9. Harmonic oscillator (representation of filling numbers)

1. Harmonic oscillator. Next we shortly discuss the representation of harmonic oscillator using raising and lowering(creation and annihilation) operators. That method is used in quantum field theory where the quantum field is interpreted as some set of microparticles.

We had the following Hamiltonian operator

$$\hat{H}=-\frac{\hbar^2}{2M}\frac{d^2}{dx^2}+\frac{M\ \omega^2 x^2}{2} \quad .$$

Let us define two new operators

$$\hat{a}=\sqrt{\frac{M\omega}{2\ \hbar}}\ x+\frac{i}{\sqrt{2M\ \hbar\ \omega}}\ \hat{p}\equiv\sqrt{\frac{M\omega}{2\ \hbar}}\ x+\sqrt{\frac{\hbar}{2M\omega}}\ \frac{d}{dx} \quad ,$$

$$\hat{a}^{+}=\sqrt{\frac{M\omega}{2\ \hbar}}\ x-\frac{i}{\sqrt{2M\ \hbar\ \omega}}\ \hat{p}\equiv\sqrt{\frac{M\omega}{2\ \hbar}}\ x-\sqrt{\frac{\hbar}{2M\omega}}\ \frac{d}{dx} \quad .$$

Direct calculation gives that $\hat{a}$ and $\hat{a}^{+}$ satisfy the following commutation relation

$$\left[\hat{a}\ ,\ \hat{a}^{+}\right]=1 \quad .$$

To prove this expression we can present firstly $\hat{a}$ operator in next form:

$$\hat{a}=\alpha\cdot x+i\cdot\beta\cdot\hat{p}\,, here\ \alpha=\sqrt{\frac{m\,\omega}{2\hbar}}\text{and}\ \beta=\frac{1}{\sqrt{2m\hbar\,\omega}}$$

$$\left[\hat{a}\ ,\ \hat{a}^{+}\right]=\hat{a}\,\hat{a}^{*}-\hat{a}^{*}\,\hat{a}=(\alpha x+i\beta\hat{p})(\alpha x-i\beta\hat{p})-(\alpha x-i\beta\hat{p})(\alpha x+i\beta\hat{p})=\alpha^2x^2+\beta^2\hat{p}^2+$$
$$i\alpha\beta(\hat{p}\,x-x\,\hat{p})-\alpha^2x^2-\beta^2\hat{p}^2-i\alpha\beta(x\,\hat{p}-\hat{p}\,x)=-2i\alpha\beta[x,\hat{p}]$$

The commutation operator $[x,\hat{p}]=i\hbar$ after substitution we have: $\left[\hat{a}\ ,\ \hat{a}^{+}\right]=1$.
Operators $\hat{a}$ and $\hat{a}^{+}$ are not Hermitean, but are conjugated to each other. Direct calculations demonstrate that applying them to eigenfunctions, the results are

$$\hat{a}\,\psi_n(x)=\sqrt{n}\ \psi_{n-1}(x) \quad ,$$

$$\hat{a}^{+}\psi_n(x)=\sqrt{n+1}\,\psi_{n+1}(x) \quad .$$

We can prove the correctness of first integral as follows. Firstly I can multiply the first integral on $\psi_{n-1}^{*}(x)$ and calculate the integral:

$$\int\psi_{n-1}^{*}\hat{a}\ \psi_n(x)\,dx=\int\psi_{n-1}^{*}\sqrt{n}\ \psi_{n-1}(x)\,dx$$

