Canonical quantization of harmonic oscillator

The method of canonical quantization is presented for the case of harmonic oscillator. Before that the classical Lagrange and Hamiltonian descriptions of the oscillator are reminded. In the first part of this lecture the natural units are not used but the Planck constant $\hbar$ is explicitly written.

Classical description

Lagrange formalism

- A classical Lagrange description of a mechanical system usually starts with the Lagrangian which in case of harmonic oscillator is

$$L(x,\dot{x}) = \frac{1}{2}m\dot{x}^2(t) - \frac{1}{2}m\omega^2 x^2(t), \tag{1}$$

  where $x(t)$ and $\dot{x}(t)$ is the time dependent position and velocity, respectively, m and ω denote the mass and frequency.

- The Euler-Lagrange equation

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 \tag{2}$$

  provides the equation of motion of harmonic oscillator which is

$$\ddot{x}(t) + \omega^2 x(t) = 0. \tag{3}$$

- Since the equation (3) is of the second order, one needs two initial conditions to uniquely determine the solution of Eq. (3). Choosing the initial conditions as

$$x(0) = x_0, \qquad \dot{x}(0) = v_0, \tag{4}$$

  the general solution of Eq. (3) reads

$$x(t) = x_0 \cos\omega t + \frac{v_0}{\omega}\sin\omega t. \tag{5}$$

- The solution (5) can be also written as

$$x(t) = Ae^{-i\omega t} + A^* e^{i\omega t}, \tag{6}$$

  where the complex constant A can be expressed through x_0, v_0 and ω. Because of our further considerations, we rewrite down the solution (5) as

$$x(t) = \sqrt{\frac{\hbar}{2m\omega}}\Big(ae^{-i\omega t} + a^* e^{i\omega t}\Big), \tag{7}$$

  where we have included the Planck constant $\hbar$ for a symmetry of classical and quantum formulas. Then, the constant a is dimensionless.

Hamilton formalism

- In a Hamiltonian (canonical) formalism one introduces a momentum conjugate to every coordinate. The momentum conjugate to x is given as

$$p(t) \equiv \frac{\partial L}{\partial \dot{x}} = m\dot{x}(t). \tag{8}$$

- One defines the Hamilton function through the Legendre transformation that is

$$H \equiv p\dot{x} - L = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2. \tag{9}$$

- The canonical equations of motion read

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}, \qquad\qquad \dot{p} = -\frac{\partial H}{\partial x} = -m\omega^2 x. \tag{10}$$

- Using the solution (7), one immediately finds that

$$p(t) = -i\sqrt{\frac{\hbar m\omega}{2}}\Big(ae^{-i\omega t} - a^* e^{i\omega t}\Big). \tag{11}$$

  Needless to say that the formulas (7, 11) satisfy the equations of motion (10).

- The Hamilton function (9) equals the constant

$$H = \hbar\omega\, aa^*, \tag{12}$$

  when the solutions (7, 11) are substituted in Eq. (9).

Exercise: Derive the formula (12).

- The Poisson bracket of the quantities $F(x,p,t)$ and $G(x,p,t)$ is defined for a system of one-pair of canonical variables as

$$\{G, F\} \equiv \frac{\partial G}{\partial x}\frac{\partial F}{\partial p} - \frac{\partial G}{\partial p}\frac{\partial F}{\partial x}. \tag{13}$$

- One observes that the pair of canonical variables obeys the relation

$$\{x, p\} = 1. \tag{14}$$

- The equations of motion (10) expressed through the Poissona brackets read

$$\dot{x} = \{x, H\}, \qquad\qquad \dot{p} = \{p, H\}. \tag{15}$$

Canonical quantization

Operators and equations of motion

- Within the canonical quantization the canonical variables $x(t), p(t)$ are changed into the operators $\hat{x}(t), \hat{p}(t)$ which act in a space of states. It is further assumed that the operators satisfy the relations obeyed by their classical counterparts with the Poisson brackets changed into the commutators. So, we have

$$\{x(t), p(t)\} \to \frac{1}{i\hbar}[\hat{x}(t), \hat{p}(t)],$$

and consequently

$$[\hat{x}(t), \hat{p}(t)] = i\hbar, \tag{16}$$

where $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$.

