PART IV

Heisenberg representation
Algebraic method for harmonic oscillator, creation and annihilation operators
Identical particles: second quantization (boson case only).

Heisenberg formulation of QM.

Consider $\hat{H}$ independent of time,

$$\frac{\partial \hat{H}}{\partial t} = 0$$

In Schroedinger picture quantum dynamics are described by time dependent wave function that obeys Schroedinger eq.

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$$

Symbolic solution of this eq reads

$$\psi(t) = e^{-i\hat{H}t/\hbar}\,\psi(0)$$

$\hat{U} = e^{-i\hat{H}t/\hbar}$ is called evolution operator.

Mathematically $e^{-i\hat{H}t/\hbar}$ is defined as series

$$e^{-i\hat{H}t/\hbar} \equiv \sum_{n=0}^{\infty} \frac{1}{n!}\left(-i\frac{\hat{H}t}{\hbar}\right)^n$$

Consider expectation value of an operator $\hat{A}$, for example

$\hat{A} = \hat{p} = -i\hbar\frac{\partial}{\partial x}$, or $\hat{A} = x$, or $A = x^2\hat{p}$...

$\psi = \psi(t, x)$

$$\langle \hat{A} \rangle_t \equiv \langle \psi(t) | \hat{A} | \psi(t) \rangle =$$

$$= \int dx \left(e^{-i\hat{H}t/\hbar}\psi(0,x)\right)^* \hat{A}\, e^{-i\hat{H}t/\hbar}\psi(0,x) =$$

$$= \int dx\, \psi^*(0,x) \underbrace{e^{i\hat{H}t/\hbar}\hat{A}\, e^{-i\hat{H}t/\hbar}} \psi(0,x) =$$

$$= \langle \psi(0)\, \hat{A}(t)\, \psi(0) \rangle$$

Let us define

$$\boxed{\hat{A}(t) = e^{i\hat{H}t/\hbar}\,\hat{A}\,e^{-i\hat{H}t/\hbar}}$$

$$\hat{A}(0) = \hat{A}$$

This is transition to the Heisenberg formulation. In this formulation operators are dependent on time while the wave function is time independent.
This is different from the Schroedinger formulation where operators are time independent and the wave function is time dependent.

Schroedinger and Heisenberg formulations are completely equivalent.

Equation of motion for an operator in Heisenberg picture

$$\hat{A}(t) = e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}$$

$$\frac{d\hat{A}(t)}{dt} = i\frac{\hat{H}}{\hbar}\underline{e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}} -$$

$$-\frac{i}{\hbar}\underline{e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}}\hat{H} =$$

$$= \frac{i}{\hbar}[\hat{H}, \hat{A}(t)]$$

$$\boxed{\frac{d\hat{A}(t)}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}(t)]}$$

Heisenberg eq. of motion

Algebraic method for Harmonic oscillator. Creation and annihilation operators (Schroedinger representation).

$$\begin{cases} \hat{H} = \dfrac{\hat{p}^2}{2m} + \dfrac{1}{2} m \omega^2 x^2 \\ [p, x] = -i\hbar \end{cases}$$

Define new operators

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega} \hat{p} \right)$$ annihilation (lowering) operator

$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega} \hat{p} \right)$$ creation (raising) operator

$\hat{a}^+$ is Hermitian conjugation to $\hat{a}$ since $\hat{x}$ and $\hat{p}$ are Hermitian

Commutation relations for $\hat{a}$

$$[\hat{a},\hat{a}] = [\hat{a}^+,\hat{a}^+] = 0$$

$$[\hat{a},\hat{a}^+] = 1$$

Proof: $[\hat{a},\hat{a}^+] = \frac{m\omega}{2\hbar}\left[\hat{x}+\frac{i}{m\omega}\hat{p},\ \hat{x}-\frac{i}{m\omega}\hat{p}\right] =$

$$= \frac{m\omega}{2\hbar}\left\{\frac{i}{m\omega}\underbrace{[\hat{p},\hat{x}]}_{-i\hbar} - \frac{i}{m\omega}\underbrace{[\hat{x},\hat{p}]}_{i\hbar}\right\} = 1.$$

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

Proof: $\hbar\omega\left\{\frac{m\omega}{2\hbar}\left(x-\frac{i}{m\omega}p\right)\left(x+\frac{i}{m\omega}p\right)+\frac{1}{2}\right\} =$

$$= \hbar\omega\left\{\frac{m\omega}{2\hbar}\left(x^2+\frac{p^2}{m^2\omega^2}-\frac{i}{m\omega}\overbrace{[p,x]}^{-i\hbar}\right)+\frac{1}{2}\right\} =$$

$$= \frac{p^2}{2m} + \frac{m\omega^2x^2}{2},\quad \underline{\underline{\text{ok}}}$$

