Introduction to Second Quantization

Lucile Chassat - Samuel Van Gele

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NOTE: This reader is an adapted, shortened version of chapter 2 of the book "Quantum Field Theory For The Gifted Amateur" by T. Lancaster and S. J. Blundell.

1 The Concept of Second Quantization

For the upcoming chapter on charge transport, we will need to get familiar with the concept of second quantization as well as the formalism of annihilation and creation operators, as these are used in the Hamiltonians describing charge transport.

The concept of second quantization is a formulation used to describe multi-body systems in quantum theory and is also known under the name of quantum field theory. This theory takes a view on physics which not only sees particles like electrons as waves ("first quantization") but also treats wave phenomena as particles ("second quantization"). This second quantization thus arises whenever we find that objects previously thought of as waves (such as electromagnetic radiation and lattice vibrations) can also act as particles (photons and phonons).

The concept of second quantization just provides a new language to describe such situations that simplifies the overall comprehension of many-body systems often encountered in physics and chemistry. The description makes use of so-called creation and annihilation operators that are introduced to insert or delete a single-particle state from the wave function.

2 The Example of Harmonic Oscillators

We will take the model of the harmonic oscillator as this is one of the simplest models to describe solids. We can regard atoms/molecules/charge sites as being interconnected by springs in the lattice and that charge transport can occur through this lattice. This model is also used at a smaller scale to describe molecular vibrations. In this context, the creation and annihilation operators can be regarded as the raising and lowering operators, which add or remove energy quanta to move from one energy level to another one.

So, in order to understand the origin of these operators, which will be useful in our charge transport models, let us recall the simple harmonic oscillator problem, a mass attached to a spring. The Hamiltonian can be written as a combination of the kinetic energy and the potential energy for the spring constant K:

$$(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}K\hat{x}^2)\Psi = E\Psi \tag{1}$$

Eigenfunctions of this harmonic oscillator have the form

$$\Psi_n(\xi) = \frac{1}{\sqrt{2^n n!}}(\frac{m\omega}{\pi\hbar})^{\frac{1}{4}} H_n(\xi) e^{\frac{-\xi^2}{2}} \tag{2}$$

with the Hermite polynomials $H_n(\xi)$ and ξ=$\sqrt{m\omega/\hbar x}$. The eigenvalues are

$$E_n = (n + \frac{1}{2})\hbar\omega \tag{3}$$

The wavefunctions as well as the energy of the system depend on an integer n. The energy levels are thus quantized and equally spaced. Moreover, there is the zero point energy, i.e., vibration in the ground state for $n = 0$.

The Hamiltonian can be rewritten as:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega\hat{x}^2 \tag{4}$$

which is tempting to factorize as:

$$\hat{H} = \frac{1}{2}m\omega^2(\hat{x} - \frac{i}{m\omega}\hat{p})(\hat{x} + \frac{i}{m\omega}\hat{p}) \tag{5}$$

However, one must be aware that $\hat{x}$ and $\hat{p}$ do not commute. This is important because by developing the above factorized Hamiltonian we obtain:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega\hat{x}^2 + \frac{i\omega}{2}[\hat{x}, \hat{p}] \tag{6}$$

Indeed, $[\hat{x}, \hat{p}] = i\hbar$, and thus by redevloping we have obtained the Hamiltonian corrected by a subtraction of the zero point energy:

$$\hat{H} - \frac{\hbar\omega}{2} = \frac{1}{2}m\omega^2(\hat{x} - \frac{i}{m\omega}\hat{p})(\hat{x} + \frac{i}{m\omega}\hat{p}) \tag{7}$$

This tells us that the operators in parenthesis $(\hat{x} \pm \frac{i}{m\omega}\hat{p})$ may be useful and we can thus define two new operators:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i}{m\omega}\hat{p}) \tag{8}$$

and

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i}{m\omega}\hat{p}) \tag{9}$$

with

$$[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1 \tag{10}$$

Putting these definitions into the Hamiltonian we get:

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}) \tag{11}$$

We have hence just rewritten our initial problem using a new language. The wavefunctions are still the same and depend on an integer n. The main operator is now $\hat{a}^\dagger\hat{a}$ that has eigenstates $|n\rangle$ with eigenvalues $\hbar\omega(n + \frac{1}{2})$, which thus renders the ladder-like energy levels much more intuitive than before.

