varphi}^\dagger_{\mathbf{k}}\hat{\varphi}_{\mathbf{k}}\,.\tag{11}$$

Altogether, the Hamiltonian (2) becomes

$$\hat{H} \;=\; \sum_{\mathbf{k}}\left(\tfrac{1}{2}\,\hat{\pi}^\dagger_{\mathbf{k}}\hat{\pi}_{\mathbf{k}} \;+\; \tfrac{1}{2}(\mathbf{k}^2+m^2)\,\hat{\varphi}^\dagger_{\mathbf{k}}\hat{\varphi}_{\mathbf{k}}\right).\tag{12}$$

Clearly, this Hamiltonian describes a bunch of harmonic oscillators with frequencies $\omega_{\mathbf{k}} = \sqrt{\mathbf{k}^2+m^2}$ (in the $\hbar = c = 1$ units). But since the mode operators are not hermitian, converting them into creation and annihilation operators takes a little more work then usual:

We define

$$\hat{a}_{\mathbf{k}} \;=\; \frac{1}{\sqrt{2\omega_{\mathbf{k}}}}\,\Big(\omega_{\mathbf{k}}\hat{\varphi}_{\mathbf{k}} \,+\, i\,\hat{\pi}_{\mathbf{k}}\Big)\,,$$

and consequently

$$\begin{aligned}
\hat{a}^{\dagger}_{\mathbf{k}} \;&=\; \frac{1}{\sqrt{2\omega_{\mathbf{k}}}}\,\Big(\omega_{\mathbf{k}}\hat{\varphi}^{\dagger}_{\mathbf{k}} \,-\, i\,\hat{\pi}^{\dagger}_{\mathbf{k}}\Big)\,,\\
\hat{a}_{-\mathbf{k}} \;&=\; \frac{1}{\sqrt{2\omega_{-\mathbf{k}}}}\,\Big(\omega_{-\mathbf{k}}\hat{\varphi}_{-\mathbf{k}} \,+\, i\,\hat{\pi}_{-\mathbf{k}}\Big) \;=\; \frac{1}{\sqrt{2\omega_{\mathbf{k}}}}\,\Big(\omega_{\mathbf{k}}\hat{\varphi}^{\dagger}_{\mathbf{k}} \,+\, i\,\hat{\pi}^{\dagger}_{\mathbf{k}}\Big)\,,\\
\hat{a}^{\dagger}_{-\mathbf{k}} \;&=\; \frac{1}{\sqrt{2\omega_{-\mathbf{k}}}}\,\Big(\omega_{-\mathbf{k}}\hat{\varphi}^{\dagger}_{-\mathbf{k}} \,-\, i\,\hat{\pi}^{\dagger}_{-\mathbf{k}}\Big) \;=\; \frac{1}{\sqrt{2\omega_{\mathbf{k}}}}\,\Big(\omega_{\mathbf{k}}\hat{\varphi}_{\mathbf{k}} \,-\, i\,\hat{\pi}_{\mathbf{k}}\Big)\,.
\end{aligned} \tag{13}$$

Note that $\hat{a}^{\dagger}_{\mathbf{k}} \neq \hat{a}_{-\mathbf{k}}$ and $\hat{a}_{-\mathbf{k}} \neq \hat{a}^{\dagger}_{\mathbf{k}}$; instead, we have independent creation and annihilation operators $\hat{a}^{\dagger}_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}$ for every mode $\mathbf{k}$.

The commutations relations between these operators are

$$[\hat{a}_{\mathbf{k}},\hat{a}_{\mathbf{k}'}] \,=\, 0, \quad [\hat{a}^{\dagger}_{\mathbf{k}},\hat{a}^{\dagger}_{\mathbf{k}'}] \,=\, 0, \quad [\hat{a}_{\mathbf{k}},\hat{a}^{\dagger}_{\mathbf{k}'}] \,=\, \delta_{\mathbf{k},\mathbf{k}'}\,. \tag{14}$$

Indeed,

$$\begin{aligned}
[\hat{a}_{\mathbf{k}},\hat{a}_{\mathbf{k}'}] \;&=\; \frac{1}{\sqrt{4\omega\omega'}}\,\Big(\omega\omega'\,[\hat{\varphi}_{\mathbf{k}},\hat{\varphi}_{\mathbf{k}'}] \,+\, i\omega'\,[\hat{\pi}_{\mathbf{k}},\hat{\varphi}_{\mathbf{k}'}] \,+\, i\omega\,[\hat{\varphi}_{\mathbf{k}},\hat{\pi}_{\mathbf{k}'}] \,-\, [\hat{\pi}_{\mathbf{k}},\hat{\pi}_{\mathbf{k}'}]\Big)\\
&=\; \frac{1}{\sqrt{4\omega\omega'}}\,\big(0 \,+\, i\omega' \times -i\delta_{\mathbf{k}+\mathbf{k}',\mathbf{0}} \,+\, i\omega \times +i\delta_{\mathbf{k}+\mathbf{k}',\mathbf{0}} \,+\, 0\big)\\
&=\; \delta_{\mathbf{k}+\mathbf{k}',\mathbf{0}} \times \frac{\omega'-\omega}{\sqrt{4\omega\omega'}}\\
&=\; 0 \qquad \text{because } \omega'=\omega \text{ when } \mathbf{k}+\mathbf{k}'=\mathbf{0}.
\end{aligned} \tag{15}$$

