Quantum Many Body Theory

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Week 3
3 Second Quantization

3.1 Creation and annihilation operators (the case of bosons)

Creation and annihilation operators were invented to simply work with many-particle wave functions. Any many-particle wave function can be written in the following way:

$$\psi(x_1, x_2, \ldots) = \sum_{k_1, k_2, \ldots} c_{k_1, k_2, \ldots} e^{i k_1 x_1 + i k_2 x_2 + \ldots},$$  \hspace{1cm} (3.1)

where $c_{k_1, k_2, \ldots}$ is either symmetric or antisymmetric with respect to interchange of $k$ (depending on whether the particles are bosons or fermions). We concentrate on the case of bosons, thus it is symmetric. This is essentially a Fourier transform of the many-particle wave function. The wave functions $e^{i k_1 x_1 + i k_2 x_2 + \ldots}$ can be described in words by listing all the values for all the $k$. For example, if $N_1$ of the particles in this wave function have momentum $k_1$, $N_2$ of the particles have momentum $k_2$ and so on, we can describe this wave function by listing all the momenta and the number of particles which have these momenta. This is called the occupation number representation. Thus a typical such wave function can be written as

$$|N_1, N_2, \ldots\rangle.$$

This notation implies that $N_1$ particles have momentum $k_1$, $N_2$ particles have momentum $k_2$ etc. It is assumed that someone already fixed once and for all the order of momenta $k_1, k_2, \text{etc}$, which the particles sitting at an i-th position in (3.2) have. An arbitrary wave function is a linear combination of such states, according to (3.1).

After (3.2) is defined, one introduces creation and annihilation operators. The creation operator $\hat{a}^\dagger_{k_i}$ is defined by how it acts on states, which for bosons takes form:

$$\hat{a}^\dagger_{k_i} |N_1, N_2, \ldots, N_{i-1}, N_i, N_{i+1}, \ldots\rangle = \sqrt{N_i} |N_1, N_2, \ldots, N_{i-1}, N_i - 1, N_{i+1}, \ldots\rangle.$$  \hspace{1cm} (3.3)

Correspondingly,

$$\hat{a}^\dagger_{k_i} |N_1, N_2, \ldots, N_{i-1}, N_i, N_{i+1}, \ldots\rangle = \sqrt{N_i + 1} |N_1, N_2, \ldots, N_{i-1}, N_i + 1, N_{i+1}, \ldots\rangle.$$  \hspace{1cm} (3.4)

(3.4) follows from (3.3) by hermitian conjugation.

It is straightforward to see that

$$\hat{a}^\dagger_{k_i} \hat{a}_{k_j} - \hat{a}^\dagger_{k_j} \hat{a}_{k_i} = \delta_{ij}.$$  \hspace{1cm} (3.5)
The operator \( \hat{a}_k \) counts the number of particles with momentum \( k \). Thus if a system of noninteracting identical bosons particles is described by the Hamiltonian

\[
\hat{H} = -\frac{1}{2m} \sum_i \frac{\partial^2}{\partial x_i^2}
\]  

(3.6)

and if \( N_1 \) of these have momentum \( k_1 \), \( N_2 \) have momentum \( k_2 \) etc, then the total energy can be obtained, obviously, as the expectation value of the Hamiltonian

\[
\hat{H} = \sum_i \frac{k_i^2}{2m} \hat{a}_k^\dagger \hat{a}_k.
\]  

(3.7)

Given the operator \( a_k \), we can define

\[
\hat{\psi}(x) = \frac{1}{\sqrt{L}} \sum_k \hat{a}_k e^{ikx}, \quad \hat{\psi}^\dagger(x) = \frac{1}{\sqrt{L}} \sum_k \hat{a}_k^\dagger e^{-ikx}.
\]  

(3.8)

These are sometimes called field operators, but basically these are creation and annihilation operators of a particle at one point, \( x \). Notice the curious factor \( 1/\sqrt{L} \), where \( L \) is the size of the system. Its presence is a standard convention, but it has a justification. Dimensionally, \( a_k^\dagger \) is a number. Indeed, \( \hat{a}_k^\dagger \hat{a}_k \) counts the number of particles with momentum \( k \), and that number is just some integer. At the same time, as we will see below, \( \hat{\psi}^\dagger(x)\hat{\psi}(x) \) counts the number of particles at a point \( x \), which cannot be just an integer, because \( x \) is an infinitesimally small point. Rather, this quantity must have dimensions of density, so that if we integrate it over some region of \( x \), we will find the total number of particles in that region. \( 1/\sqrt{L} \) is the factor which gives it dimensions of density.

