Classical & Quantum Faces of Harmonic Oscillator

– Lecture notes –

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A one-dimensional harmonic oscillator is first described in terms of classical Lagrange and Hamiltonian formalisms and then it is quantized in three ways: referring to the Schrödinger's wave mechanics, using the method of canonical quantization, and finally, applying the path-integral technique.

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1. INTRODUCTION

A one-dimensional harmonic oscillator is presumably the most frequently discussed quantum physical system. It is simple, exactly solvable but still nontrivial. Therefore, various methods of theoretical physics are often explained in the context harmonic oscillator before they are applied to more complex systems. In this note we explain how to quantize the harmonic oscillator in three ways: referring to the Schrödinger's wave mechanics, using the method of canonical quantization, and finally, applying the path-integral technique. The three methods can be then easily extended to quantize a relativistic noninteracting fields.

2. CLASSICAL DESCRIPTION

Let us first remind a reader how the one-dimensional harmonic oscillator is described within the classical physics. In this way we will also fix the notation which is used further on.

A. Lagrange formalism

A classical description of mechanical systems, which is given in terms of the Lagrange formalism, usually starts with writing down the Lagrangian. In case of harmonic oscillator it is given as

$$L(x,\dot{x}) = \frac{1}{2}m\dot{x}^{2}(t) - \frac{1}{2}m\omega^{2}x^{2}(t), \qquad (2.1)$$

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

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 \tag{2.2}$$

provides the equation of motion of harmonic oscillator which is

$$\ddot{x}(t) + \omega^2 x(t) = 0.$$
(2.3)

Since the equation (2.3) is of the second order, one needs two initial conditions to uniquely determine the solution of Eq. (2.3). Choosing the initial conditions as

$$x(0) = x_0, \qquad \dot{x}(0) = v_0, \qquad (2.4)$$

the general solution of Eq. (2.3) reads

$$x(t) = x_0 \cos \omega t + \frac{v_0}{\omega} \sin \omega t.$$
(2.5)

The solution (2.5) can be also written as

$$x(t) = Ae^{-i\omega t} + A^* e^{i\omega t}, (2.6)$$

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 (2.5) as

$$x(t) = \sqrt{\frac{\hbar}{2m\omega}} \left(ae^{-i\omega t} + a^* e^{i\omega t} \right), \tag{2.7}$$

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

B. Hamilton formalism

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

$$p(t) \equiv \frac{\partial L}{\partial \dot{x}} = m \dot{x}(t), \qquad (2.8)$$

and one defines the Hamilton function through the Legendre transformation that is

$$H \equiv p\dot{x} - L = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2.$$
 (2.9)

The canonical equations of motion read

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}, \qquad \dot{p} = -\frac{\partial H}{\partial x} = -m\omega^2 x.$$
 (2.10)

Using the solution (2.7), one immediately finds that

$$p(t) = -i\sqrt{\frac{\hbar m\omega}{2}} \left(ae^{-i\omega t} - a^* e^{i\omega t} \right).$$
(2.11)

Needless to say that the formulas (2.7, 2.11) satisfy the equations of motion (2.10). The Hamilton function (2.9) equals the constant

$$H = \hbar\omega \, aa^*,\tag{2.12}$$

when the solutions (2.7, 2.11) are substituted in Eq. (2.9).

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

$$\{G,F\} \equiv \frac{\partial G}{\partial x}\frac{\partial F}{\partial p} - \frac{\partial G}{\partial p}\frac{\partial F}{\partial x}.$$
(2.13)

One observes that the pair of variables obeys the relation

$$\{x, p\} = 1 \tag{2.14}$$

and the equations of motion (2.10) expressed through the Poissona brackets read

$$\dot{x} = \{x, H\}, \qquad \dot{p} = \{p, H\}.$$
 (2.15)

3. SCHRÖDINGER'S WAVE MECHANICS

After a brief reminder of the Schrödinger's wave mechanics, the problem of harmonic oscillator is solved.

A. Formulation

A central object of the Schrödinger's wave mechanics is a complex valued wave function which provides a complete information about a physical system. In case of a system with one degree of freedom such as the harmonic oscillator, the wave function is $\Psi(t, x)$ and it is the quantum counterpart of a solution of classical equation of motion x(t). The wave functions form a vector space of quantum states which is also called the Fock space.

One introduces a scalar product of the functions $\Psi_1(t,x)$ and $\Psi_2(t,x)$ in the following way

$$(\Psi_1, \Psi_2) \equiv \int dx \ \Psi_1^*(t, x) \Psi_2(t, x).$$
 (3.1)

As long as the integration limits are not specified, it is understood that the integration extends form $-\infty$ to ∞ . It can be easily checked that the definition satisfies the required relations

$$(\Psi_1, \Psi_2)^* = (\Psi_2, \Psi_1),$$
(3.2)

$$\left(\Psi, \alpha_1 \Psi_1 + \alpha_2 \Psi_2\right) = \alpha_1 \left(\Psi, \Psi_1\right) + \alpha_2 \left(\Psi, \Psi_2\right),\tag{3.3}$$

where α_1, α_2 are complex numbers. When $(\Psi_1, \Psi_2) = 0$ the wave functions are called mutually *orthogonal*.

The wave functions are assumed to obey the normalization condition

$$\left(\Psi,\Psi\right) = \int dx \ \Psi^*(t,x)\Psi(t,x) = 1, \tag{3.4}$$

which allows for a probabilistic interpretation of $|\Psi(t,x)|^2$.

Observable physical quantities – observables – are represented by hermitian operators acting in the space of wave functions. An operator corresponding to a classical quantity A is denoted as \hat{A} and the fact that the operator is hermitian means

$$\left(\Psi_1, \hat{A}\Psi_2\right) = \left(\hat{A}\Psi_1, \Psi_2\right),\tag{3.5}$$

which holds for any functions $\Psi_1(t, x)$ and $\Psi_2(t, x)$.

There are three important properties of a hermitian operator. Its eigenvalues are real and eigenvectors corresponding to eigenvalues, which differ from each other, are mutually orthogonal. A set of eigenvectors of a hermitian operator constitutes a basis of the vector space of states.

The momentum and position operators are defined as

$$\hat{p}\Psi(t,x) \equiv -i\hbar \frac{\partial}{\partial x}\Psi(t,x), \qquad \hat{x}\Psi(t,x) \equiv x\Psi(t,x).$$
(3.6)

The wave function is postulated to obey the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(t,x) = \hat{H}\Psi(t,x),$$
(3.7)

where the energy operator - hamiltonian - is defined as

$$\hat{H} \equiv \frac{\hat{p}^2}{2m} + V(t,x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(t,x), \qquad (3.8)$$

with V(t, x) being the potential energy.