Similarly, $[\hat{a}^{\dagger}_{\mathbf{k}},\hat{a}^{\dagger}_{\mathbf{k}'}] = 0$. Finally,

$$\begin{aligned}
[\hat{a}_{\mathbf{k}},\hat{a}^{\dagger}_{\mathbf{k}'}] \;&=\; \frac{1}{\sqrt{4\omega\omega'}}\,\Big(\omega\omega'\,[\hat{\varphi}_{\mathbf{k}},\hat{\varphi}^{\dagger}_{\mathbf{k}'}] \,+\, i\omega'\,[\hat{\pi}_{\mathbf{k}},\hat{\varphi}^{\dagger}_{\mathbf{k}'}] \,-\, i\omega\,[\hat{\varphi}_{\mathbf{k}},\hat{\pi}^{\dagger}_{\mathbf{k}'}] \,+\, [\hat{\pi}_{\mathbf{k}},\hat{\pi}^{\dagger}_{\mathbf{k}'}]\Big)\\
&=\; \frac{1}{\sqrt{4\omega\omega'}}\,\big(0 \,+\, i\omega' \times -i\delta_{\mathbf{k},\mathbf{k}'} \,-\, i\omega \times +i\delta_{\mathbf{k},\mathbf{k}'} \,+\, 0\big)\\
&=\; \delta_{\mathbf{k},\mathbf{k}'} \times \frac{\omega+\omega'}{\sqrt{4\omega\omega'}}\\
&=\; \delta_{\mathbf{k},\mathbf{k}'} \qquad \text{because } \omega'=\omega \text{ when } \mathbf{k}'=\mathbf{k}.
\end{aligned} \tag{16}$$

To re-obtain the field mode operators $\hat{\varphi}_{\mathbf{k}}$ and $\hat{\pi}_{\mathbf{k}}$ from the creation and annihilation operators, let us combine the first and the last equations (13) for the $\hat{a}_{\mathbf{k}}$ and $\hat{a}^{\dagger}_{-\mathbf{k}}$. Adding and subtracting those equations, we find

$$\hat{a}_{\mathbf{k}} + \hat{a}^\dagger_{-\mathbf{k}} = \sqrt{2\omega_{\mathbf{k}}} \times \hat{\varphi}_{\mathbf{k}}\,, \qquad -i\hat{a}_{\mathbf{k}} + i\hat{a}^\dagger_{-\mathbf{k}} = \sqrt{\frac{2}{\omega_{\mathbf{k}}}} \times \hat{\pi}_{\mathbf{k}}\,. \tag{17}$$

Consequently,

$$\begin{aligned}
\omega^2\hat{\varphi}^\dagger_{\mathbf{k}}\hat{\varphi}_{\mathbf{k}} &= \frac{\omega_{\mathbf{k}}}{2} \times (\hat{a}^\dagger_{\mathbf{k}} + \hat{a}_{-\mathbf{k}})(\hat{a}_{\mathbf{k}} + \hat{a}^\dagger_{-\mathbf{k}}) \\
&= \frac{\omega_{\mathbf{k}}}{2} \times \left(\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}^\dagger_{\mathbf{k}}\hat{a}^\dagger_{-\mathbf{k}} + \hat{a}_{-\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}\hat{a}^\dagger_{-\mathbf{k}}\right), \\
\hat{\pi}^\dagger_{\mathbf{k}}\hat{\pi}_{\mathbf{k}} &= \frac{\omega_{\mathbf{k}}}{2} \times (i\hat{a}^\dagger_{\mathbf{k}} - i\hat{a}_{-\mathbf{k}})(-i\hat{a}_{\mathbf{k}} + i\hat{a}^\dagger_{-\mathbf{k}}) \\
&= \frac{\omega_{\mathbf{k}}}{2} \times \left(\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} - \hat{a}^\dagger_{\mathbf{k}}\hat{a}^\dagger_{-\mathbf{k}} - \hat{a}_{-\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}\hat{a}^\dagger_{-\mathbf{k}}\right),
\end{aligned} \tag{18}$$

hence

$$\begin{aligned}
\omega^2\hat{\varphi}^\dagger_{\mathbf{k}}\hat{\varphi}_{\mathbf{k}} + \hat{\pi}^\dagger_{\mathbf{k}}\hat{\pi}_{\mathbf{k}} &= \omega_{\mathbf{k}} \times \left(\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}\hat{a}^\dagger_{-\mathbf{k}}\right) \\
&= \omega_{\mathbf{k}} \times \left(\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}^\dagger_{-\mathbf{k}}\hat{a}_{-\mathbf{k}} + 1\right).
\end{aligned} \tag{19}$$

Altogether, the Hamiltonian (12) becomes

$$\hat{H} = \sum_{\mathbf{k}} \tfrac{1}{2}\omega_{\mathbf{k}} \times \left(\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}^\dagger_{-\mathbf{k}}\hat{a}_{-\mathbf{k}} + 1\right) = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \tfrac{1}{2}\right). \tag{20}$$

In light of the commutation relations (14), this Hamiltonian clearly describes an infinite family of harmonic oscillators, one oscillator for each plane-wave mode $\mathbf{k}$.