Define operator $\hat{N}$ as $\underline{\underline{\hat{N} = a^+a}}$

$$\hat{H} = \hbar\omega(\hat{N} + \tfrac{1}{2})$$

Let us find eigenstates of $\hat{N}$

$$\Psi_n = |n\rangle, \qquad \underline{\hat{N}|n\rangle = n|n\rangle}$$

n is eigenvalue of $\hat{N}$

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① $\underline{n \text{ is nonnegative}}$

Proof:

$$\langle n|\hat{N}|n\rangle = n\langle n|n\rangle = n$$

on the other hand

$$\langle n|\hat{N}|n\rangle = \langle n|a^+a|n\rangle = \langle\tilde{n}|\tilde{n}\rangle \geq 0$$

where $|\tilde{n}\rangle = a|n\rangle$

$$\langle\tilde{n}| = (a|n\rangle)^+ = \langle n|a^+$$

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② $|\tilde{n}\rangle = a|n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue $(n-1)$

$|\tilde{\tilde{n}}\rangle = a^+|n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue $(n+1)$

Proof. $[a,a^+] = aa^+ - a^+a = 1 \Rightarrow a^+a = aa^+ - 1$

$\hat{N}|\tilde{n}\rangle = \hat{N}a|n\rangle = a^+ a a|n\rangle =$

$= (-1 + \hat{a}\hat{a}^+)\hat{a}|n\rangle = -|\tilde{n}\rangle + \hat{a}\hat{N}|n\rangle =$

$= -|\tilde{n}\rangle + \hat{a}n|n\rangle = (n-1)|\tilde{n}\rangle$, ok.

Similarly $\hat{N}a^+|n\rangle = (n+1)a^+|n\rangle$

Thus eigenvalues of N differ by 1.

③ The eigenvalues of n are integer:

Proof.
Suppose we have a particular state $|n\rangle$.
By repeated application of $\hat{a}$ we generate eigenstates with eigenvalues $(n-1), (n-2), (n-3), \ldots$
This cannot continue indefinetely because all eigenvalues are ≥ 0 (point ① page 75)

Hence there must be a <u>lowest eigenstate</u> $|0\rangle$ (ground state)

with the property that $\boxed{\hat{a}|0\rangle = 0}$

So this state has eigenvalue $n=0$

Hence in general n is integer and nonnegative.

Spectrum of Hamiltonian

$$\hat{H}|n\rangle = \hbar\omega(\hat{N}+\tfrac{1}{2})|n\rangle = \hbar\omega(n+\tfrac{1}{2})|n\rangle$$

$$\underline{\varepsilon_n = \hbar\omega(n+\tfrac{1}{2})}$$

Wave function of the ground state

$$0 = \hat{a}|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)\psi_0 \Longrightarrow$$

$$\Longrightarrow \left(x + \frac{\hbar}{m\omega}\frac{d}{dx}\right)\psi_0 = 0$$

Solution is: $\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$

Normalization of eigenstates

$$|n+1\rangle = \overset{\swarrow \text{ some constant}}{C}\, a^{+}|n\rangle \qquad \boxed{aa^{+}-a^{+}a=1}$$

$$1 = \langle n+1|n+1\rangle = |C|^{2}\langle n|\hat{a}\,\hat{a}^{+}|n\rangle =$$

$$= |C|^{2}\langle n|1+\underbrace{\hat{a}^{+}\hat{a}}_{\hat{N}}|n\rangle = |C|^{2}(1+n) \Longrightarrow$$

$$\Longrightarrow |C|^{2} = \frac{1}{1+n}$$

$$\boxed{\sqrt{n+1}\,|n+1\rangle = a^{+}|n\rangle}$$

Similarly $\boxed{\sqrt{n}\,|n-1\rangle = a|n\rangle}$

From here we find

$$\boxed{|n\rangle = \frac{1}{\sqrt{n!}}(a^{+})^{n}|0\rangle}$$

Harmonic oscillator in Heisenberg picture

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

$$\frac{da}{dt} = \frac{i}{\hbar}[H, a] = \frac{i}{\hbar}\hbar\omega\left[\left(a^+a + \frac{1}{2}\right), a\right] =$$

$$= i\omega[a^+a, a] = i\omega[a^+, a]a = i\omega a$$

Hence $\underline{\hat{a}(t) = e^{-i\omega t}\hat{a}(0)}$

$$\underline{a^+(t) = e^{i\omega t}a^+(0)}$$

Alternatively

$$\hat{H} = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}, \quad [p, x] = -i\hbar$$

$$\frac{dp}{dt} = \frac{i}{\hbar}[H, p] = \frac{im\omega^2}{2\hbar}[x^2, p] =$$

$$= \frac{im\omega^2}{2\hbar}\left\{x[xp] + [x, p]x\right\} = -m\omega^2 x$$

$$\frac{dx}{dt} = \frac{i}{\hbar}[H, x] = \frac{i}{2m\hbar}[p^2, x] = \frac{p}{m}$$

$$\boxed{\begin{aligned} \frac{d\hat{p}}{dt} &= -m\omega^2 \hat{x} \\ \frac{d\hat{x}}{dt} &= \frac{\hat{p}}{m} \end{aligned}}$$

look exactly like classical eqs., but these are operator eqs!