If the hamiltonian is time independent, a solution of the Schrödinger equation can be written as

$$\Psi(t,x) = e^{-i\frac{Et}{\hbar}}\phi(x),\tag{3.9}$$

where $\phi(x)$ is an eigenfunction of \hat{H} with the eigenvalue E that is

$$\hat{H}\phi(x) = E\phi(x), \tag{3.10}$$

which is called the time-independent Schrödinger equation.

B. Application to harmonic oscillator

In case of harmonic oscillator we have

$$V(x) = \frac{1}{2}m\omega^2 x^2,$$
 (3.11)

and the Schrödinger equation to be solved is

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 - E\right)\phi(x) = 0.$$
(3.12)

Before we start solving the equation, let us write it in a simpler form. For this purpose one introduces the new variable z = ax. Then,

$$\left(\frac{\partial^2}{\partial z^2} - \frac{m^2 \omega^2}{a^4 \hbar^2} z^2 + \frac{2mE}{a^2 \hbar^2}\right) \phi(z) = 0.$$
(3.13)

Choosing $a = \sqrt{\frac{m\omega}{\hbar}}$, the equation gets the desired form

$$\left(\frac{\partial^2}{\partial z^2} - z^2 + \lambda\right)\phi(z) = 0, \qquad (3.14)$$

where $\lambda \equiv \frac{2E}{\hbar\omega}$.

We first look for the solution of Eq. (3.14) when $z^2 \to \infty$. Then, λ can be omitted in Eq. (3.14) and the approximate solution is

$$\phi(z) \approx C e^{\pm \frac{1}{2}z^2}.\tag{3.15}$$

where C is a constant. Since the wave function has to be normalizable according to Eq. (3.4), the solution (3.15) with sign plus is rejected. Once the long-distance behavior of the function $\phi(z)$ is found, we look for a solution of Eq. (3.14) in the form

$$\phi(z) = H(z) e^{-\frac{1}{2}z^2},\tag{3.16}$$

which converts Eq. (3.14) into

$$\left(\frac{\partial^2}{\partial z^2} - 2z\frac{\partial}{\partial z} + \lambda - 1\right)H(z) = 0.$$
(3.17)

We look for a solution of Eq. (3.17) in the form of power series

$$H(z) = \sum_{k=0}^{\infty} a_k z^k, \qquad (3.18)$$

which substituted in Eq. (3.17) gives

$$\sum_{k=0}^{\infty} \left(k(k-1)a_k z^{k-2} - 2ka_k z^k + (\lambda - 1)a_k z^k \right) = 0.$$
(3.19)

One observes that the first term vanishes for k = 0 and k = 1. Shifting the index k of the first term by 2 and keeping in mind that the equation (3.19) holds for any z, which means that the coefficients at every power of z must vanish, we get the equation

$$(k+2)(k+1)a_{k+2} - (2k - \lambda + 1)a_k = 0, (3.20)$$

which gives the recurrence relation

$$a_{k+2} = \frac{2k - \lambda + 1}{(k+2)(k+1)}a_k.$$
(3.21)

When $k \gg 1$ we have

$$a_{k+2} \approx \frac{2}{k} a_k,\tag{3.22}$$

which coincides in the limit $k \gg 1$ with the expansion of the function e^{z^2} . If $H(z) \sim e^{z^2}$, we have $\phi(z) = H(z) e^{-\frac{1}{2}z^2} \sim e^{\frac{1}{2}z^2}$. However, such a wave function is not normalizable. So, we conclude that the series (3.18) has to terminate or equivalently the function H(z) is a polynomial of order n which is denoted as $H_n(z)$. The polynomials, which are solutions of Eq (3.20), are known as the Hermite polynomials. They can be found from the formula

$$H_n(z) = (-1)^n e^{z^2} \frac{\partial^n}{\partial z^n} e^{-z^2},$$
(3.23)

which gives $H_0(z) = 1$, $H_1(z) = 2z$, $H_2(z) = 4z^2 - 2$, etc.

Since $H_n(z)$ is the polynomial of order n, the coefficient a_{n+2} must vanish and consequently, the recurrence relation (3.21) gives

$$2n - \lambda + 1 = 0. \tag{3.24}$$

Because $\lambda \equiv \frac{2E}{\hbar\omega}$, we find the quantized energy of the harmonic oscillator as

$$E_n = \hbar \omega \left(n + \frac{1}{2} \right). \tag{3.25}$$

As follows from the above reasoning, the quantization of energy occurs because the wave functions must decrease as $x \to \pm \infty$ which is required by the normalization condition (3.4).

The normalized wave function of the n-state is

$$\phi_n(x) = \sqrt{\frac{a}{\sqrt{\pi} \ 2^n n!}} \ H_n(ax) \ e^{-\frac{1}{2}a^2 x^2}, \tag{3.26}$$

where, as previously, $a = \sqrt{\frac{m\omega}{\hbar}}$. As it seen in Eq. (3.25), the minimal or ground state energy E_0 , which is also known as the energy of zero-point oscillations or zero-point fluctuations, is nonzero. It occurs as staying at the bottom of the potential would require a perfect localization x = 0. The ground state energy results from the compromise of the position and momentum localizations. To better explain what is meant here let us consider the ground state wave function which in the coordinate space is

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}.$$
(3.27)

The wave function in the momentum space is found to be

$$\phi_0(k) = \int dx \, e^{-i\frac{kx}{\hbar}} \phi_0(x) = \sqrt{2} \left(\frac{\pi\hbar}{m\omega}\right)^{1/4} e^{-\frac{k^2}{2\hbar m\omega}}.$$
(3.28)

The position and momentum probability distributions are

$$|\phi_0(x)|^2 = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{m\omega x^2}{\hbar}}, \qquad |\phi_0(k)|^2 = 2\sqrt{\frac{\pi\hbar}{m\omega}} e^{-\frac{k^2}{m\hbar\omega}}.$$
(3.29)

One checks that

$$\int dx \, |\phi_0(x)|^2 = 1 = \int \frac{dk}{2\pi\hbar} \, |\phi_0(k)|^2.$$
(3.30)

The widths of the distributions (3.29) read

$$\sigma_x \equiv \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{\hbar}{2m\omega}}, \qquad \sigma_k \equiv \sqrt{\langle k^2 \rangle - \langle k \rangle^2} = \sqrt{\frac{m\omega}{2\hbar}}. \tag{3.31}$$

As seen, the product of the widths

$$\sigma_x \sigma_k = \frac{\hbar}{2},\tag{3.32}$$

which is the minimal value allowed by the uncertainty principle.

