Lecture 4

Learning goals

- To define annihilation and creation operators for fermions.
- To learn the very basics of quantum field theory, namely the concept of field operators.
- To understand how equation of motion is derived for field operators.

8 Second quantization continued

8.1 Fermions

For fermions, the antisymmetric states can be written using the Slater determinant:

$$S_- |i_1, i_2, \ldots, i_N\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} |i_1\rangle_1 & |i_1\rangle_2 & \ldots & |i_1\rangle_N \\ \vdots & \vdots & \ddots & \vdots \\ |i_N\rangle_1 & |i_N\rangle_2 & \ldots & |i_N\rangle_N \end{vmatrix}. \tag{8.1}$$

This fulfills the Pauli principle: no two identical fermions in the same state. In addition

$$S_- |i_2, i_1, \ldots, i_N\rangle = -S_- |i_1, i_2, \ldots, i_N\rangle. \tag{8.2}$$

As for bosons, one can define the Fock space. The orthogonality relation is the same as for bosons (compare with Equation (7.13) for bosons):

$$\langle n_1, n_2, \ldots | n_1', n_2', \ldots\rangle = \delta_{n_1 n_1'} \delta_{n_2 n_2'} \ldots \tag{8.3}$$

The completeness relation is different since **the occupation number for fermions can be only zero or one** (compare with Equation (7.14) for bosons):

$$\sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \cdots \sum_{n_N=0}^{1} |n_1, n_2, \ldots n_N\rangle \langle n_1, n_2, \ldots n_N| = \hat{1}. \tag{8.4}$$

Now let us introduce the creation operators. For fermions, applying them twice must give zero, due to the Pauli exclusion principle. Also, the order in which they are applied must play a role in order to get the minus signs related to permutations. Let us define the creation operators by:

$$S_- |i_1, i_2, \ldots, i_N\rangle = a_{i_1}^\dagger a_{i_2}^\dagger \ldots a_{i_N}^\dagger |0\rangle \tag{8.5}$$

$$S_- |i_2, i_1, \ldots, i_N\rangle = a_{i_2}^\dagger a_{i_1}^\dagger \ldots a_{i_N}^\dagger |0\rangle. \tag{8.6}$$

These states must be equal except a minus sign, therefore the operators must anti-commute:

$$\left\{a_i^\dagger, a_j^\dagger\right\} = 0, \qquad a_i^\dagger a_j^\dagger = -a_j^\dagger a_i^\dagger. \tag{8.7}$$

This implies also that double occupation is impossible:

$$a_i^\dagger a_j^\dagger = -a_j^\dagger a_i^\dagger \Rightarrow \left(a_i^\dagger\right)^2 = 0. \tag{8.8}$$

Notation:

$$\{A, B\} \equiv [A, B]_+ = AB + BA \tag{8.9}$$

$$[A, B] \equiv [A, B]_- = AB - BA. \tag{8.10}$$

Since ordering matters, one must choose some ordering in the beginning and then keep it fixed. Then (compare with Equation (7.24) for bosons)

$$|n_1, n_2, \ldots\rangle = \left(a_1^\dagger\right)^{n_1} \left(a_2^\dagger\right)^{n_2} \ldots |0\rangle\,, \qquad n_i = 0, 1. \tag{8.11}$$

The creation operator $a_i^\dagger$ must be (compare with Equation (7.15) for bosons):

$$a_i^\dagger\, |\ldots, n_i, \ldots\rangle = (1 - n_i)\,(-1)^{\sum_{j<i} n_j}\, |\ldots, n_i + 1, \ldots\rangle \tag{8.12}$$

The reason for the term $(-1)^{\sum_{j<i} n_j}$ is that the operator $a_i^\dagger$ has to be brought to the position i and along the way commuted with the other operators $a_j^\dagger$.