Now consider the eigenvalues and the eigenstates of the multi-oscillator Hamiltonian (20). A single harmonic oscillator has eigenvalues $E_n = \omega(n + \frac{1}{2})$ where $n = 0, 1, 2, 3, \ldots$. For the multi-oscillator system at hand, each $\hat{n}_{\mathbf{k}} = \hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}}$ commutes with all the other $\hat{n}_{\mathbf{k}'}$, so we may diagonalize them all at the same time. This gives us eigenstates

$$|\{n_{\mathbf{k}} \text{ for all } \mathbf{k}\}\rangle = \bigotimes_{\mathbf{k}} |n_{\mathbf{k}}\rangle \qquad \text{of energy} \quad E_{\{n_{\mathbf{k}}\}} = \sum_{\mathbf{k}} \omega_{\mathbf{k}}(n_{\mathbf{k}} + \tfrac{1}{2}). \tag{21}$$

where each $n_{\mathbf{k}}$ is an integer ≥ 0. Moreover, all combinations of the $n_{\mathbf{k}}$ are allowed because the $\hat{a}^\dagger_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}$ operators can change a particular $n_{\mathbf{k}} \to n_{\mathbf{k}} \pm 1$ without affecting any other

$n_{\mathbf{k}'}$. (This follows from $[\hat{a}_{\mathbf{k}}, \hat{n}_{\mathbf{k}'}] = 0$ and $[\hat{a}^\dagger_{\mathbf{k}}, \hat{n}_{\mathbf{k}'}] = 0$ for $\mathbf{k}' \neq \mathbf{k}$.) Thus, the Hilbert space of the multi-oscillator system — and hence of the free quantum field theory — is a direct product of Hilbert spaces for each oscillator,

$$\mathcal{H}(\text{QFT}) \;=\; \bigotimes_{\mathbf{k}} \mathcal{H}(\text{harmonic oscillator for mode } \mathbf{k}). \tag{22}$$

From the Multi-Oscillator System to Identical Bosons

A constant term in the Hamiltonian of a quantum system does not affect its dynamics in any way, it simply shifts energies of all states by the same constant amount. So to simplify our analysis of the multi-oscillator system in particle terms, let's subtract the infinite zero-point energy $E_0 = \sum_{\mathbf{k}} \frac{1}{2}\omega_{\mathbf{k}}$ from the Hamiltonian (20), thus

$$\hat{H} \;\to\; \hat{H} \;-\; E_0 \;=\; \sum_{\mathbf{k}} \omega_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}}\,. \tag{23}$$

I'll come back to the zero-point energy, but right now let's focus on other issues.

In the multi-oscillator Hilbert space (22) each *occupation number* $n_{\mathbf{k}}$ is independent from all others. However, *states of finite energy must have finite* $N = \sum_{\mathbf{k}} n_{\mathbf{k}}$, so let us re-organize the Hilbert space into eigenspaces of the $\hat{N} = \sum_{\mathbf{k}} \hat{n}_{\mathbf{k}}$ operator,

$$\mathcal{H}(\text{QFT}) \;=\; \bigotimes_{\mathbf{k}} \mathcal{H}(\text{mode } \mathbf{k}) \;=\; \bigoplus_{N=0}^{\infty} \mathcal{H}_N\,, \tag{24}$$

and consider what do those eigenspaces look like for different N. For $N = 0$, the $\mathcal{H}_0$ spans a single state, the *vacuum* $|0\rangle = |\text{all } n_{\mathbf{k}} = 0\rangle$. For $N = 1$, the $\mathcal{H}_1$ spans eigenstates with a single $n_{\mathbf{k}} = 1$ while all other $n_{\mathbf{k}'} = 0$. Renaming such eigenstates $|n_{\mathbf{k}} = 1, \text{other } n = 0\rangle \to |\mathbf{k}\rangle$ and noting their energies

$$E(|\mathbf{k}\rangle) \;=\; \omega_{\mathbf{k}} \;=\; \sqrt{\mathbf{k}^2 + m^2}\,, \tag{25}$$

we identify the $\mathcal{H}_1$ as a Hilbert space of a free relativistic particle with Hamiltonian

$$\hat{H}^{\text{particle}} \;=\; \sqrt{\hat{\mathbf{P}}^2 + m^2}\,. \tag{26}$$

For $N > 1$, we may have several modes with $n_{\mathbf{k}} > 0$, but for a finite N there can be only a finite number of such modes. So we rename such a state $|\mathbf{k}_1, \ldots, \mathbf{k}_N\rangle$ by listing only the modes $\mathbf{k}$ with $n_{\mathbf{k}} > 0$ and repeating each $\mathbf{k}$ $n_{\mathbf{k}}$ times. For example,

$$\left|3_{\mathbf{k}}, 2_{\mathbf{k}'}, 2_{\mathbf{k}''}, 1_{\mathbf{k}'''}, 0_{\text{everything else}}\right\rangle \;=\; \left|\mathbf{k}, \mathbf{k}, \mathbf{k}, \mathbf{k}', \mathbf{k}', \mathbf{k}'', \mathbf{k}'', \mathbf{k}'''\right\rangle . \tag{27}$$

In such notations, the $\mathcal{H}_N$ Hilbert space spans eigenstates $|\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_N\rangle$ labeled by N modes $\mathbf{k}_1, \ldots, \mathbf{k}_N$ (such modes may coincide but do not have to). The energy of such an eigenstate is

$$E(|\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_N\rangle) \;=\omega_{\mathbf{k}_1} + \omega_{\mathbf{k}_2} + \cdots + \omega_{\mathbf{k}_N}\,, \tag{28}$$

which allows us to identify the $\mathcal{H}_N$ as the Hilbert space of N free relativistic particles with the Hamiltonian

$$\hat{H}^{N\,\text{particles}} \;=\sum_{i=1}^{N} \sqrt{\hat{\mathbf{P}}^2(i^{\text{th}}) \,+\, m^2}\,. \tag{29}$$