4. CANONICAL QUANTIZATION

The canonical quantization offers an alternative method to describe a quantum system starting with its classical counterpart.

A. 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

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

and consequently

$$[\hat{x}(t), \hat{p}(t)] = i\hbar, \tag{4.1}$$

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. (2.15), the operators $\hat{x}(t), \hat{p}(t)$ should obey the equations

$$i\hbar \dot{\hat{x}}(t) = [\hat{x}(t), \hat{H}], \qquad i\hbar \dot{\hat{p}}(t) = [\hat{p}(t), \hat{H}].$$
(4.2)

Knowing the solutions of classical equations of motion (2.7, 2.11), the corresponding quantum solutions are expected to be

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2m\omega}} \Big(\hat{a}e^{-i\omega t} + \hat{a}^{\dagger}e^{i\omega t} \Big), \tag{4.3}$$

and

$$\hat{p}(t) = -i\sqrt{\frac{m\omega\hbar}{2}} \Big(\hat{a}e^{-i\omega t} - \hat{a}^{\dagger}e^{i\omega t} \Big), \tag{4.4}$$

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 (4.3, 4.4) satisfy the quantum equations of motion (4.2). For this purpose one observes that the relation (4.1) implies the commutation relation for the creation and annihilation operators

$$[\hat{a}, \hat{a}^{\dagger}] = 1.$$
 (4.5)

Consequently, the quantum Hamiltonian, which is an analog of the classical expression (2.9), equals

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2 = \frac{\hbar\omega}{2} \left(\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a}\right), \tag{4.6}$$

which, using the relation (4.5), is rewritten as

$$\hat{H} = \hbar \omega \left(\hat{a}^{\dagger} \hat{a} + \frac{1}{2} \right). \tag{4.7}$$

One checks that there hold the relations

$$[\hat{a}, \hat{H}] = \hbar \omega \,\hat{a}, \qquad \qquad [\hat{a}^{\dagger}, \hat{H}] = -\hbar \omega \,\hat{a}^{\dagger}, \qquad (4.8)$$

which allow one to prove immediately that the expressions (4.3, 4.4) satisfy the quantum equations of motion (4.2). This happens because the Poisson brackets and commutator have the same algebraic structure.

B. 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

$$\hat{H}|E\rangle = E|E\rangle. \tag{4.9}$$

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

$$\hat{H}\hat{a}|E\rangle = \left(\hat{a}\hat{H} + [\hat{H},\hat{a}]\right)|E\rangle = (\hat{a}\hat{H} - \hbar\omega\hat{a})|E\rangle = (\hat{a}E - \hbar\omega\hat{a})|E\rangle = (E - \hbar\omega)\hat{a}|E\rangle$$
(4.10)

and

$$\hat{H}\hat{a}^{\dagger}|E\rangle = \left(\hat{a}^{\dagger}\hat{H} + [\hat{H}, \hat{a}^{\dagger}]\right)|E\rangle = \left(\hat{a}^{\dagger}\hat{H} + \hbar\omega\hat{a}^{\dagger}\right)|E\rangle = \left(\hat{a}^{\dagger}E + \hbar\omega\hat{a}^{\dagger}\right)|E\rangle = (E + \hbar\omega)\hat{a}^{\dagger}|E\rangle.$$
(4.11)

Therefore, 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

$$\hat{a}|E\rangle = |E - \hbar\omega\rangle,\tag{4.12}$$

$$\hat{a}^{\dagger}|E\rangle = |E + \hbar\omega\rangle. \tag{4.13}$$

As seen, 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 (4.6) – cannot be decreased. Therefore, we demand the property

$$\hat{a}|0\rangle = \langle 0|\hat{a}^{\dagger} = 0, \tag{4.14}$$

where $|0\rangle$ denotes the ground state. Its energy eigenvalue is then found as

$$\hat{H}|0\rangle = \hbar\omega \left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2}\right)|0\rangle = \frac{\hbar\omega}{2}|0\rangle.$$
(4.15)

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 $n\hbar\omega$. Its energy eigenvalue is $\hbar\omega(n + 1/2)$ and its normalization is determined by the condition $\langle n|n\rangle = 1$. Then, we can easily find how the annihilation and creation operators act on $|n\rangle$. We write

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

$$(4.16)$$

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

$$\langle n|\hat{a}^{\dagger}\hat{a}|n\rangle = n\langle n|n\rangle = n = |C_n|^2\langle n-1|n-1\rangle = |C_n|^2.$$
(4.17)

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

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle. \tag{4.18}$$

Analogously one finds

$$\hat{a}^{\dagger}|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{4.19}$$

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

$$\hat{a}^{\dagger}\hat{a}|n\rangle = n|n\rangle. \tag{4.20}$$

5. SCHRÖDINGER'S AND HEISENBERG'S PICTURES

One asks how the Schrödinger's wave mechanics is related to the quantum canonical formalism. As will be show here these are two different but equivalent approaches connected to each other by a unitary transformation.

In this section we start using the Dirac notation which is introduced and explained in detail in Appendix A. We also use the natural units with $\hbar = 1$ to simplify the formulas.

A. Schrödinger's picture

As we already know, the wave mechanics is based on the Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi(t)\rangle_{\rm S} = \hat{H}|\psi(t)\rangle_{\rm S}.$$
(5.1)

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 (5.1) is

$$|\psi(t)\rangle_{\mathrm{S}} = e^{-iHt}|\psi(0)\rangle_{\mathrm{S}},\tag{5.2}$$

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

$${}_{\mathrm{S}}\!\langle\phi(t)|\hat{\Omega}_{\mathrm{S}}|\psi(t)\rangle_{\mathrm{S}} = {}_{\mathrm{S}}\!\langle\phi(0)|e^{iHt}\hat{\Omega}_{\mathrm{S}}e^{-iHt}|\psi(0)\rangle_{\mathrm{S}}.$$
(5.3)

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.