The adjoint (annihilation) operator is

$$\langle \ldots, n_i, \ldots|\, a_i = (1 - n_i)\,(-1)^{\sum_{j<i} n_j}\, \langle \ldots, n_i + 1, \ldots| \tag{8.13}$$

$$\Rightarrow \langle \ldots, n_i, \ldots|\, a_i\, |\ldots, n'_i, \ldots\rangle = (1 - n_i)\,(-1)^{\sum_{j<i} n_j}\, \delta_{n_i+1, n'_i} \tag{8.14}$$

$$\Rightarrow a_i\, |\ldots, n'_i, \ldots\rangle = \sum_{n_i} |n_i\rangle \langle n_i|\, a_i\, |n'_i\rangle = n'_i\,(-1)^{\sum_{j<i} n_j}\, |\ldots, n'_i - 1, \ldots\rangle \tag{8.15}$$

$$\begin{aligned} \Rightarrow a_i a_i^\dagger\, |\ldots, n_i, \ldots\rangle &= a_i\,(1 - n_i)\,(-1)^{\sum_{j<i} n_j}\, |\ldots, n_i + 1, \ldots\rangle \\ &= (1 - n_i)\,(n_i + 1)\, |\ldots, n_i, \ldots\rangle \\ &= (1 - n_i)\, |\ldots, n_i, \ldots\rangle \end{aligned} \tag{8.16}$$

$$a_i^\dagger a_i\, |\ldots, n_i, \ldots\rangle = n_i\, |\ldots, n_i, \ldots\rangle \tag{8.17}$$

($n_i^2 = n_i$ for $n_i = 0, 1$). From here, one obtains the anticommutation rules for fermions (take sums of Equations (8.16) and (8.17), compare with (7.20) for bosons):

$$[a_i, a_j]_+ = 0, \qquad \left[a_i^\dagger, a_j^\dagger\right]_+ = 0, \qquad \left[a_i, a_j^\dagger\right]_+ = \delta_{ij}. \tag{8.18}$$

Note that quite often fermionic annihilation and creation operators are denoted by the letter c: c_i, $c_i^\dagger$, and the bosonic ones by a (or b): a_i, $a_i^\dagger$ (b_i, $b_i^\dagger$). In these lecture notes, we will also sometimes (as above) use a_i for fermions, because some of the results we derive are the same or similar for bosons and fermions. Always remember whether you are dealing with bosons or fermions, in this course and afterwards!

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8.2 Field operators

The annihilation and creation operators a_i, $a_i^\dagger$ operate in some given basis of states. However, as usual, the basis can be changed through unitary transformations. By changing to the position basis, one defines the so-called field operators. They often give an intuitive and clear formulation of the physical problem in question, and, importantly, they are the basic entities of quantum field theories. We will now learn the basics of field operators.

Given a single-particle basis set $\{|i\rangle\}$ and the corresponding annihilation and creation operators, a_i and $a_i^\dagger$, we can move to a new basis $\{|\lambda\rangle\}$ with new annihilation and creation operators b_λ and $b_\lambda^\dagger$ as follows:
First expand the basis states

$$|\lambda\rangle = \sum_i |i\rangle\langle i|\lambda\rangle. \tag{8.19}$$

The new basis states are $|\lambda\rangle = b_\lambda^\dagger|0\rangle$. We assume that the vacuum state in both bases is the same. Then one obtains

$$b_\lambda^\dagger|0\rangle = \sum_i \langle i|\lambda\rangle a_i^\dagger|0\rangle, \tag{8.20}$$

which gives the creation and annihilation operators

$$b_\lambda^\dagger = \sum_i \langle i|\lambda\rangle a_i^\dagger, \tag{8.21}$$

and

$$b_\lambda = \sum_i \langle \lambda|i\rangle a_i. \tag{8.22}$$

Now we transform into the position basis $\{|\mathbf{x}\rangle\}$. The corresponding annihilation and creation operators are called (annihilation and creation) **field operators**:

$$\psi^\dagger(\mathbf{x}) = \sum_i \langle i|\mathbf{x}\rangle a_i^\dagger = \sum_i \varphi_i^*(\mathbf{x}) a_i^\dagger, \tag{8.23}$$

where $\varphi_i(\mathbf{x})$ is the wave function of the single-particle state $|i\rangle$. Field operators satisfy the usual (anti)commutation relations for (fermions) bosons:

$$[\psi(\mathbf{x}), \psi(\mathbf{x}')]_\pm = \sum_{ij} \varphi_i(\mathbf{x})\varphi_j(\mathbf{x}')\,[a_i, a_j]_\pm = 0, \tag{8.24}$$

$$\left[\psi^\dagger(\mathbf{x}), \psi^\dagger(\mathbf{x}')\right]_\pm = \sum_{ij} \varphi_i^*(\mathbf{x})\varphi_j^*(\mathbf{x}')\left[a_i^\dagger, a_j^\dagger\right]_\pm = 0, \tag{8.25}$$

and

$$\left[\psi(\mathbf{x}), \psi^\dagger(\mathbf{x}')\right]_\pm = \sum_{ij} \varphi_i(\mathbf{x})\varphi_j^*(\mathbf{x}')\left[a_i, a_j^\dagger\right]_\pm = \sum_i \varphi_i(\mathbf{x})\varphi_i^*(\mathbf{x}') = \delta^{(3)}(\mathbf{x}-\mathbf{x}') \tag{8.26}$$

One can now express various operators in terms of these field operators. Let us start with the kinetic energy operator:

$$
\begin{aligned}
H_{kin} &= \sum_{ij} a_i^\dagger \langle i|T|j\rangle a_j \\
&= \sum_{ij} a_i^\dagger a_j \int d^3x\, \varphi_i^*(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \varphi_j(\mathbf{x}) \\
&= \int d^3x \left(\sum_i a_i^\dagger \varphi_i^*(\mathbf{x})\right) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \left(\sum_j a_j \varphi_j(\mathbf{x})\right) \\
&= \int d^3x\, \psi^\dagger(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \psi(\mathbf{x}).
\end{aligned} \tag{8.27}
$$

By integration in parts, and assuming that the field $\psi(\mathbf{x})$ goes to zero at infinity (the integration limits are plus minus infinity), this can also be written in the form

$$
H_{kin} = \frac{\hbar^2}{2m} \int d^3x\, \nabla\psi^\dagger(\mathbf{x})\nabla\psi(\mathbf{x}). \tag{8.28}
$$

In the same way we obtain the expression for a single-particle potential

$$
\begin{aligned}
H_{pot} &= \sum_{ij} a_i^\dagger U_{ij} a_j \\
&= \int d^3x\, U(\mathbf{x})\psi^\dagger(\mathbf{x})\psi(\mathbf{x}).
\end{aligned} \tag{8.29}
$$

And the two-particle interaction is expressed as (derivation in **Exercise set 4**)

$$
H_{\text{int}} = \frac{1}{2} \int d^3x \int d^3x'\, \psi^\dagger(\mathbf{x})\psi^\dagger(\mathbf{x}')V(\mathbf{x},\mathbf{x}')\psi(\mathbf{x}')\psi(\mathbf{x}), \tag{8.30}
$$

and the total Hamiltonian in the field operator formulation is the sum of these (plus any other part such as some electromagnetic fields):

$$
\begin{aligned}
H &= H_{kin} + H_{pot} + H_{int} \\
&= \int d^3x \left(\frac{\hbar^2}{2m}\nabla\psi^\dagger(\mathbf{x})\nabla\psi(\mathbf{x}) + U(\mathbf{x})\psi^\dagger(\mathbf{x})\psi(\mathbf{x})\right) \\
&+ \frac{1}{2}\int d^3x \int d^3x'\, \psi^\dagger(\mathbf{x})\psi^\dagger(\mathbf{x}')V(\mathbf{x},\mathbf{x}')\psi(\mathbf{x}')\psi(\mathbf{x}).
\end{aligned} \tag{8.31}
$$