- In the classical limit $\hbar \to 0$, the operators $\hat{x}, \hat{p}$ commute and thus they behave as classical variables.

- Since the classical equations of motion are given by Eqs. (15), the operators $\hat{x}(t), \hat{p}(t)$ should obey the equations

$$i\hbar\,\dot{\hat{x}}(t) = [\hat{x}(t), \hat{H}], \qquad\qquad i\hbar\,\dot{\hat{p}}(t) = [\hat{p}(t), \hat{H}]. \tag{17}$$

- Knowing the solutions of classical equations of motion (7, 11), the corresponding quantum solutions are expected to be

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2m\omega}}\Big(\hat{a}e^{-i\omega t} + \hat{a}^\dagger e^{i\omega t}\Big), \tag{18}$$

and

$$\hat{p}(t) = -i\sqrt{\frac{m\omega\hbar}{2}}\Big(\hat{a}e^{-i\omega t} - \hat{a}^\dagger e^{i\omega t}\Big), \tag{19}$$

where $\hat{a}^\dagger$ and $\hat{a}$ is the creation and annihilation operator, respectively. As we will show further on, the operators create and annihilate, respectively, a quantum of energy $\hbar\omega$.

- Now we are going to prove that the operators (18, 19) satisfy the quantum equations of motion (17). For this purpose one observes that the relation (16) implies the commutation relation for the creation and annihilation operators

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{20}$$

- Consequently, the quantum Hamiltonian, which is an analog of the classical expression (9), equals

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \frac{\hbar\omega}{2}\,(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}), \tag{21}$$

which, using the relation (20), is rewritten as

$$\hat{H} = \hbar\omega\Big(\hat{a}^\dagger\hat{a} + \frac{1}{2}\Big). \tag{22}$$

- One checks that there hold the relations

$$[\hat{a}, \hat{H}] = \hbar\omega\, \hat{a}, \qquad [\hat{a}^\dagger, \hat{H}] = -\hbar\omega\, \hat{a}^\dagger, \tag{23}$$

which allow one to prove immediately that the expressions (18, 19) satisfy the quantum equations of motion (17). This happens because the Poisson brackets and commutator have the same algebraic structure.

Construction of space of states

- We are now going to construct the space of states, also called the Fock space, by looking for the energy eigenstates

$$\hat{H}|E\rangle = E|E\rangle. \tag{24}$$

- One finds that if $|E\rangle$ is the energy eigenstate, so are both $\hat{a}|E\rangle$ and $\hat{a}^\dagger|E\rangle$. Indeed

$$\hat{H}\hat{a}|E\rangle = \Big(\hat{a}\hat{H} + [\hat{H}, \hat{a}]\Big)|E\rangle = (\hat{a}\hat{H} - \hbar\omega\hat{a})|E\rangle = (\hat{a}E - \hbar\omega\hat{a})|E\rangle = (E - \hbar\omega)\hat{a}|E\rangle \tag{25}$$

and

$$\hat{H}\hat{a}^\dagger|E\rangle = \Big(\hat{a}^\dagger\hat{H} + [\hat{H}, \hat{a}^\dagger]\Big)|E\rangle = (\hat{a}^\dagger\hat{H} + \hbar\omega\hat{a}^\dagger)|E\rangle = (\hat{a}^\dagger E + \hbar\omega\hat{a}^\dagger)|E\rangle = (E + \hbar\omega)\hat{a}^\dagger|E\rangle. \tag{26}$$

- The energy eigenvalue of $\hat{a}|E\rangle$ is $(E - \hbar\omega)$ and that of $\hat{a}^\dagger|E\rangle$ is $(E + \hbar\omega)$, and we write

$$\hat{a}|E\rangle = |E - \hbar\omega\rangle, \tag{27}$$
$$\hat{a}^\dagger|E\rangle = |E + \hbar\omega\rangle. \tag{28}$$

- The annihilation operator $\hat{a}$ decreases the energy of the state $|E\rangle$ by $\hbar\omega$ and the creation operator $\hat{a}^\dagger$ increases the energy of the state $|E\rangle$ by $\hbar\omega$. The energy of the ground state – its existence follows from the positivity of Hamiltonian (22) – cannot be decreased.