B. Heisenberg's picture

The matrix element (5.3) can be also written as

$${}_{\mathrm{S}}\!\langle\phi(t)|\hat{\Omega}_{\mathrm{S}}|\psi(t)\rangle_{\mathrm{S}} = {}_{\mathrm{H}}\!\langle\phi|\hat{\Omega}_{\mathrm{H}}(t)|\psi\rangle_{\mathrm{H}},\tag{5.4}$$

where

$$|\psi\rangle_{\rm H} \equiv |\psi(0)\rangle_{\rm S} = e^{iHt} |\psi(t)\rangle_{\rm S} \tag{5.5}$$

is the state in the Heisenberg's picture, and

$$\hat{\Omega}_{\rm H}(t) \equiv e^{i\hat{H}t}\hat{\Omega}_{\rm S} \ e^{-i\hat{H}t} \tag{5.6}$$

is the observable in the Heisenberg's picture. The equation (5.4) shows that going from the Schrödinger's to Heisenberg's picture the time dependence is transferred from the states to the observable.

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

$$\frac{d}{dt}\hat{\Omega}_{\rm H}(t) = \left(\frac{d}{dt}e^{i\hat{H}t}\right)\hat{\Omega}_{\rm S} \ e^{-i\hat{H}t} + e^{i\hat{H}t}\hat{\Omega}_{\rm S}\left(\frac{d}{dt}e^{-i\hat{H}t}\right) = ie^{i\hat{H}t}\hat{H}\hat{\Omega}_{\rm S} \ e^{-i\hat{H}t} - ie^{i\hat{H}t}\hat{\Omega}_{\rm S} \ \hat{H} \ e^{-i\hat{H}t}.$$
(5.7)

Since the operators \hat{H} and $e^{-i\hat{H}t}$ commute with each other and consequently can be interchanged, the equality (5.7) becomes the equation of motion of the observable $\hat{\Omega}_{\rm H}(t)$ that is

$$\frac{d}{dt}\hat{\Omega}_{\rm H}(t) = i[\hat{H}, \hat{\Omega}_{\rm H}(t)].$$
(5.8)

We note that the Hamiltonian \hat{H} is the same in the Schrödinger's and Heisenberg's picture and for this reason it does not carry the index S or H. Writing down the equation (5.8) for the position $\hat{x}_{\rm H}(t)$ and momentum $\hat{p}_{\rm H}(t)$ operators, we find the equations

$$\frac{d}{dt}\hat{x}_{\rm H}(t) = i[\hat{H}, \hat{x}_{\rm H}(t)], \qquad \qquad \frac{d}{dt}\hat{p}_{\rm H}(t) = i[\hat{H}, \hat{p}_{\rm H}(t)], \qquad (5.9)$$

which were obtained in Sec. 4 due to the canonical quantization of the classical equations of motion. Needless to say the operators $\hat{x}_{\rm H}(t)$ and $\hat{p}_{\rm H}(t)$ obey the commutation relation

$$[\hat{x}_{\rm H}(t), \hat{p}_{\rm H}(t)] = i. \tag{5.10}$$

So, we conclude that the wave mechanics presented in Sec. 3 and the canonical quantization discussed in Sec. 4 are the two equivalent approaches to quantum mechanics connected to each other by the unitary transformation:

$$|\psi\rangle_{\rm H} = e^{iHt} |\psi(t)\rangle_{\rm S} \tag{5.11}$$

$$\hat{\Omega}_{\rm H}(t) = e^{i\hat{H}t}\hat{\Omega}_{\rm S} \ e^{-i\hat{H}t}.$$
(5.12)

6. PATH INTEGRAL FORMULATION

In this section we discuss the third approach to quantum mechanics which is known as the path integral formulation. The eigenstates of position operator \hat{x} play a crucial role here. In the Schrödinger's picture \hat{x}_S is time independent and so are the eigenstates $|x\rangle_S$ which by definition obey

$$\hat{x}_S |x\rangle_S = x|x\rangle_S. \tag{6.1}$$

In case of the Heisenberg's picture we have

$$\hat{x}_H(t) = e^{iHt} \hat{x}_S e^{-iHt}, \qquad |x,t\rangle_H = e^{iHt} |x\rangle_S, \qquad \hat{x}_H(t) |x,t\rangle_H = x |x,t\rangle_H.$$
(6.2)

As previously, we use the hats to distinguish operators from their eigenvalues or classical counterparts. The Dirac notation, which is used here, is introduced and explained in detail in Appendix A. As in Sec. 5 we keep $\hbar = 1$.

A. Transition amplitude

We consider the transition amplitude $\langle x, t | x_0, t_0 \rangle$ where the states are in the Heisenberg's picture. Since $\langle x, t | = \langle x | e^{-i\hat{H}t}$ and $|x_0, t_0 \rangle = e^{i\hat{H}t_0} |x_0 \rangle$, where the states with no time argument are in the Schrödinger's picture, we have

$$\langle x, t | x_0, t_0 \rangle = \langle x | e^{-iH(t-t_0)} | x_0 \rangle.$$
(6.3)

To compute it we split the time interval $[t, t_0]$ into N pieces of the length Δt in such a way that $t_j = t_0 + j\Delta t$ with j = 0, 1, 2, ..., N and $\Delta t \equiv (t - t_0)/N$. As seen $t_{j=0} = t_0$ and $t_N = t$. Then, referring to the completeness of the position eigenstates

$$\int dx |x, t\rangle \langle x, t| = 1 \tag{6.4}$$

one writes the expression of interest as

$$\langle x, t | x_0, t_0 \rangle = \int dx_{N-1} \int dx_{N-2} \cdots \int dx_1 \tag{6.5}$$

 $\times \langle x, t | x_{N-1}, t_{N-1} \rangle \langle x_{N-1}, t_{N-1} | x_{N-2}, t_{N-2} \rangle \cdots \langle x_2, t_2 | x_1, t_1 \rangle \langle x_1, t_1 | x_0, t_0 \rangle.$

We compute

$$\langle x_{j+1}, t_j | x_j, t_j \rangle = \langle x_{j+1} | e^{-i\hat{H}\Delta t} | x_j \rangle = \langle x_{j+1} | 1 - i\hat{H}\Delta t | x_j \rangle + \mathcal{O}(\Delta t^2).$$
(6.6)

Since $\langle x|x'\rangle = \delta(x-x')$, one gets

$$\langle x_{j+1}, t_j | x_j, t_j \rangle = \delta(x_{j+1} - x_j) - i \langle x_{j+1} | \hat{H} | x_j \rangle \Delta t + \mathcal{O}(\Delta t^2).$$
(6.7)