Notice that the above applies equally to fermions and bosons.
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8.2.1 Field equations

Further insight into the field operators can be obtained by calculating their equations of motion. We consider the field operators in the Heisenberg picture:

$$
\psi(\mathbf{x},t) = e^{iHt/\hbar}\psi(\mathbf{x},0)e^{-iHt/\hbar}. \tag{8.32}
$$

The we start from the Heisenberg equation of motion

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = -[H,\psi(\mathbf{x},t)] = -e^{iHt/\hbar}[H,\psi(\mathbf{x},0)]e^{-iHt/\hbar}. \tag{8.33}$$

Therefore, one needs to just calculate the commutator at time $t = 0$. Let us first consider the kinetic energy part of the Hamiltonian.

The kinetic energy part of the commutator becomes (below, $\pm$ refers to fermions and bosons, respectively)

$$\begin{aligned}
-[H_{kin},\psi(\mathbf{x},0)] = [\psi(\mathbf{x}),H_{kin}] &= \int d^3x' \left[\psi(\mathbf{x}),\psi^\dagger(\mathbf{x}')\left(-\frac{\hbar^2\nabla'^2}{2m}\right)\psi(\mathbf{x}')\right] \\
&= \frac{\hbar^2}{2m}\int d^3x' \left[\psi(\mathbf{x}),\nabla'\psi^\dagger(\mathbf{x}')\nabla'\psi(\mathbf{x}')\right] \\
&= \frac{\hbar^2}{2m}\int d^3x' \left\{\psi(\mathbf{x})\nabla'\psi^\dagger(\mathbf{x}')\nabla'\psi(\mathbf{x}') - \nabla'\psi^\dagger(\mathbf{x}')\nabla'\psi(\mathbf{x}')\psi(\mathbf{x})\right\} \\
&= \frac{\hbar^2}{2m}\int d^3x' \left\{\nabla'\psi(\mathbf{x})\psi^\dagger(\mathbf{x}')\nabla'\psi(\mathbf{x}') \pm \nabla'\psi^\dagger(\mathbf{x}')\psi(\mathbf{x})\nabla'\psi(\mathbf{x}')\right\} \\
&= \frac{\hbar^2}{2m}\int d^3x'\, \nabla' \left[\psi(\mathbf{x}),\psi^\dagger(\mathbf{x}')\right]_{\pm} \nabla'\psi(\mathbf{x}') \\
&= \frac{\hbar^2}{2m}\int d^3x'\, \nabla'\delta^{(3)}(\mathbf{x}-\mathbf{x}')\nabla'\psi(\mathbf{x}') \\
&= -\frac{\hbar^2}{2m}\int d^3x'\, \delta^{(3)}(\mathbf{x}-\mathbf{x}')\nabla'^2\psi(\mathbf{x}') \\
&= -\frac{\hbar^2\nabla^2}{2m}\psi(\mathbf{x}),
\end{aligned} \tag{8.34}$$

where the second last line was obtained by partial integration. In a very similar way, one can obtain the part of the equation of motion from the potential energy term. To calculate the part corresponding to the interaction term is an exercise in **Exercise set 4**. Combining these, the equation of motion (8.33) for the field operator becomes

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) &= \left(-\frac{\hbar^2\nabla^2}{2m} + U(\mathbf{x})\right)\psi(\mathbf{x},t) \\
&+ \int d^3x'\psi^\dagger(\mathbf{x}',t)V(\mathbf{x},\mathbf{x}')\psi(\mathbf{x}',t)\psi(\mathbf{x},t).
\end{aligned} \tag{8.35}$$