The integral on right side is equal to $\sqrt{n}$ and

$$\int\psi_{n-1}^{*}\hat{a}\ \psi_n(x)\,dx=\sqrt{n}$$

The left integral is equal:

$$\int \psi_{n-1}^{*} \hat{a}\, \psi_n(x)\, dx = \int \psi_{n-1}^{*} \left(\sqrt{\frac{M\omega}{2\hbar}} x + \sqrt{\frac{\hbar}{2M\omega}} \frac{d}{dx}\right) \psi_n\, dx =$$

$$\int \psi_{n-1}^{*} \sqrt{\frac{M\omega}{2\hbar}} x\, \psi_n\, dx + \int \psi_{n-1}^{*} \sqrt{\frac{\hbar}{2M\omega}} \frac{d}{dx} \psi_n dx = \sqrt{\frac{M\omega}{2\hbar}} \int \psi_{n-1}^{*} x\, \psi_n\, dx + \sqrt{\frac{\hbar}{2M\omega}} \int \psi_{n-1}^{*} \frac{d}{dx} \psi_n\, dx =$$

$$\sqrt{\frac{M\omega}{2\hbar}} \int \psi_{n-1}^{*} x\, \psi_n\, dx + \sqrt{\frac{\hbar}{2M\omega}} \int \psi_{n-1}^{*} \frac{d}{dx} \psi_n\, dx = \frac{\sqrt{n}}{2} + \frac{\sqrt{n}}{2} = \sqrt{n}$$

Here we see that operator $\hat{a}$ acting on state $\psi_n(x)$ with energy E_n leads to state $\psi_{n-1}(x)$ with energy $E_{n-1} = E_n - \hbar\omega$ and operator $\hat{a}^{+}$ similarly to state $\psi_{n+1}(x)$ with energy $E_{n+1} = E_n + \hbar\omega$. Therefore they are lowering and raising operators (in quantum field theory these operators are called annihilation and creation operators).

Using operators $\hat{a}$ and $\hat{a}^{+}$ the Hamiltonia operator is expressed as

$$\hat{H} = \frac{\hbar\omega}{2} (\hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a}) \ .$$

Using commutation relations ($\hat{a}\hat{a}^{+} = \hat{a}^{+}\hat{a} + 1$) it is also expressed as

$$\hat{H} = \hbar\,\omega \left(\hat{a}^{+}\, \hat{a} + \frac{1}{2}\right)$$

Since $(\hat{a}^{+}\hat{a})\psi_n = \sqrt{n}\,\hat{a}^{+}\psi_{n-1} = n\psi_n$, it is easy to verify that $\hat{H}\, \psi_n = \hbar\,\omega\,(n + 1/2)\, \psi_n$. If we treat the radiation as a systems of particles (similarly, as A. Einstein interpreted electromagnetic radiation as a set of photons), we may interprete *n* as a number of particles or filling number and then the operator

$$\hat{N} = \hat{a}^{+}\hat{a}$$

as a particle number operator, since $\hat{N}\psi_n = n\, \psi_n$.

This operators have one very useful propertie, the $\hat{a}^{*}\, \psi_0 = 1 \cdot \psi_1$ if we apply this operator two times $\hat{a}^{*}\hat{a}^{*}\, \psi_0 = (\hat{a}^{*})^2\, \psi_0 = \sqrt{1 \cdot 2} \cdot \psi_2$ and n-times $(\hat{a}^{*})^n\, \psi_0 = \sqrt{n!} \cdot \psi_n$ or $\psi_n = \frac{1}{\sqrt{n!}} (\hat{a}^{*})^n\, \psi_0$. The creation operator can be used to generate wave functions for any state based on the wave function for the ground state.

This approach is called "secondary quantization". An increase in the energy of a harmonic oscillator can be interpreted as the creation or destruction of formal particles (in the case of vibrations) of **phonons.** If the harmonic oscillator jumps from a level with a quantum number n = 2 to a level with n = 5 in the scheme of this approach, we can say that 3 phonons with energy $\hbar \cdot \omega$ were created.The transition from level with n=5 to level with n=2 means that 3 phonons were annihilated. This formalizm is very useful to describe the vibration of atoms in crystals. If a photon is a quantum of energy for an electromagnetic field, the phonon is a quantum of energy for oscillations. To describe the vibration properties of crystals, the harmonic waves moving in the crystals can be replaced by moving phonons, particles with a momentum $\vec{p} = \hbar\vec{k}$.