Now one introduces the complete set of momentum eigenstates $|p\rangle$ and writes

$$\langle x_{j+1}|\hat{H}|x_j\rangle = \int \frac{dp_j}{2\pi} \langle x_{j+1}|p_j\rangle \langle p_j|\hat{H}|x_j\rangle.$$
(6.8)

Assuming that $\hat{H} = f(\hat{p}) + g(\hat{x})$, where f and g are arbitrary functions, one gets

$$\langle p|\hat{H}|x\rangle = \langle p|f(\hat{p}) + g(\hat{x})|x\rangle = (f(p) + g(x))\langle p|x\rangle = H(p,x)\langle p|x\rangle,$$
(6.9)

where H(p, x) is the classical Hamiltonian. Since $\langle p | x \rangle = e^{-ipx}$, we obtain

$$\langle p|\hat{H}|x\rangle = H(p,x)e^{-ipx} \tag{6.10}$$

and

$$\langle x_{j+1} | \hat{H} | x_j \rangle = \int \frac{dp_j}{2\pi} e^{ip_j(x_{j+1} - x_j)} H(p_j, x_j).$$
(6.11)

Consequently

$$\langle x_{j+1}, t_j | x_j, t_j \rangle = \int \frac{dp_j}{2\pi} e^{ip_j(x_{j+1} - x_j)} \left[1 - iH(p_j, x_j) \Delta t \right] + \mathcal{O}(\Delta t^2) = \int \frac{dp_j}{2\pi} e^{i[p_j(x_{j+1} - x_j) - H(p_j, x_j) \Delta t]} + \mathcal{O}(\Delta t^2)$$
(6.12)

and

$$\langle x,t|x_0,t_0\rangle = \int dx_{N-1} \int dx_{N-2} \cdots \int dx_1 \int \frac{dp_N}{2\pi} \int \frac{dp_{N-1}}{2\pi} \cdots \int \frac{dp_1}{2\pi} \int \frac{dp_0}{2\pi}$$

$$\times \exp\left\{i\sum_{j=0}^N \left[p_j \frac{x_{j+1}-x_j}{\Delta t} - H(p_j,x_j)\right] \Delta t\right\}.$$
(6.13)

The initial and final values of x are fixed but the momenta are not. For this reason the number of momentum integrations is two more than that of the position integrations. In the continuum limit, we write the result (6.13) as

$$\langle x, t | x_0, t_0 \rangle = \int \mathcal{D}x(t') \int \frac{\mathcal{D}p(t')}{2\pi} \exp\left\{ i \int_{t_0}^t dt' \Big[p(t') \dot{x}(t') - H\big(p(t'), x(t')\big) \Big] \right\},\tag{6.14}$$

where $\dot{x} \equiv \frac{dx}{dt}$ and

$$\int \mathcal{D}x(t)\cdots = \lim_{N \to \infty} \int dx_{N-1} \int dx_{N-2}\cdots \int dx_1 \dots$$
(6.15)

denotes the functional integration with the boundary condition $x(t' = t_0) = x_0$ and x(t' = t) = x. There are no boundary conditions for the momentum functional integration.

It is tempting to identify $p\dot{x} - H(p, x)$ with the classical Lagrangian L. In the Lagrangian formalism the energy E indeed equals

$$E = p(t) \dot{x}(t) - L(t), \tag{6.16}$$

where $p \equiv \frac{dL}{dx}$. However, *E* has a meaning of the conserved energy provided x(t) satisfies the equation of motion. The trajectories x(t) and p(t) from Eq. (6.14) are *not* required to obey the equations of motion.

When H(p, x) quadratically depends on p as in the non-relativistic Hamiltonian

$$H(p,x) = \frac{p^2}{2m} + V(x), \tag{6.17}$$

the momentum integral in Eq. (6.14) is Gaussian and it can be explicitly computed. Starting with the formula (6.13), we have

$$\langle x, t | x_0, t_0 \rangle = \int dx_{N-1} \int dx_{N-2} \cdots \int dx_1 \int \frac{dp_N}{2\pi} \int \frac{dp_{N-1}}{2\pi} \cdots \int \frac{dp_1}{2\pi} \int \frac{dp_0}{2\pi}$$
(6.18)

$$\times \exp \Big\{ i \sum_{j=0}^N \Big[p_j \frac{x_{j+1} - x_j}{\Delta t} - \frac{p_j^2}{2m} - V(x_j) \Big] \Delta t \Big\}.$$

Keeping in mind that

$$\int_{-\infty}^{\infty} dp \ e^{ipx-ap^2} = \sqrt{\frac{\pi}{a}} \ e^{-\frac{x^2}{4a}},\tag{6.19}$$

one computes

$$\int \frac{dp}{2\pi} \exp\left\{i\left[p\dot{x} - \frac{p^2}{2m}\right]\Delta t\right\} = \sqrt{\frac{m}{2\pi i \Delta t}} e^{i\Delta t \frac{m\dot{x}^2}{2}},\tag{6.20}$$

which gives

$$\langle x,t|x_0,t_0\rangle = \left(\frac{m}{2\pi i\Delta t}\right)^{\frac{N}{2}} \int dx_{N-1} \int dx_{N-2} \cdots \int dx_1 \exp\left\{i\sum_{j=0}^N \left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\Delta t}\right)^2 - V(x_j)\right]\Delta t\right\}.$$
 (6.21)

In the continuum limit we get

$$\langle x, t | x_0, t_0 \rangle = C \int \mathcal{D}x(t') \exp\left\{ i \int_{t_0}^t dt' \left[\frac{m \dot{x}^2(t')}{2} - V(x) \right] \right\},$$
(6.22)

where the normalization constant C is

$$C = \lim_{N \to \infty} \left(\frac{m}{2\pi i \Delta t}\right)^{\frac{N}{2}} = \int \frac{\mathcal{D}p(t')}{2\pi} \exp\left[-i \int_{t_0}^t dt' \frac{p^2(t')}{2m}\right].$$
 (6.23)

Since

$$L(t) \equiv \frac{m\dot{x}^{2}(t)}{2} - V(x), \qquad (6.24)$$

we finally find

$$\langle x, t | x_0, t_0 \rangle = C \int \mathcal{D}x(t') \exp\left\{i \int_{t_0}^t dt' L(t')\right\},\tag{6.25}$$

which is the key object of the path integral formulation of quantum mechanics.