The inverse transformations read

\[
\hat{a}_k = \frac{1}{\sqrt{L}} \int dx \ \hat{\psi}(x) e^{-ikx}, \quad \hat{a}_k^\dagger = \frac{1}{\sqrt{L}} \int dx \ \hat{\psi}^\dagger(x) e^{ikx}.
\]  

(3.9)

Using these, we can check that for example

\[
\sum_k \hat{a}_k^\dagger \hat{a}_k = \int dx \ \hat{\psi}^\dagger(x)\hat{\psi}(x)
\]  

(3.10)

confirming that \( \hat{\psi}^\dagger(x)\hat{\psi}(x) \) is the density of particles.

We can also check that for the free particle Hamiltonian (3.7)

\[
\hat{H} = \int dx \ \frac{1}{2m} \frac{\partial \hat{\psi}^\dagger(x) \partial \hat{\psi}(x)}{\partial x}
\]  

(3.11)

Finally, we can check that

\[
\hat{\psi}(x)\hat{\psi}^\dagger(y) - \hat{\psi}^\dagger(y)\hat{\psi}(x) = \delta(x - y).
\]  

(3.12)
Now suppose we have interacting particles, with the Hamiltonian

\[ \hat{H} = -\frac{1}{2m} \sum_i \frac{\partial^2}{\partial x_i^2} + \sum_{i<j} U(|x_i - x_j|). \]  \hspace{1cm} (3.13)

It describes particles (bosons, since we are considering only bosons here), which interact via pair-wise interactions \( U(|x|) \) which depend on the distance \(|x|\) between the particles. Let us write this Hamiltonian in the form similar to (3.7). While the first term (kinetic energy) still takes the form (3.11), the interaction term can be rewritten using the notion of the density of particles at a point, to give

\[ \hat{H} = \int dx \, \frac{1}{2m} \frac{\partial \hat{\psi}^\dagger(x)}{\partial x} \frac{\partial \hat{\psi}(x)}{\partial x} + \frac{1}{2} \int dx_1 dx_2 \, \hat{\psi}^\dagger(x_1) \hat{\psi}(x_1) U(|x_1 - x_2|) \, \hat{\psi}^\dagger(x_2) \hat{\psi}(x_2). \]  \hspace{1cm} (3.14)

The coefficient \( 1/2 \) in front of the interaction term prevents overcounting. Indeed, as we integrate over \( x_1 \) and \( x_2 \) we count the interactions between particles at two points, let’s say \( y_1 \) and \( y_2 \), twice. Once when \( x_1 = y_1 \) and \( x_2 = y_2 \). Second time when \( x_1 = y_2 \) and \( x_2 = y_1 \). \( 1/2 \) removes this overcounting. Note that in (3.13) this problem was taken care of by summing over \( i < j \), that is, each pair of particles was counted only once.

For various reasons, often one wants to put all the creation operators to the left of the annihilation operators in the Hamiltonian (it’s easier to do calculations this way). We can do it by employing the commutation relations (3.12) on the two operators, one just to the left of \( U \) and one just to the right of \( U \) in (3.14) to move the operators around as in

\[ \int dx_1 dx_2 \, \hat{\psi}^\dagger(x_1) \hat{\psi}(x_1) U(|x_1 - x_2|) \, \hat{\psi}^\dagger(x_2) \hat{\psi}(x_2) = \int dx_1 dx_2 U(|x_1 - x_2|) \, \hat{\psi}^\dagger(x_1) \hat{\psi}(x_1) \hat{\psi}^\dagger(x_2) \hat{\psi}(x_2) + \int dx \, U(0) \hat{\psi}^\dagger(x) \hat{\psi}(x). \]  \hspace{1cm} (3.15)