However, treating the $\mathbf{k}_1, \ldots, \mathbf{k}_N$ momenta of N particles as independent over-counts the quantum states because the occupation numbers $n_{\mathbf{k}}$ do not specify the *order* in which we list the modes $\mathbf{k}_i$. For example, both $|\mathbf{k}_1, \mathbf{k}_2\rangle$ and $|\mathbf{k}_2, \mathbf{k}_1\rangle$ both correspond to the same state $\left|1_{\mathbf{k}_1}, 1_{\mathbf{k}_2}, 0_{\text{others}}\right\rangle$. More generally,

$$|\{n_{\mathbf{k}}\}\rangle \;=\; |\mathbf{k}_1, \ldots, \mathbf{k}_N\rangle \;=\; |\text{any permutation of the } \mathbf{k}_1, \ldots, \mathbf{k}_N\rangle\,. \tag{30}$$

In other words, the N relativistic particles in the $\mathcal{H}_N$ are *identical bosons.*

Altogether, we have

$$\mathcal{H}(\text{QFT}) \;=\; \bigotimes_{\mathbf{k}} \mathcal{H}(\text{harmonic oscillator } \#\mathbf{k}) \;=\; \bigoplus_{N=0}^{\infty} \mathcal{H}(N \text{ identical bosons}). \tag{31}$$

Hilbert spaces of this kind — any number N of identical bosons (or fermions) are known as *Fock spaces.* So the Hilbert space of the quantum field is the same as the Fock space of particles, and the Hamiltonians are also the same:

$$\hat{H}[\hat{\varphi}(\mathbf{x}), \hat{\pi}(\mathbf{x})] \;=\sum_{i=0}^{\hat{N}} \sqrt{\hat{\mathbf{P}}_i^2 \,+\, m^2}\,. \tag{32}$$

In other words, the quantum theory of the free field is identical to the quantum theory of (any number of) free identical bosons. For the theory in question, the field is a relativistic scalar

$\varphi(x)$ and the bosons are spinless relativistic particles. But in exactly the same manner, the quantum theory of Maxwell fields $F^{\mu\nu}(x)$ is identical to the quantum theory of (any number of) photons — which are massless relativistic particles with two polarizations states (per photon) and obey Bose statistics.

Quantization of field theories with non-quadratic Hamiltonians (and hence non-linear classical equations of motion) also leads to theories equivalent to theories of quantum particles, but this time the particles are not free but interact with each other. In relativistic theories, the interactions also allow for creation and destruction of particles; such processes have to be described in terms of the Fock space rather than a fixed–N Hilbert space. In non-relativistic theories, the net particle number N is sometimes conserved, sometimes not, but even when it is conserved, the Fock-space formalism is often convenient.

Finally, a few words about the zero-point energy $E_0 = \sum_{\mathbf{k}} \frac{1}{2}\omega_{\mathbf{k}}$. From the particles' point of view, E_0 is the vacuum energy. It does not affect any properties of the individual particles or the way they interact with each other, so one usually simply ignores the E_0 and proceeds as if it was not there. However, in some situations E_0 becomes important: (1) When one couples a quantum field theory to general relativity, vacuum energy density becomes the cosmological constant. (2) When a QFT has some variable parameters, the vacuum energy acts as an effective potential for those parameters. This is important for cosmology of the early Universe, and also for the Casimir effect. Note that while the E_0 itself is infinite (except in supersymmetric theories where infinities cancel out between the bosonic and fermionic fields), it can be written as a sum of an infinite *constant* and a finite part which changes with parameters by a finite amount ΔE_0 — it's the finite part that's responsible for the effective potential and for the Casimir effect.

From Identical Bosons back to Creation and Annihilation Operators.

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 this section, I will develop the second quantization formalism for the ordinary non-relativistic particles (for example, helium atoms), although it works in the same way for all kinds of particles, or even for the quasiparticles such as phonons.

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

$$\mathcal{F} \;=\; \bigoplus_{N=0}^{\infty} \mathcal{H}(N\,\text{bosons}), \tag{33}$$

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.[†]

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 $\hat{H}_2 = \hat{H}_1(1^{\text{st}}) + \hat{H}_1(2^{\text{nd}})$. 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*:

$$|\alpha,\beta\rangle \;=\; |\beta,\alpha\rangle \;=\begin{cases} \dfrac{|\alpha\rangle\otimes|\beta\rangle \,+\, |\beta\rangle\otimes|\alpha\rangle}{\sqrt{2}} & \text{for } \beta\neq\alpha, \\[2ex] |\alpha\rangle\otimes|\alpha\rangle & \text{for } \beta=\alpha, \end{cases} \tag{34}$$

or in the wave-function Language

$$\phi_{\alpha\beta}(\mathbf{x}_1,\mathbf{x}_2) \;=\; \phi_{\beta\alpha}(\mathbf{x}_1,\mathbf{x}_2) \;=\begin{cases} \dfrac{\phi_\alpha(\mathbf{x}_1)\phi_\beta(\mathbf{x}_2) \,+\, \phi_\beta(\mathbf{x}_1)\phi_\alpha(\mathbf{x}_2)}{\sqrt{2}} & \text{for } \beta\neq\alpha, \\[2ex] \phi_\alpha(\mathbf{x}_1)\phi_\alpha(\mathbf{x}_2) & \text{for } \beta=\alpha, \end{cases} \tag{35}$$

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

† 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.