B. From path integrals to Schrödinger equation

A variety of information is encoded in the transition amplitude (6.25). However, let us first discuss how the amplitude is related to the Schrödinger equation (3.7). The relation is presumably most easily obtained when one considers the wave function $\Psi(t, x)$ and the function at an infinitesimally later time $\Psi(t + \varepsilon, y)$ which are connected by the amplitude (6.25) in the following way

$$\Psi(t+\varepsilon,y) = \int_{-\infty}^{\infty} dx \,\langle y,t+\varepsilon | x,t \rangle \,\Psi(t,x).$$
(6.26)

Since

$$\int_{t}^{t+\varepsilon} dt' L(t') = \int_{t}^{t+\varepsilon} dt' \left(\frac{m\dot{x}^2}{2} - V(x)\right) = \left(\frac{m\dot{x}^2}{2} - V(x)\right)\varepsilon,\tag{6.27}$$

we have

$$\langle y, t+\varepsilon | x, t \rangle = C \int_{x(t)=x}^{x(t+\varepsilon)=y} \mathcal{D}x(t') \exp\left[i\left(\frac{m\dot{x}^2}{2} - V(x)\right)\varepsilon\right] = \left(\frac{m}{2\pi i\varepsilon}\right)^{1/2} \exp\left[i\left(\frac{m(x-y)^2}{2\varepsilon^2} - V(x)\right)\varepsilon\right], \quad (6.28)$$

where according to Eq. (6.23)

$$C = \left(\frac{m}{2\pi i\varepsilon}\right)^{1/2}.\tag{6.29}$$

Substituting the result (6.28) into Eq. (6.26), one gets

$$\Psi(t+\varepsilon,y) = \left(\frac{m}{2\pi i\varepsilon}\right)^{1/2} \int_{-\infty}^{\infty} dx \, \exp\left[-\frac{m(x-y)^2}{2i\varepsilon}\right] \, \exp\left[-i\varepsilon V(x)\right] \Psi(t,x). \tag{6.30}$$

Now we change the integration variable to $\Delta = x - y$ and the integral (6.30) reads

$$\Psi(t+\varepsilon,y) = \left(\frac{m}{2\pi i\varepsilon}\right)^{1/2} \int_{-\infty}^{\infty} d\Delta \exp\left[-\frac{m\Delta^2}{2i\varepsilon}\right] \exp\left[-i\varepsilon V(y+\Delta)\right] \Psi(t,y+\Delta).$$
(6.31)

Because of the infinite simally small element ε the factor $\exp\left[i\frac{m\Delta^2}{2\varepsilon}\right]$ oscillates fast as Δ varies, and consequently the contribution to the integral (6.31) comes only from a small domain around $\Delta = 0$. So, we expand the wave function and the factor $\exp[-i\varepsilon V(y + \Delta)]$ around y as

$$\Psi(t, y + \Delta) = \Psi(t, y) + \Delta \frac{\partial}{\partial y} \Psi(t, y) + \frac{1}{2} \Delta^2 \frac{\partial^2}{\partial y^2} \Psi(t, y) + \dots$$
(6.32)

$$\exp[-i\varepsilon V(y+\Delta)] = 1 - i\varepsilon V(y) + \dots$$
(6.33)

which substituted into Eq. (6.31) provide

$$\Psi(t+\varepsilon,y) = \left(\frac{m}{2\pi i\varepsilon}\right)^{1/2} \left(1-i\varepsilon V(y)\right) \int_{-\infty}^{\infty} d\Delta \exp\left[-\frac{m\Delta^2}{2i\varepsilon}\right] \left(\Psi(t,y) + \Delta\frac{\partial}{\partial y}\Psi(t,y) + \frac{1}{2}\Delta^2\frac{\partial^2}{\partial y^2}\Psi(t,y)\right).$$
(6.34)

The integral of the term with the first derivative of the wave function vanishes because the integrand is odd as a function of Δ . The remaining two elementary Gaussian integrals give the equation

$$\Psi(t+\varepsilon,y) = \left(1-i\varepsilon V(y)\right) \left(\Psi(t,y) + \frac{i\varepsilon}{2m}\frac{\partial^2}{\partial y^2}\Psi(t,y)\right) = \Psi(t,y) - i\varepsilon \left(-\frac{1}{2m}\frac{\partial^2}{\partial y^2} + V(y)\right)\Psi(t,y), \tag{6.35}$$

which can be written as

$$i\frac{\Psi(t+\varepsilon,y)-\Psi(t,y)}{\varepsilon} = \left(-\frac{1}{2m}\frac{\partial^2}{\partial y^2} + V(y)\right)\Psi(t,y).$$
(6.36)

Taking the limit $\varepsilon \to 0$ we get the Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(t,y) = \left(-\frac{1}{2m}\frac{\partial^2}{\partial y^2} + V(y)\right)\Psi(t,y).$$
(6.37)

So, we conclude that the Schrödinger equation is encoded in the transition amplitude (6.25).

C. Explicit form of the transition amplitude

Let us look for an explicit expression of the amplitude (6.25) for the case of harmonic oscillator. One option is to perform the path integral in the expression (6.25) discretizing the time and space variables and then taking the continuum limit.

However, there is a simpler method which relies on our knowledge of the exact solution of the classical equation of motion (2.5). Specifically, we intend to change the variable of functional integration from x(t') to $\xi(t') \equiv x(t') - x_{cl}(t')$, where $x_{cl}(t')$ is the classical solution which obeys the conditions

$$x_{\rm cl}(t_0) = x_0, \qquad \qquad x_{\rm cl}(t) = x.$$
 (6.38)

Then, $\xi(t) = \xi(t_0) = 0$.