The last term is equal to \( U(0)N \), where \( N \) is the total number of particles. It represents just a constant which is being added to the Hamiltonian and is thus irrelevant. So we can rewrite the many-body Hamiltonian (3.14) as in

\[ \hat{H} = \int dx \, \frac{1}{2m} \frac{\partial \hat{\psi}^\dagger(x)}{\partial x} \frac{\partial \hat{\psi}(x)}{\partial x} + \frac{1}{2} \int dx_1 dx_2 U(|x_1 - x_2|) \, \hat{\psi}^\dagger(x_1) \hat{\psi}^\dagger(x_2) \hat{\psi}(x_1) \hat{\psi}(x_2). \]  \hspace{1cm} (3.16)

### 3.2 Practical usage of the creation and annihilation operators

We replaced (3.13) with (3.14) or (3.16). But why is the new form better than the old one? The short answer is, there are many tricks which allow to manipulate creation and annihilation operators to understand the behavior of complicated systems.
Another question is, what does it mean to “solve” a problem such as (3.16)? This depends. If one especially lucky, then the “solution” could mean the following. One is able to find some new creation and annihilation operators, let’s call them $\hat{b}_i$ and $\hat{b}_i^\dagger$, which still satisfy the right commutation relations, such that in terms of them the Hamiltonian takes the form of a "free" Hamiltonian

$$\hat{H} = \sum_i \epsilon_i \hat{b}_i^\dagger \hat{b}_i. \quad (3.17)$$

Then this Hamiltonian describes free (noninteracting) particles with energies $\epsilon_i$ and is completely understood (solved). The new particles $b$ may have very little to do with the original particles $a$.

Typically we say that if the Hamiltonian is quadratic in creation and annihilation operators, it is completely solvable ((3.14) or (3.16) clearly do not belong in this category).

Even if the Hamiltonian is quadratic, but does not take the form (3.17), such as this one

$$\hat{H} = \sum_i \epsilon_i \hat{b}_i^\dagger \hat{b}_i + \sum_j t_j \left( \hat{b}_j^2 + \hat{b}_j^\dagger 2 \right), \quad (3.18)$$

it is still solvable by a straightforward technique called Bogoliubov transformation (see problem 3 of the problem set 1).

Here is another example. The Hamiltonian (3.11) looks quadratic, but does not take the form (3.17). How would one solve it? One recognizes that the transformation (3.8) brings it to the form (3.7), which is obviously solvable.

In general, a Hamiltonian of the form

$$\hat{H} = \sum_{ij} \hat{a}_i^\dagger h_{ij} \hat{a}_j \quad (3.19)$$

where $h_{ij}$ is some hermitian matrix, is solvable by a unitary transformation. Linear algebra tells us there exists a unitary matrix $U$ such that $U^\dagger h U$ is a diagonal matrix, with the diagonal entries $\epsilon_i$. Then in terms of new operators $\hat{a}_i = \sum_j U_{ij} \hat{b}_j$, $\hat{b}_i = \sum_j U_{ij}^\dagger \hat{a}_j$ (this is a unitary matrix, so $U^\dagger = U^{-1}$) the Hamiltonian becomes

$$\hat{H} = \sum_i \epsilon_i \hat{b}_i^\dagger \hat{b}_i, \quad (3.20)$$

that is, it is solved.

How does one know that $\hat{b}$ are legitimate operators? One checks their commutation relations

$$[\hat{b}_i^\dagger, \hat{b}_j] = \sum_{lk} [\hat{a}_l^\dagger U_{li}, U_{jk}^\dagger \hat{a}_k] = \sum U_{ki} U_{jk}^\dagger = \delta_{ij}. \quad (3.21)$$
Thus the commutation relations work. (Here $[\hat{a}, \hat{b}] \equiv \hat{a}\hat{b} - \hat{b}\hat{a}$ is a convenient shorthand notation, and we used that by the definition of a unitary matrix $\sum_k U_{jk}^\dagger U_{ki} = \delta_{ij}$).