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

$$\psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \;=\; \psi(\text{any permutation of the } \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N). \tag{36}$$

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

$$\hat{H}_N \;=\; \sum_{i=1}^{N} \hat{H}_1(i^{\text{th}}\,\text{particle}). \tag{37}$$

Without the symmetry requirement (36), 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

$$\begin{aligned}
|\alpha, \beta, \ldots, \omega\rangle \;&=\; \frac{|\alpha\rangle \otimes |\beta\rangle \otimes \cdots \otimes |\omega\rangle \;+\; \text{all } \textit{distinct} \text{ permutations of } \alpha, \beta, \ldots, \omega}{\sqrt{\#\text{ of distinct permutations}}}\,, \\
\phi_{\alpha\beta\cdots\omega}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \;&=\; \frac{\phi_\alpha(\mathbf{x}_1)\phi_\beta(\mathbf{x}_2)\cdots\phi_\omega(\mathbf{x}_N) \;+\; \text{all } \textit{distinct} \text{ permutations of } \alpha, \beta, \ldots, \omega}{\sqrt{\#\text{ of distinct permutations}}}\,.
\end{aligned} \tag{38}$$

Consequently, the *order* of the N single-particle labels $\alpha, \beta, \ldots, \omega$ of a state (38) does not matter,

$$|\alpha, \beta, \ldots, \omega\rangle \;=\; |\text{any permutation of the } \alpha, \beta, \ldots, \omega\rangle\,, \tag{39}$$

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,

$$|\alpha, \alpha, \alpha, \beta, \beta, \gamma, \gamma, \delta, \epsilon\rangle \;=\big|3_\alpha, 2_\beta, 2_\gamma, 1_\delta, 1_\epsilon, 0_{\text{all others}}\big\rangle\,. \tag{40}$$

Formally,

$$|\alpha_1 \;\ldots, \alpha_N\rangle \;=\; \big|\{n_\beta\}\big\rangle \qquad \text{where} \quad n_\beta \;= \sum_{i=1}^{N} \delta_{\alpha_i,\beta}\,. \tag{41}$$

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

The states (38) are eigenstates of the Hamiltonian (37) 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 $\big|\{n_\beta\}\big\rangle$ 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 $\big|\{n_\beta\}\big\rangle$ with all values of the $N = \sum_\beta n_\beta$. Physically, this space is the Fock space

$$\mathcal{F} \;=\; |\text{vacuum}\rangle \;\oplus\; \mathcal{H}_1 \;\oplus\; \mathcal{H}_2 \;\oplus\; \mathcal{H}_3 \;\oplus\; \cdots \;=\; \bigoplus_{N=0}^{\infty} \mathcal{H}_N \tag{42}$$

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

In other words, what we have done thus far is to construct a basis of the entire Fock space comprising states $\big|\{n_\beta\}\big\rangle$ with definite occupation numbers. We can think of this basis as a common eigenbasis of a family of commuting hermitian operators $\hat{n}_\beta$ with eigenvalues $n_\beta = 0, 1, 2, \ldots$. Such operators are very useful for extending additive operators such as (37) to the whole Fock space and for writing them in compact form

$$\hat{H}\Big|_{\text{whole}\,\mathcal{F}} \;=\; \sum_\beta \epsilon_\beta \hat{n}_\beta\,. \tag{43}$$

Indeed, the operators (37) and (43) have the same eigenstates $|\alpha_1, \cdots, \alpha_N\rangle$ and the same eigenvalues $\sum_\beta \epsilon_\beta n_\beta = \epsilon_{\alpha_1} + \cdots + \epsilon_{\alpha_N}$.

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

$$\hat{H}_{\text{tot}} \;=\; \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} \times \hat{n}_{\mathbf{p}} \tag{44}$$

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

$$\hat{\mathbf{P}}_{\text{tot}} \;=\; \sum_{\mathbf{p}} \mathbf{p} \times \hat{n}_{\mathbf{p}} \tag{45}$$

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

$\star \quad \star \quad \star$

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 $\hat{a}_\alpha$. 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 $\big|\{n_\beta\}\big\rangle \in \mathcal{F}$, we may change one particular $n_\alpha \to n'_\alpha \pm 1$ 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,

$$\mathcal{F} \;=\; \bigotimes_\beta \mathcal{H}(\text{mode }\beta) \qquad \text{where} \quad \mathcal{H}(\text{mode }\beta)\text{ spans }\big|n_\beta\big\rangle \text{ for } n_\beta = 0,1,2,3,\ldots. \tag{46}$$

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

$$\hat{a}^\dagger\,|n\rangle \;\stackrel{\rm def}{=}\; \sqrt{n+1}\,|n+1\rangle\,, \qquad \hat{a}\,|n\rangle \;\stackrel{\rm def}{=}\; \begin{cases} \sqrt{n}\,|n-1\rangle & \text{for } n>0,\\ 0 & \text{for } n=0, \end{cases} \tag{47}$$

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. (46) 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

$$\begin{aligned} \hat{a}^\dagger_\alpha\,\big|\{n_\beta\}\big\rangle \;&\stackrel{\rm def}{=}\; \sqrt{n_\alpha+1}\,\big|\{n'_\beta = n_\beta + \delta_{\alpha\beta}\}\big\rangle\,,\\ \hat{a}_\alpha\,\big|\{n_\beta\}\big\rangle \;&\stackrel{\rm def}{=}\; \begin{cases} \sqrt{n_\alpha}\,\big|\{n'_\beta = n_\beta - \delta_{\alpha\beta}\}\big\rangle & \text{for } n_\alpha>0,\\ 0 & \text{for } n_\alpha=0, \end{cases}\\ \hat{n}_\alpha \;&=\; \hat{a}^\dagger_\alpha\hat{a}_\alpha\,. \end{aligned} \tag{48}$$