We write the classical solution (2.5) as

$$x_{\rm cl}(t') = A\cos(\omega t') + B\sin(\omega t'), \tag{6.39}$$

where A and B are constants to be found from the conditions (6.38). Once it is achieved the solution reads

$$x_{\rm cl}(t') = x_0 \frac{\sin\left(\omega(t-t')\right)}{\sin(\omega T)} + x \frac{\sin\left(\omega(t'-t_0)\right)}{\sin(\omega T)}.$$
(6.40)

where $T \equiv t - t_0$. The classical action corresponding to the solution (6.40) is easily computed as

$$S_{\rm cl} = \int_{t_0}^t dt' L\big(x_{\rm cl}(t'), \dot{x}_{\rm cl}(t')\big) = \frac{m}{2} \int_{t_0}^t dt' \big[\dot{x}_{\rm cl}^2(t') - \omega^2 x_{\rm cl}^2(t') \big] = \frac{m\omega}{2\sin(\omega T)} \Big[(x^2 + x_0^2)\cos(\omega T) - 2xx_0 \Big].$$
(6.41)

We are now ready to change the variable of functional integration from x(t') to $\xi(t') \equiv x(t') - x_{cl}(t')$ in Eq. (6.25). The Lagrange function equals

$$L(\xi(t') + x_{\rm cl}(t'), \dot{\xi}(t') + \dot{x}_{\rm cl}(t')) = \frac{m}{2} \Big[(\dot{\xi}(t') + \dot{x}_{\rm cl}(t'))^2 - \omega^2 (\xi(t') + x_{\rm cl}(t'))^2 \Big]$$

$$= \frac{m}{2} \big[\dot{\xi}^2(t') - \omega^2 \xi^2(t') \big] + \frac{m}{2} \big[\dot{x}_{\rm cl}^2(t') - \omega^2 x_{\rm cl}^2(t') \big]$$

$$+ m \big[\dot{\xi}(t') \, \dot{x}_{\rm cl}(t') - \omega^2 \xi(t') \, x_{\rm cl}(t') \big].$$
(6.42)

Since $x_{\rm cl}(t')$ obeys the equation of motion (2.3), the last term in Eq. (6.42) can be rewritten as

$$m[\dot{\xi}(t')\,\dot{x}_{\rm cl}(t') + \xi(t')\,\ddot{x}_{\rm cl}(t')] \tag{6.43}$$

and it vanishes when partially integrated over t' from t_0 to t because $\xi(t) = \xi(t_0) = 0$. Therefore, the action equals

$$S = \int_{t_0}^t dt' L\big(\xi(t') + x_{\rm cl}(t'), \dot{\xi}(t') + \dot{x}_{\rm cl}(t')\big) = S_{\rm cl} + \frac{m}{2} \int_{t_0}^t dt' \big[\dot{\xi}^2(t') - \omega^2 \xi^2(t')\big]$$
(6.44)

and the amplitude (6.25) is

$$\langle x, t | x_0, t_0 \rangle = e^{iS_{\rm cl}} C \int \mathcal{D}\xi(t') \exp\left\{ i \frac{m}{2} \int_{t_0}^t dt' \left[\dot{\xi}^2(t') - \omega^2 \xi^2(t') \right] \right\}.$$
(6.45)

The factor $e^{iS_{cl}}$ is already known due to Eq. (6.41) while the remaining factor is independent of x and x_0 . It can depend solely on $T \equiv t - t_0$ because of the temporal translation invariance of the whole problem. So, we write

$$\langle x, t | x_0, t_0 \rangle = f(T) \exp \left\{ i \frac{m\omega}{2\sin(\omega T)} \left[(x^2 + x_0^2) \cos(\omega T) - 2xx_0 \right] \right\}.$$
 (6.46)

The unknown factor f(T) can be found from the requirement

$$\langle x_1, t_1 | x_0, t_0 \rangle = \int dx \, \langle x_1, t_1 | x, t \rangle \langle x, t | x_0, t_0 \rangle, \tag{6.47}$$

which comes from the very meaning of the transition amplitude. It leads to the equation

$$f(t_{1} - t_{0}) \exp\left\{i\frac{m\omega}{2\sin(\omega(t_{1} - t_{0}))}\left[(x_{1}^{2} + x_{0}^{2})\cos(\omega(t_{1} - t_{0})) - 2x_{1}x_{0}\right]\right\}$$

$$= f(t_{1} - t) f(t - t_{0}) \int dx \exp\left\{i\frac{m\omega}{2\sin(\omega(t_{1} - t))}\left[(x_{1}^{2} + x^{2})\cos(\omega(t_{1} - t)) - 2x_{1}x\right]\right\}$$

$$\times \exp\left\{i\frac{m\omega}{2\sin(\omega(t - t_{0}))}\left[(x^{2} + x_{0}^{2})\cos(\omega(t - t_{0})) - 2xx_{0}\right]\right\}.$$
(6.48)

Performing the Gaussian integral over x the equation becomes

$$f(t_1 - t_0) = f(t_1 - t) f(t - t_0) \left(\frac{2\pi i}{m\omega}\right)^{1/2} \left(\frac{\sin\left(\omega(t_1 - t)\right)\sin\left(\omega(t - t_0)\right)}{\sin\left(\omega(t_1 - t_0)\right)}\right)^{1/2},\tag{6.49}$$

which is solved by

$$f(t - t_0) = \left(\frac{m\omega}{2\pi i \sin(\omega(t - t_0))}\right)^{1/2}.$$
(6.50)

Finally, the transition amplitude equals

$$\langle x, t | x_0, t_0 \rangle = \left(\frac{m\omega}{2\pi i \sin(\omega T)}\right)^{1/2} \exp\left\{i\frac{m\omega}{2\sin(\omega T)}\left[(x^2 + x_0^2)\cos(\omega T) - 2xx_0\right]\right\}.$$
(6.51)

D. Energy levels

To get the energy levels from the transition amplitude (6.51), we first return to Eq. (6.3) and express the amplitude through the energy eigenstates $|E_n\rangle$ as

$$\langle x, t | x_0, t_0 \rangle = \langle x | e^{-i\hat{H}(t-t_0)} | x_0 \rangle = \sum_{n,m} \langle x | E_n \rangle \langle E_n | e^{-i\hat{H}(t-t_0)} | E_m \rangle \langle E_m | x_0 \rangle$$
$$= \sum_{n,m} \langle x | E_n \rangle \langle E_n | E_m \rangle e^{-iE_m(t-t_0)} \langle E_m | x_0 \rangle = \sum_{n,m} \langle x | E_n \rangle \delta^{nm} e^{-iE_m T} \langle E_m | x_0 \rangle$$
$$= \sum_n \langle x | E_n \rangle e^{-iE_n T} \langle E_n | x_0 \rangle = \sum_n e^{-iE_n T} \phi_n(x) \phi_n^*(x_0), \qquad (6.52)$$

where, as previously, $T \equiv t - t_0$ and $\phi_n(x) \equiv \langle x | E_n \rangle$ is the wave function which is the energy eigenfunction.