The equation of motion for the field operator $\psi(\mathbf{x},t)$ looks like the Schrödinger equation for a wave function except that we are now in the Heisenberg picture and $\psi(\mathbf{x},t)$ is an operator. The field operator describes a **quantum field**, for instance an electron field. In quantum field theory, quantum mechanical systems (like electronic, photonic, etc. systems) are parametrized (or represented) by an infinite number of degrees of freedom: in $\psi(\mathbf{x})$, the position is a continuous variable, therefore the infinite number of degrees of freedom. Note that here $\mathbf{x}$ is a parameter characterizing the field, not an operator. **Quanta of the field** are what we understand as individual particles, like electrons, photons, etc. This field theoretical approach is often used in condensed matter and high-energy physics. One reason for the name "second quantization" is that we obtained for the quantum field operators an equation that looks exactly like the (non-linear) Schrödinger equation for wavefunctions.

8.2.2 Momentum representation

The field operator formulation is often the starting point for many problems. However, eventually the continuous basis $\{|\mathbf{x}\rangle\}$ is not very useful and the field operators will be expanded in some suitable (usually discrete) basis. In the absence of an external potential the basis of choice is (often) the plane wave basis, i.e. one expands

$$\psi(\mathbf{x}) = \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} a_{\mathbf{k}}, \tag{8.36}$$

where V is the volume normalization factor and $\mathbf{k}$ is the momentum. Calculations will be more convenient if the system is put in a box of volume $V = L_x L_y L_z$. In the end one can then take the thermodynamic limit $V \to \infty$, while keeping the density N/V fixed (N is the number of particles).

Using periodic boundary conditions, the allowed momentum eigenstates for each direction in the box are

$$\mathbf{k} = 2\pi \left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right). \tag{8.37}$$

where $n_i \in \mathcal{Z}$. The eigenfunctions are

$$\varphi_{\mathbf{k}} = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}}, \tag{8.38}$$

and they are orthonormal. Expanding now the field operators in this basis gives (**Exercise set 4**) the Hamiltonian

$$H = \sum_{\mathbf{k}} \frac{\hbar^2\mathbf{k}^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{1}{V} \sum_{\mathbf{k},\mathbf{k}'} U_{\mathbf{k}'-\mathbf{k}} a^\dagger_{\mathbf{k}'} a_{\mathbf{k}} + \frac{1}{2V} \sum_{\mathbf{k},\mathbf{p},\mathbf{q}} V_{\mathbf{q}} a^\dagger_{\mathbf{p}+\mathbf{q}} a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}} a_{\mathbf{p}}, \tag{8.39}$$

where $V_{\mathbf{q}}$ is the Fourier transformation of the interaction potential (it has been assumed that $V(\mathbf{x}, \mathbf{x}')$ is translationally invariant $V(\mathbf{x}, \mathbf{x}') = V(\mathbf{x} - \mathbf{x}')$)

$$V(\mathbf{x} - \mathbf{x}') = \frac{1}{V} \sum_{\mathbf{q}} V_{\mathbf{q}} e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}. \tag{8.40}$$

The Fourier transformation of the single particle potential, $U_{\mathbf{k}}$, is defined similarly. The annihilation and creation operators for a particle with a wave vector $\mathbf{k}$ (i.e. in the state $\varphi_{\mathbf{k}}$) obey the usual commutation relations:

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}]_\pm = 0 \tag{8.41}$$

$$\left[a^\dagger_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}\right]_\pm = 0 \tag{8.42}$$

$$\left[a_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}\right]_\pm = \delta_{\mathbf{k}\mathbf{k}'}. \tag{8.43}$$

The interaction term has a nice pictorial interpretation, in terms of so called diagrams. It causes the annihilation of two particles with wave vectors $\mathbf{k}$ and $\mathbf{p}$ and creates in their place two particles with wave vectors $\mathbf{k} - \mathbf{q}$ and $\mathbf{p} + \mathbf{q}$.
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