It is easy to see from these definitions that the operators $\hat{a}^\dagger_\alpha$, $\hat{a}_\alpha$, and $\hat{n}_\alpha$ 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*

$$[\hat{a}_\alpha,\hat{a}_\beta] \;=\; 0, \qquad [\hat{a}^\dagger_\alpha,\hat{a}^\dagger_\beta] \;=\; 0, \qquad [\hat{a}_\alpha,\hat{a}^\dagger_\beta] \;=\; \delta_{\alpha\beta}\,. \tag{49}$$

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

$$\hat{N}\hat{a}_\alpha^\dagger \;=\; \hat{a}_\alpha^\dagger(\hat{N}+1) \quad \text{and} \quad \hat{N}\hat{a}_\alpha \;=\; \hat{a}_\alpha(\hat{N}-1), \tag{50}$$

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

Of particular interest to QM of many-particle systems are operator products $\hat{a}_\alpha^\dagger \hat{a}_\beta$, $\hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \hat{a}_\gamma \hat{a}_\delta$, *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)

$$\widehat{H}_{\rm tot} \;=\; \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m}\, \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}\,, \qquad \widehat{\mathbf{P}}_{\rm tot} \;=\; \sum_{\mathbf{p}} \mathbf{p}\, \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}\,, \tag{51}$$

cf. eqs. (44) and (45).

More generally, consider any one-body (*i.e.*, one body at a time) additive operator which acts on N-particle states as

$$\hat{A}^{\rm tot}(N \text{ particles}) \;=\; \sum_{i=1}^{N} \hat{A}_1(i^{\rm th} \text{ particle}) \tag{52}$$

where $\hat{A}_1$ is some kind of a single-particle operator. Let $\langle\alpha|\,\hat{A}_1\,|\beta\rangle$ be its matrix elements. Then in the Fock space formalism, the net operator (52) acts as

$$\hat{A}^{\rm tot} \;=\; \sum_{\alpha,\beta} \langle\alpha|\,\hat{A}_1\,|\beta\rangle \times \hat{a}_\alpha^\dagger \hat{a}_\beta\,. \tag{53}$$

In particular, when the 1-particle states $|\alpha\rangle$ are eigenstates of the $\hat{A}_1$, this formula reduces to

$$\hat{A}^{\rm tot} \;=\; \sum_{\alpha} (\text{eigenvalue})_\alpha \times \hat{a}_\alpha^\dagger \hat{a}_\alpha\,. \tag{54}$$

At this point in the argument, the special case (54) should be obvious to you. The more general case (53) including the non-diagonal matrix elements $\langle\alpha|\,\hat{A}_1\,|\beta\rangle$ is not obvious, but the proof involves techniques which outside of the main line of our QFT class. So instead of presenting them in this set of notes, I made a separate set of notes on operators in wave-function and Fock-space languages. We shall not have time to cover these notes in class, so I ask you to read them on your own, whenever you have time for this.

In the same set of notes, you will also see that if three single-particle operators $\hat{A}_1$, $\hat{B}_1$, and $\hat{C}_1$ are related via commutation relation $[\hat{A}_1,\hat{B}_1]=\hat{C}_1$, then the corresponding Fock-space operators $\hat{A}^{\rm tot}$, $\hat{B}^{\rm tot}$, and $\hat{C}^{\rm tot}$ defined according to eq. (53) obey the same commutation relation $[\hat{A}^{\rm tot},\hat{B}^{\rm tot}]=\hat{C}^{\rm tot}$. For example, consider a gas of free atoms with nonzero integer spin $s=1,2,\ldots$. In terms of the creation and annihilation operators, the net spin operator for the whole gas becomes

$$\widehat{\mathbf{S}}_{\rm net} \;=\; \sum_{\mathbf{p}}\sum_{m_s,m'_s}\langle s,m_s|\,\hat{\mathbf{S}}_1\,|s,m'_s\rangle\times\hat{a}^\dagger_{\mathbf{p},m_s}\hat{a}_{\mathbf{p},m'_s}\,, \tag{55}$$

and since the single atom's spin operator obeys the angular momentum commutation relations $[\hat{S}^i_1,\hat{S}^j_1]=i\epsilon^{ijk}\hat{S}^k_1$, the net spin operator satisfies the same relations $[\hat{S}^i_{\rm net},\hat{S}^j_{\rm net}]=i\epsilon^{ijk}\hat{S}^k_{\rm net}$.

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

$$\hat{V}_{\rm net}\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) \;=\; \tfrac12\sum_{i\neq j}^{i,j=1,\ldots,N}V_2(\mathbf{x}_i-\mathbf{x}_j)\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N). \tag{56}$$

In the Fock-space formalism, this operator becomes

$$\widehat{V}_{\rm net} \;=\; \tfrac12\sum_{\alpha,\beta,\gamma,\delta}V_{\alpha,\beta,\gamma,\delta}\times\hat{a}^\dagger_\alpha\hat{a}^\dagger_\beta\hat{a}_\delta\hat{a}_\gamma \tag{57}$$

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

$$V_{\alpha,\beta,\gamma,\delta} \;=\; \int\!d\mathbf{x}_1\!\int\!d\mathbf{x}_2\,\phi^*_\alpha(\mathbf{x}_1)\phi^*_\beta(\mathbf{x}_2)\times V_2(\mathbf{x}_1-\mathbf{x}_2)\times\phi_\gamma(\mathbf{x}_1)\phi_\delta(\mathbf{x}_2). \tag{58}$$