The easiest way to extract the energy levels is to consider the equality

$$\int dx \,\langle x, t | x, t_0 \rangle = \sum_n e^{-iE_n T},\tag{6.53}$$

which follows from Eq. (6.52) because

$$\int dx \, |\phi_n(x)|^2 = 1. \tag{6.54}$$

Using the amplitude (6.51), one finds

$$\int dx \,\langle x, t | x, t_0 \rangle = \frac{1}{2i \sin(\omega T/2)} = e^{-\frac{i\omega T}{2}} \frac{1}{1 - e^{-i\omega T}} = \sum_{n=0}^{\infty} e^{-i(n + \frac{1}{2})\omega T},\tag{6.55}$$

and consequently we get the well-known energy levels

$$E_n = \left(n + \frac{1}{2}\right)\omega\tag{6.56}$$

with n = 0, 1, 2... One may wonder whether the energies (6.56) are uniquely determined by the l.h.s. of Eq. (6.55). To show that this is indeed the case one expands the function in the l.h.s. of Eq. (6.55) into a Fourier series, observing that it is the periodic function of T with the period $P = 4\pi/\omega$. Thus, we write

$$\frac{1}{2i\sin(\omega T/2)} = \sum_{k=-\infty}^{\infty} c_k \, e^{ik\Omega T},\tag{6.57}$$

where $\Omega \equiv 2\pi/P = \omega/2$ and

$$c_k \equiv \frac{1}{P} \int_{-P/2}^{P/2} \frac{dT}{2i\sin(\omega T/2)} e^{-ik\Omega T} = -\frac{1}{2\pi} \int_0^{\pi} dx \, \frac{\sin(kx)}{\sin(x)} = \begin{cases} 0 & \text{for } k \text{ even,} \\ -\frac{1}{2}\operatorname{sgn}(k) & \text{for } k \text{ odd.} \end{cases}$$
(6.58)

Substituting the coefficients (6.58) into the expansion (6.57), one finds

$$\frac{1}{2i\sin(\omega T/2)} = -\frac{1}{2}\sum_{n=0}^{\infty} \left(e^{i(2n+1)\omega T/2} - e^{-i(2n+1)\omega T/2} \right) = -i\sum_{n=0}^{\infty} \sin\left(\left(n + \frac{1}{2} \right) \omega T \right), \tag{6.59}$$

which actually equals the r.h.s. of Eq. (6.55). The equality is evident observing that the real part of the r.h.s. of Eq. (6.55) vanishes, as the function in the l.h.s. of Eq. (6.55) is purely imaginary.

At the end we note that one can also show that the wave functions, which enter the amplitude (6.51), coincide with the functions (3.26) derived in Sec. 3 B as solutions of the Schrödinger equation.

We explain here the so-called Dirac notation which was introduced by Paul Dirac in 1939. The notation is commonly used in quantum mechanics and quantum field theory.

- A quantum state is denoted as $|\Psi\rangle$ and it is called *ket*.
- The state conjugate to $|\Psi\rangle$ is denoted as $\langle\Psi|$ and its called *bra*.
- The scalar product of the states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ is $\langle \Psi_1|\Psi_2\rangle$. One observes that

$$(\langle \Psi_1 | \Psi_2 \rangle)^* = \langle \Psi_2 | \Psi_1 \rangle$$

as it should be.

• The states are normalized to unity that is

$$\langle \Psi | \Psi \rangle = 1.$$

• An eigenstate of the (one-dimensional) position operator \hat{x} is denoted as $|x\rangle$ and by definition

$$\hat{x}|x\rangle = x|x\rangle.$$

• The states $|x_1\rangle$, $|x_2\rangle$ are orthonormal that is

$$\langle x_1 | x_2 \rangle = \delta(x_1 - x_2).$$

• An eigenstate of the (one-dimensional) momentum operator \hat{p} is denoted as $|p\rangle$ and by definition

$$\hat{p}|p\rangle = p|p\rangle$$

• The states $|p_1\rangle$, $|p_2\rangle$ are orthogonal that is

$$\langle p_1 | p_2 \rangle = \# \delta(p_1 - p_2).$$

The numerical factor # will be found later on.

- The wave function in coordinate space is defined as $\Psi(x) \equiv \langle x | \Psi \rangle$.
- If the state is time dependent, which is denoted as $|\Psi(t)\rangle$, so is the wave function that is $\Psi(t,x) \equiv \langle x|\Psi(t)\rangle$.
- The wave function in momentum space is defined as $\Psi(p) \equiv \langle p | \Psi \rangle$.
- The wave function in coordinate space, which is the eigenfunction of momentum operator, is $\Psi_p(x) \equiv \langle x | p \rangle$.
- The position operator, which acts on the wave functions in coordinate space, is defined as $\hat{x}\Psi(x) \equiv x\Psi(x)$.
- The momentum operator, which acts on the wave functions in coordinate space, is defined as $\hat{p}\Psi(x) \equiv -i\frac{\partial}{\partial x}\Psi(x)$.
- Since the wave function $\Psi_p(x)$ satisfies the equation

$$-i\frac{\partial}{\partial x}\Psi_p(x) = p\Psi_p(x)$$

it equals $\Psi_p(x) = Ce^{ipx}$ where C is the normalization constant which is assumed to be real. It is found from the condition

$$1 = \int dx \, \Psi_p^*(x) \Psi_p(x) = C^2 \int dx = C^2 L,$$

where L is the length of the box where the normalization is done. Therefore $C = 1/\sqrt{L}$ and

$$\Psi_p(x) \equiv \langle x | p \rangle = \frac{1}{\sqrt{L}} e^{ipx}$$

• One observes that

$$1 = \int dx \, \Psi_p^*(x) \Psi_p(x) = \int dx \, \langle p | x \rangle \langle x | p \rangle$$

and thus

$$1 = \int dx \, |x\rangle \langle x|,$$

which is the *completeness condition* of the position eigenstates.

• Let us compute

$$\langle p_1 | p_2 \rangle = \int dx \, \langle p_1 | x \rangle \langle x | p_2 \rangle = \int dx \, \Psi_{p_1}^*(x) \Psi_{p_2}(x) = \frac{1}{L} \int dx \, e^{i(p_1 - p_2)x} = \frac{2\pi}{L} \delta(p_1 - p_2).$$

• Finally, we compute

$$\Psi(p) \equiv \langle p | \Psi \rangle = \int dx \, \langle p | x \rangle \langle x | \Psi \rangle = \frac{1}{\sqrt{L}} \int dx \, e^{-ipx} \, \langle x | \Psi \rangle = \frac{1}{\sqrt{L}} \int dx \, e^{-ipx} \, \Psi(x).$$

The final formula expresses the well-known fact that $\Psi(p)$ equals the Fourier transform of $\Psi(x)$.