Solution

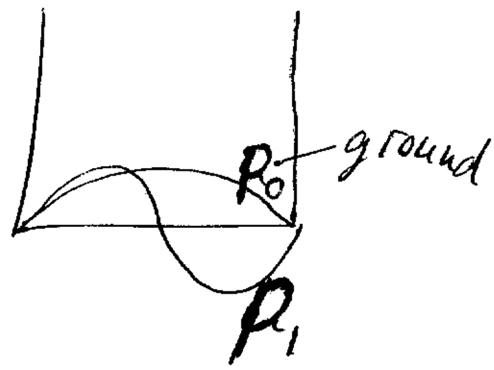
$$\begin{cases} \hat{p}(t) = \hat{p}(0)\cos\omega t - m\omega\, \hat{x}(0)\sin\omega t \\ \hat{x}(t) = \hat{x}(0)\cos\omega t + \frac{1}{m\omega}\hat{p}(0)\sin\omega t \end{cases}$$

Identical particles.

Second quantization

Bosons

Example: 3 particles in a box, 2 particles in the ground state and 1 in the first excited state



$$\Psi(x_1, x_2, x_3) = A\left[\psi_{\mathbf{p}_0}(x_1)\psi_{\mathbf{p}_0}(x_2)\psi_{\mathbf{p}_1}(x_3) + \right.$$

$$\left. + \psi_{\mathbf{p}_0}(x_3)\psi_{\mathbf{p}_0}(x_2)\psi_{\mathbf{p}_1}(x_1) + \psi_{\mathbf{p}_0}(x_3)\psi_{\mathbf{p}_0}(x_1)\psi_{\mathbf{p}_1}(x_2)\right]$$

$A = \frac{1}{\sqrt{3}}$ - normalization

$$\frac{1}{\sqrt{3}} = \sqrt{\frac{2!\,1!}{3!}}$$

general case

$\psi_{p_0}(x), \psi_{p_1}(x), \psi_{p_2}(x) \ldots$ are orthonormalized single particle states in arbitrary potential.

Let us consider N identical particles. Out of these n_0 are in the p_0 state, n_1 are in p_1 state etc. so $\boxed{N = \sum_i n_i}$

The wave function of the many-body system is

$$\text{(A)} \quad \Psi = \sqrt{\frac{n_0!\, n_1! \ldots}{N!}} \sum \psi_{p_0}(x_1)\psi_{p_1}(x_2) \ldots \psi_{p_N}(x_N)$$

summation over all nontrivial permutations of $x_1, x_2 \ldots x_N$

The number of terms in the wave function is $\dfrac{N!}{n_0!\, n_1! \ldots} \gg 1$

Second quantization representation

$|0\rangle$ - ground state (vacuum) =
= state without particles.

(B) $$|n_0, n_1, \ldots\rangle = \frac{1}{\sqrt{n_0!}}(a_0^+)^{n_0} \frac{1}{\sqrt{n_1!}}(a_1^+)^{n_1} \cdots \quad |0\rangle$$

the many body state

a_0^+ - creation operator of the particle in the state ψ_{p_0}

a_1^+ creation operator of the particle in the state ψ_{p_1}

etc.

In the second quantization representation the many-body state (B) has only one term instead of very many terms in the usual representation (A)

This is possible if the creation and annihilation operators obey commutation relations that we derived for harmonic oscillator

$$\boxed{\begin{array}{l} [a_i, a_j] = [a_i^+, a_j^+] = 0 \\ [a_i, a_j^+] = \delta_{ij} \end{array}} \quad (C)$$

These are called Bose commutation relations.

<u>Note</u> that we <u>do not</u> have a harmonic oscillator now.
We base on a purely mathematical fact that if we have operators that obey (C) then we **can** introduce states $|n_i\rangle = \frac{1}{\sqrt{n_i!}} (a_i^+)^{n_i} |0\rangle$

that obeys the following relations

$$\boxed{\begin{aligned} \sqrt{n_i+1}\,|n_i+1\rangle &= a_i^+\,|n_i\rangle \\ \sqrt{n_i}\,|n_i-1\rangle &= a_i\,|n_i\rangle \end{aligned}}$$

That is all we need for many-body physics.

We learned the math fact using oscillator as an example but now we can forget the oscillator.

Example: Operator of number of particles

$$\hat{N} = \sum_i a_i^+ a_i$$

$$\langle n_0, n_1, \ldots | \hat{N} | n_0\, n_1 \ldots \rangle =$$

$$= n_0 + n_1 + \ldots$$ — by construction.

Other operators can be also rewritten in second quantization representation