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

$$\begin{aligned} V_{\mathbf{p}'_1,\mathbf{p}'_2,\mathbf{p}_1,\mathbf{p}_2} &= L^{-3}\delta_{\mathbf{p}'_1+\mathbf{p}'_2,\mathbf{p}_1+\mathbf{p}_2} \times W(\mathbf{q}) \\ \text{where} \quad \mathbf{q} = \mathbf{p}'_1 - \mathbf{p}_1 = \mathbf{p}_2 - \mathbf{p}'_2 & \quad \text{and} \quad W(\mathbf{q}) = \int d\mathbf{x}\, e^{-i\mathbf{q}\mathbf{x}}\, V_2(\mathbf{x}), \end{aligned} \tag{59}$$

hence

$$\widehat{V}_{\text{net}} = \tfrac{1}{2} L^{-3} \sum_{\mathbf{q}} W(\mathbf{q}) \sum_{\mathbf{p}_1,\mathbf{p}_2} \hat{a}^\dagger_{\mathbf{p}_1+\mathbf{q}} \hat{a}^\dagger_{\mathbf{p}_2-\mathbf{q}} \hat{a}_{\mathbf{p}_2} \hat{a}_{\mathbf{p}_1} . \tag{60}$$

More generally, a two-body additive operator of the form

$$\hat{B}_{\text{net}}(N \text{ particles}) = \tfrac{1}{2} \sum_{i\neq j}^{i,j=1,\ldots,N} \hat{B}_2(i^{\text{th}} \text{ and } j^{\text{th}} \text{ particles}) \tag{61}$$

in the Fock space formalism becomes

$$\widehat{B}_{\text{net}} = \tfrac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} B_{\alpha,\beta,\gamma,\delta} \times \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_\delta \hat{a}_\gamma \qquad \text{where} \quad B_{\alpha,\beta,\gamma,\delta} = (\langle\alpha| \otimes \langle\beta|)\hat{B}_2(|\gamma\rangle \otimes |\delta\rangle). \tag{62}$$

Note that the matrix elements $B_{\alpha,\beta,\gamma,\delta}$ are not symmetrized with respect to particle permutations $\gamma \leftrightarrow \delta$ and $\alpha \leftrightarrow \beta$; instead, the operator product $\hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_\delta \hat{a}_\gamma$ takes care of the symmetrization thanks to $\hat{a}_\delta \hat{a}_\gamma = \hat{a}_\gamma \hat{a}_\delta$ and $\hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta = \hat{a}^\dagger_\beta \hat{a}^\dagger_\alpha$.

Again, the proof of eq. (62) involve techniques I do not wish to develop here, so I present it in my notes on operators in wave-function and Fock-space languages.

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 $\hat{a}_\alpha$ to $\hat{a}^\dagger_\mu$ and $\hat{a}_\mu$, namely

$$\hat{a}^\dagger_\mu \;=\; \sum_\alpha \hat{a}^\dagger_\alpha \times \langle\alpha|\mu\rangle\,, \qquad \hat{a}_\mu \;=\; \sum_\alpha \hat{a}_\alpha \times \langle\mu|\alpha\rangle\,. \tag{63}$$

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 $\hat{a}_\mu$ and the $\hat{a}^\dagger_\mu$ obey the same bosonic commutation relations (49) as the $\hat{a}_\alpha$ 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*

$$\widehat{\Psi}^\dagger(\mathbf{x}) \;\equiv\; \hat{a}^\dagger_{\mathbf{x}} \;=\; \sum_\alpha \hat{a}^\dagger_\alpha \times \phi_\alpha(\mathbf{x}) \tag{64}$$

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

$$\widehat{\Psi}(\mathbf{x}) \;\equiv\; \hat{a}_{\mathbf{x}} \;=\; \sum_\alpha \hat{a}_\alpha \times \phi^*_\alpha(\mathbf{x}) \tag{65}$$

which annihilates a particle at point $\mathbf{x}$. These fields obey the continuous version of the bosonic commutation relations (49), namely

$$\left[\widehat{\Psi}(\mathbf{x}),\widehat{\Psi}(\mathbf{x}')\right] \;=\; 0, \qquad \left[\widehat{\Psi}^\dagger(\mathbf{x}),\widehat{\Psi}^\dagger(\mathbf{x}')\right] \;=\; 0, \qquad \left[\widehat{\Psi}(\mathbf{x}),\widehat{\Psi}^\dagger(\mathbf{x}')\right] \;=\; \delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{66}$$

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

$$\hat{N} \;=\; \sum_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha \;=\; \int d^3\mathbf{x}\,\widehat{\Psi}^\dagger(\mathbf{x})\widehat{\Psi}(\mathbf{x}), \tag{67}$$

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

$$\hat{V}_{\rm net} \;=\int\!d^3\mathbf{x}\,V_e(\mathbf{x})\times\hat{n}(\mathbf{x}) \;=\int\!d^3\mathbf{x}\,V_e(\mathbf{x})\times\widehat{\Psi}^\dagger(\mathbf{x})\widehat{\Psi}(\mathbf{x}). \tag{68}$$

Similarly, the net momentum operator is

$$\widehat{\mathbf{P}}_{\rm net} \;=\;\sum_{\mathbf{p}}\mathbf{p}\,\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} \;=\int\!d^3\mathbf{x}\,\widehat{\Psi}^\dagger(\mathbf{x})\left(-i\nabla\widehat{\Psi}(\mathbf{x})\right), \tag{69}$$

and the net *non-relativistic* kinetic energy operator is

$$\hat{H}^{\rm kin}_{\rm net} \;=\;\sum_{\mathbf{p}}\frac{\mathbf{p}^2}{2m}\,\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} \;=\int\!d^3\mathbf{x}\,\widehat{\Psi}^\dagger(\mathbf{x})\left(\frac{-\nabla^2}{2m}\,\widehat{\Psi}(\mathbf{x})\right) \;=\;+\frac{1}{2m}\int\!d^3\mathbf{x}\,\nabla\widehat{\Psi}^\dagger(\mathbf{x})\cdot\nabla\widehat{\Psi}(\mathbf{x}). \tag{70}$$