- An operator $\hat{A}$ is positive definite if

$$\langle\alpha|\hat{A}|\alpha\rangle \geqslant 0 \tag{29}$$

for any $|\alpha\rangle$. The Hamiltonian (22) is positive definite because $\omega > 0$ and

$$\langle\alpha|\hat{H}|\alpha\rangle = \omega\langle\alpha|\Big(\hat{a}^\dagger\hat{a} + \frac{1}{2}\Big)|\alpha\rangle = \omega\langle\beta|\beta\rangle + \frac{1}{2}\omega\langle\alpha|\alpha\rangle \geqslant 0, \tag{30}$$

where $|\beta\rangle \equiv \hat{a}|\alpha\rangle$. We note that $\langle\alpha|\alpha\rangle \geqslant 0$, $\langle\beta|\beta\rangle \geqslant 0$.

- We demand the property

$$\hat{a}|0\rangle = \langle 0|\hat{a}^\dagger = 0, \tag{31}$$

where $|0\rangle$ denotes the ground state.

- The ground state energy eigenvalue is found as

$$\hat{H}|0\rangle = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|0\rangle = \frac{\hbar\omega}{2}|0\rangle. \tag{32}$$

- The construction of the space of energy eigenstates starts with the ground state $|0\rangle$. Then, we see that the energy eigenvalues are $\hbar\omega/2$, $\hbar\omega(1+1/2)$, $\hbar\omega(2+1/2)$, etc. which correspond to $|0\rangle$, $\hat{a}^\dagger|0\rangle$, $\hat{a}^\dagger\hat{a}^\dagger|0\rangle$, etc.

- We define the state $|n\rangle$ of n quanta of energy $\hbar\omega$. Its energy eigenvalue is $\hbar\omega(n+1/2)$ and its normalization is determined by the condition $\langle n|n\rangle = 1$.
- We compute $\langle n|\hat{a}^\dagger\hat{a}|n\rangle$ as

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = \langle n|\Big(\frac{\hat{H}}{\omega} - \frac{1}{2}\Big)|n\rangle = \Big(n + \frac{1}{2}\Big) - \frac{1}{2} = n. \tag{33}$$

- The annihilation operator acts on $|n\rangle$ as

$$\hat{a}|n\rangle = C_n|n-1\rangle, \qquad \langle n|\hat{a}^\dagger = \langle n-1|C_n^*, \tag{34}$$

  where C_n is the unknown constant. The energy eigenvalue tells us that $\langle n|\hat{a}^\dagger\hat{a}|n\rangle = n\langle n|n\rangle$ and thus

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = n\langle n|n\rangle = n = |C_n|^2\langle n-1|n-1\rangle = |C_n|^2. \tag{35}$$

  Consequently, $|C_n|^2 = n$ and the simplest choice is $C_n = \sqrt{n}$. So, we have

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle. \tag{36}$$

- Analogously one finds

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{37}$$

- The product $\hat{a}^\dagger\hat{a}$ is called the particle number operator as

$$\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle. \tag{38}$$

Schrödinger's and Heisenberg's pictures

We return here to natural units with $\hbar = 1$.

Schrödinger's picture

- The wave mechanics is based on the Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi(t)\rangle_{\mathrm{S}} = \hat{H}|\psi(t)\rangle_{\mathrm{S}}. \tag{39}$$

  where the Hamiltonian $\hat{H}$ is assumed, for simplicity, to be time-independent. The states carry the index S as they belong to the *Schrödinger's picture* – a meaning of this statement will be explained soon.
- Since the formal solution of the equation (39) is

$$|\psi(t)\rangle_{\mathrm{S}} = e^{-i\hat{H}t}|\psi(0)\rangle_{\mathrm{S}}, \tag{40}$$

  a matrix element of the observable $\hat{\Omega}_{\mathrm{S}}$, which is also assumed to be time-independent, can be written as

$${}_{\mathrm{S}}\langle\phi(t)|\hat{\Omega}_{\mathrm{S}}|\psi(t)\rangle_{\mathrm{S}} = {}_{\mathrm{S}}\langle\phi(0)|e^{i\hat{H}t}\hat{\Omega}_{\mathrm{S}}e^{-i\hat{H}t}|\psi(0)\rangle_{\mathrm{S}}. \tag{41}$$

- The evolution operator $\hat{U}(t) \equiv e^{-i\hat{H}t}$ is unitary, that is $\hat{U}^{-1}(t) = \hat{U}^\dagger(t)$, because $\hat{H}$ is hermitian.

