

Review of Quantum Mechanics

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Quantum mechanics is a modern mathematical theory used to describe the quantum phenomena. Although many scientists think it is not the ultimate theory, it is the most accurate theory today that describes the experiments. Quantum mechanics is formulated under the postulates, which are derived after many attempts to explain the experiments. In classical mechanics, a physical system consists of physical quantities which have definite values. For examples, the position x and the momentum p of a particle at any given time t are assumed to be some numbers. On the contrary, a physical system in quantum mechanics is described by a state $|\psi\rangle$. The notation $|\psi\rangle$ is called a ket. In a closed system, the state $|\psi\rangle$ contains all the information of the systems. The exotic part of quantum mechanics is that even $|\psi\rangle$ is complete, the outcome of observed quantities are still probabilistic.

1 Wavefunction

Let's use the wavefunction to elaborate the nature of probability. The wavefunction of a particle is obtained by writing $|\psi\rangle$ in the x basis $|x\rangle$,

$$\psi(x) \equiv \langle x|\psi\rangle. \quad (1)$$

For a given wavefunction $\psi(x)$, the probability to find the particle to be at x is $|\psi(x)|^2 dx$. Since the total probability is one, the normalization of a state requires that

$$\int |\psi(x)|^2 dx = 1. \quad (2)$$

The average position $\langle x \rangle$ (expectation value) of the particle is

$$\langle x \rangle = \int x |\psi(x)|^2 dx. \quad (3)$$

With the definitions, the well known Schrödinger's equation reads

$$i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V(x)\psi. \quad (4)$$

The representation of a state $|\psi\rangle$ is not unique. For example, we can use the momentum basis $|p\rangle$ to write $|\psi\rangle$,

$$\phi(p) \equiv \langle p|\psi\rangle, \quad (5)$$

and

$$\int |\phi(p)|^2 dp = 1. \quad (6)$$

Eq. (4) is only one example of the Schrödinger's equation. We will learn more general approaches to write the equations of quantum mechanics. There, we will start from the **Hamiltonian** of a system.

2 Dirac Notations

In quantum mechanics, the Bra-Ket notations are convenient tools. Any states are written as Kets $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, \dots$. You can think a Ket as a column vector. However, the representation of a column vector depends on the bases. For example, in the position basis, Kets can be defined as:

$$|\psi\rangle = \begin{pmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_N) \end{pmatrix}. \quad (7)$$

whereas in the momentum basis

$$|\psi\rangle = \begin{pmatrix} \phi(p_1) \\ \phi(p_2) \\ \vdots \\ \phi(p_N) \end{pmatrix} \quad (8)$$

The role of a Bra is similar to row vectors in linear algebra. In the position basis, Bra can be defined as:

$$\langle\psi| = \left(\psi^*(x_1) \quad \psi^*(x_2) \quad \dots \quad \psi^*(x_N) \right). \quad (9)$$

whereas in the momentum basis

$$\langle\psi| = \left(\phi^*(p_1) \quad \phi^*(p_2) \quad \dots \quad \phi^*(p_N) \right). \quad (10)$$

The inner product of two states $|\psi\rangle$ and $|\phi\rangle$ is

$$\langle\psi|\phi\rangle, \quad (11)$$

which is a complex number. The inner product $\langle\psi_i|\psi_i\rangle$ is the probability to find the particle in the i th state. The outer product of two states $|\psi\rangle$ and $|\phi\rangle$ is

$$|\phi\rangle\langle\psi| \quad (12)$$

which is a matrix.

Exercise 1: Calculation of bras and kets

Let

$$|a\rangle = \begin{pmatrix} 1 \\ 2i \\ 3 \end{pmatrix} \quad (13)$$

$$|b\rangle = \begin{pmatrix} i \\ 0 \\ 2 \end{pmatrix} \quad (14)$$

1. What are $\langle a|$ and $\langle b|$?
2. Calculate $\langle a|a\rangle$, $\langle b|b\rangle$, $\langle a|b\rangle$ and $\langle b|a\rangle$?
3. Calculate $|a\rangle\langle b|$ and $|b\rangle\langle a|$. Are they complex conjugate of each other?