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

$$\begin{aligned}\hat{H} \;=\; \hat{H}^{\rm kin}_{\rm net} \,+\, \hat{V}_{\rm net} \;&=\int\!d^3\mathbf{x}\left(\frac{1}{2m}\,\nabla\widehat{\Psi}^\dagger(\mathbf{x})\cdot\nabla\widehat{\Psi}(\mathbf{x}) \,+\, V_e(\mathbf{x})\widehat{\Psi}^\dagger(\mathbf{x})\widehat{\Psi}(\mathbf{x})\right)\\ &=\int\!d^3\mathbf{x}\,\widehat{\Psi}^\dagger(\mathbf{x})\left(-\frac{\nabla^2}{2m}\,+\,V_e(\mathbf{x})\right)\widehat{\Psi}(\mathbf{x}).\end{aligned} \tag{71}$$

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

$$\begin{aligned} i\frac{\partial}{\partial t}\widehat{\Psi}(\mathbf{x},t) \;&=\; \left[\widehat{\Psi}(\mathbf{x},t),\hat{H}\right] \;=\; \left(-\frac{\nabla^2}{2m}\,+\,V_e(\mathbf{x})\right)\widehat{\Psi}(\mathbf{x},t),\\ -i\frac{\partial}{\partial t}\widehat{\Psi}^\dagger(\mathbf{x},t) \;&=\; \left[\hat{H},\widehat{\Psi}(\mathbf{x},t)\right] \;=\; \left(-\frac{\nabla^2}{2m}\,+\,V_e(\mathbf{x})\right)\widehat{\Psi}^\dagger(\mathbf{x},t).\end{aligned} \tag{72}$$

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 $\hat{\Psi}$ does not preserve N). (3) Adding interactions to the Hamiltonian (71) would make eqs. (72) non-linear, while the true Schrödinger equations are always linear, no matter what.

Indeed, let the particles have a two-body interaction potential (56). In terms of the quantum creation and annihilation fields, the Fock-space two-body potential becomes

$$\widehat{V}_{\rm int} \;=\; \tfrac{1}{2}\!\int\! d^3\mathbf{x}_1\!\int\! d^3\mathbf{x}_2\, V_2(\mathbf{x}_1-\mathbf{x}_2)\times \widehat{\Psi}^\dagger(\mathbf{x}_1)\widehat{\Psi}^\dagger(\mathbf{x}_2)\widehat{\Psi}(\mathbf{x}_2)\widehat{\Psi}(\mathbf{x}_1). \tag{73}$$

Adding this interaction to the free Hamiltonian (71) makes the Heisenberg equations for the quantum fields nonlinear (and non-local), namely:

$$\begin{aligned}
i\frac{\partial}{\partial t}\widehat{\Psi}(\mathbf{x},t) \;&=\; \left[\widehat{\Psi}(\mathbf{x},t),\hat{H}\right] \;=\; \left(-\frac{\nabla^2}{2m}+V_e(\mathbf{x})\right)\widehat{\Psi}(\mathbf{x},t)\\
&\qquad +\int\! d^3\mathbf{x}'\, V_2(\mathbf{x}'-\mathbf{x})\widehat{\Psi}^\dagger(\mathbf{x}')\widehat{\Psi}(\mathbf{x}')\times\widehat{\Psi}(\mathbf{x}),\\
-i\frac{\partial}{\partial t}\widehat{\Psi}^\dagger(\mathbf{x},t) \;&=\; -\left[\widehat{\Psi}^\dagger(\mathbf{x},t),\hat{H}\right] \;=\; \left(-\frac{\nabla^2}{2m}+V_e(\mathbf{x})\right)\widehat{\Psi}^\dagger(\mathbf{x},t)\\
&\qquad +\;\widehat{\Psi}^\dagger(\mathbf{x})\times\int\! d^3\mathbf{x}'\, V_2(\mathbf{x}'-\mathbf{x})\widehat{\Psi}^\dagger(\mathbf{x}')\widehat{\Psi}(\mathbf{x}').
\end{aligned} \tag{74}$$

However, without the two-body (or multi-body) interactions between the particles, the Heisenberg equations (72) are linear and look just like Schrödinger equation for a single-particle 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

$$\mathcal{L}_{\rm Schr} \;=\; -\hbar\,{\rm Im}(\psi^*\dot{\psi}) \;-\; \frac{\hbar^2}{2m}\nabla\psi^*\nabla\psi \;-\; V_e(\mathbf{x})\times\psi^*\psi\,. \tag{75}$$

(Note, $-\hbar\,{\rm Im}(\psi^*\dot{\psi}) = i\hbar\psi^*\dot{\psi} +$ 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

$$H \;=\; \int\! d^3\mathbf{x}\left(i\hbar\psi^*\times\dot{\psi} \,-\, \mathcal{L}\right) \;=\; \int\! d^3\mathbf{x}\left(\frac{\hbar^2}{2m}\nabla\psi^*\nabla\psi \,+\, V_e(\mathbf{x})\times\psi^*\psi\right). \tag{76}$$

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 (66) (which follow from the $i\hbar\psi^*(\mathbf{x})$ being the canonical conjugate of $\psi(\mathbf{x})$), and the classical Hamiltonian (76) becomes the Hamiltonian operator (71).

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.