If the main operator is a product of two operators, we can define a new number operator:

$$\hat{n} = \hat{a}^\dagger \hat{a} \tag{12}$$

When $\hat{n}$ operates on an eigenstate, it returns the integer of the energy level of the system

$$\hat{n}|n\rangle = n|n\rangle \tag{13}$$

The Hamiltonian becomes:

$$\hat{H} = \hbar\omega(\hat{n} + \frac{1}{2}) \tag{14}$$

and the Schrödinger equation now reads:

$$\hat{H}|n\rangle = \hbar\omega(\hat{n} + \frac{1}{2})|n\rangle \tag{15}$$

Now we would like to see what $\hat{a}^\dagger$ and $\hat{a}$ actually do. We can operate $\hat{a}^\dagger$ on the eigenstate $|n\rangle$ and then the number operator to see what the value of the integer is. We find that

$$\hat{n}\hat{a}^\dagger|n\rangle = \hat{a}^\dagger\hat{a}\hat{a}^\dagger|n\rangle \tag{16}$$

$$\hat{n}\hat{a}^\dagger|n\rangle = \hat{a}^\dagger(\hat{a}\hat{a}^\dagger)|n\rangle \tag{17}$$

And with the commutator

$$\hat{n}\hat{a}^\dagger|n\rangle = \hat{a}^\dagger(1 + \hat{a}^\dagger\hat{a})|n\rangle \tag{18}$$

$$\hat{n}\hat{a}^\dagger|n\rangle = \hat{a}^\dagger(1 + \hat{n})|n\rangle \tag{19}$$

$$\hat{n}\hat{a}^\dagger|n\rangle = (1 + n)\hat{a}^\dagger|n\rangle \tag{20}$$

So operating $\hat{a}^\dagger$ on a state $|n\rangle$ gives us a state whose integer is one higher and $\hat{a}^\dagger|n\rangle$ creates a vector that is also an eigenstate of the operator $\hat{n}$. This is why we call $\hat{a}^\dagger$ the "raising" or "creation" operator. By analogy, operating $\hat{a}$ on a state $|n\rangle$ gives us a state whose integer is one lower and $\hat{a}|n\rangle$ creates a vector that is also an eigenstate of the operator $\hat{n}$, which is why $\hat{a}$ is called the "lowering" or "annihilation" operator.

We now know the eigenstates of the operator $\hat{n}$ which are the eigenstates $|n\rangle$ that verify equation 13, so that equation 20 tells us that

$$\hat{a}^\dagger|n\rangle = k|n+1\rangle \tag{21}$$

with a constant k. This equation needs to be normalized by taking the norm of the state (multiplying by the adjoint):

$$|\hat{a}^\dagger|n\rangle|^2 = \langle n|\hat{a}\hat{a}^\dagger|n\rangle = |k|^2\langle n+1|n+1\rangle = |k|^2 \tag{22}$$

With the commuter, we have

$$\langle n|\hat{a}\hat{a}^\dagger|n\rangle = \langle n|1 + \hat{a}^\dagger\hat{a}|n\rangle = \langle n|1 + \hat{n}|n\rangle = (1+n)\langle n|n\rangle \tag{23}$$

So we have

$$n + 1 = k^2 \tag{24}$$

$$\sqrt{n+1} = k \tag{25}$$

and thus

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1}|n+1\rangle \tag{26}$$

A similar treatment can be performed for $\hat{a}$.

In conclusion, operating $\hat{a}^\dagger$ on an eigenstate $|n\rangle$ gives a new state $|n+1\rangle$

3 The Mathematical Properties of Creation and Annihilation Operators

Further mathematical properties and functioning of the new operators are discussed in the paper "Introduction to the "second quantization" formalism for non-relativistic quantum mechanics" by Tasaki, pages 4–9 .