Heisenberg's picture

- The matrix element (41) can be also written as

$$_{\rm S}\langle\phi(t)|\hat{\Omega}_{\rm S}|\psi(t)\rangle_{\rm S} = \ _{\rm H}\langle\phi|\hat{\Omega}_{\rm H}(t)|\psi\rangle_{\rm H}, \tag{42}$$

where

$$|\psi\rangle_{\rm H} \equiv |\psi(0)\rangle_{\rm S} = e^{i\hat{H}t}|\psi(t)\rangle_{\rm S} \tag{43}$$

is the state in the *Heisenberg's picture*, and

$$\hat{\Omega}_{\rm H}(t) \equiv e^{i\hat{H}t}\hat{\Omega}_{\rm S}\, e^{-i\hat{H}t} \tag{44}$$

is the observable in the Heisenberg's picture.

- The equation (42) shows that going from the Schrödinger's to Heisenberg's picture the time dependence is transfered from the states to the observables.

- Let us compute the time derivative of $\hat{\Omega}_{\rm H}(t)$

$$\frac{d}{dt}\hat{\Omega}_{\rm H}(t) = \left(\frac{d}{dt}e^{i\hat{H}t}\right)\hat{\Omega}_{\rm S}\, e^{-i\hat{H}t} + e^{i\hat{H}t}\hat{\Omega}_{\rm S}\left(\frac{d}{dt}e^{-i\hat{H}t}\right) = ie^{i\hat{H}t}\hat{H}\hat{\Omega}_{\rm S}\, e^{-i\hat{H}t} - ie^{i\hat{H}t}\,\hat{\Omega}_{\rm S}\,\hat{H}\, e^{-i\hat{H}t}. \tag{45}$$

- Since the operators $\hat{H}$ and $e^{-i\hat{H}t}$ commute with each other and consequently can be interchanged, the equality (45) becomes the equation of motion of the observable $\hat{\Omega}_{\rm H}(t)$ that is

$$\frac{d}{dt}\hat{\Omega}_{\rm H}(t) = i[\hat{H}, \hat{\Omega}_{\rm H}(t)]. \tag{46}$$

- The Hamiltonian $\hat{H}$ is the same in the Schrödinger's and Heisenberg's pictures and for this reason it does not carry the index S or H.

- Writing down the equation (46) for the position $\hat{x}_{\rm H}(t)$ and momentum $\hat{p}_{\rm H}(t)$ operators, we find the equations

$$\frac{d}{dt}\hat{x}_{\rm H}(t) = i[\hat{H}, \hat{x}_{\rm H}(t)], \qquad \frac{d}{dt}\hat{p}_{\rm H}(t) = i[\hat{H}, \hat{p}_{\rm H}(t)], \tag{47}$$

which we already know as Eqs. (17) obtained due to the canonical quantization of the classical equations of motion.

- The operators $\hat{x}_{\rm H}(t)$ and $\hat{p}_{\rm H}(t)$ obviously obey the commutation relation

$$[\hat{x}_{\rm H}(t), \hat{p}_{\rm H}(t)] = i. \tag{48}$$

- The Schrödinger's picture (wave mechanics) and the Heisenberg's picture (operator formalism) are the two equivalent approaches to quantum mechanics connected to each other by the unitary transformation:

$$|\psi\rangle_{\rm H} = e^{i\hat{H}t}|\psi(t)\rangle_{\rm S} \tag{49}$$

$$\hat{\Omega}_{\rm H}(t) = e^{i\hat{H}t}\hat{\Omega}_{\rm S}\, e^{-i\hat{H}t}. \tag{50}$$