If $|\psi\rangle$ is to describe a single particle, the normalization of a state requires the inner product

$$\langle\psi|\psi\rangle = 1 \quad (15)$$

or in a specific basis

$$\sum_i |\psi_i|^2 = 1, \quad (16)$$

and for a continuous variable like x ,

$$\int dx |\psi(x)|^2 = 1. \quad (17)$$

In the position basis, the position is a operator \hat{x} (a matrix).

$$\hat{x} = \begin{pmatrix} x_1 & 0 & 0 & 0 \\ 0 & x_2 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & x_N \end{pmatrix} \quad (18)$$

As it should be, the operator \hat{x} is a diagonal matrix in the position basis. In the Dirac's notation, the expectation value of x is

$$\langle x \rangle = \langle\psi|\hat{x}|\psi\rangle \quad (19)$$

$$= \sum_i x_i |\psi_i|^2 \quad (20)$$

$$= \int x |\psi(x)|^2 dx. \quad (21)$$

3 Postulates of Quantum Mechanics

Postulate 1: State Vector

A physical system is completely described by a **complex** state vector $|\psi\rangle$ in the Hilbert space.

The state vector $|\psi\rangle$ contains all the information. The state vector can be written as a sum of other (basis) vectors.

$$|\psi\rangle = \sum_i \alpha_i |\psi_i\rangle \quad (22)$$

The probability to find the system in the i th state is $|\alpha_i|^2$. The simplest example is the qubit,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle. \quad (23)$$

Without losing the generality, the qubit can be written as ($|\alpha|^2 + |\beta|^2 = 1$)

$$|\psi\rangle = e^{i\phi_g} \left(\cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} e^{i\phi_r} |1\rangle \right), \quad (24)$$

where ϕ_g is the global phase, and ϕ_r is the relative phase between the $|0\rangle$ and $|1\rangle$ states. Without comparing with another qubit, the phase ϕ_g does not have much meaning. The degrees of freedoms of a qubit are given by θ and ϕ_r , which correspond to a surface of a sphere. The space of a qubit is called the Bloch sphere.

Postulate 2: Temporal Evolution

The evolution of a closed quantum state is described by the unitary transformation.

The state $|\psi(t')\rangle$ is related to the state $|\psi(t)\rangle$ by

$$|\psi(t')\rangle = \hat{U}(t, t') |\psi(t)\rangle, \quad (25)$$

where $U(t, t')$ is a unitary operator (a matrix), $U^\dagger U = \mathbb{1}$.¹

The postulate comes from the conservation of total probabilities,

$$\langle \psi(t') | \psi(t') \rangle = \langle \psi(t) | \psi(t) \rangle = 1 \quad (26)$$

The unitary operator can be written as

¹For the sake of simplicity, I won't use a hat for an operator all the time unless there will be confusion.

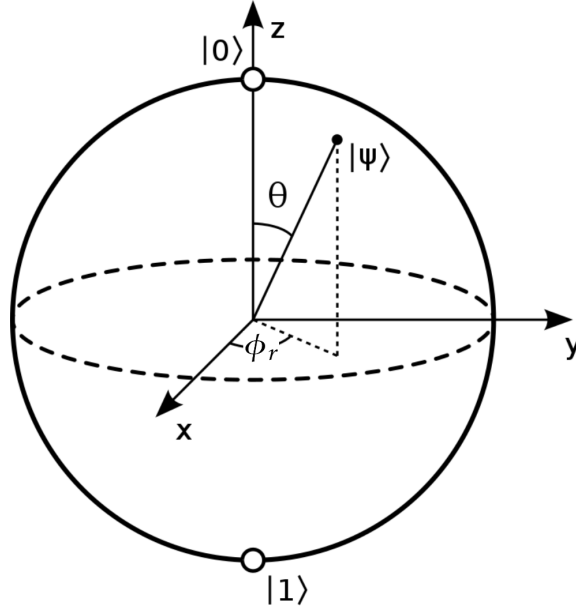


Figure 1: Bloch sphere.

$$U(t, t') = e^{-i\frac{\mathcal{H}}{\hbar}(t'-t)}, \quad (27)$$

where \mathcal{H} has to be hermitian, $\mathcal{H} = \mathcal{H}^\dagger$, to make $U(t', t)$ unitary.

Exercise 2: Exponential Function of Matrices

Show that the operator defined by Eq. (27) is unitary. Use the following facts,

- $e^A = \mathbb{1} + A + \frac{A^2}{2!} + \dots$
- $e^A e^B = e^{A+B}$ if $[A, B] \equiv AB - BA = 0$.
- $\mathcal{H} = \mathcal{H}^\dagger$

The postulate gives rise to the general form of the time-dependent Schrödinger's equation,

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \mathcal{H} |\psi\rangle. \quad (28)$$

The operator \mathcal{H} is called the “**Hamiltonian**” of the system. The Hamiltonian, coming from the classical mechanics, typically is the total energy of the system. For example, for a particle, the Hamiltonian $\mathcal{H} = \frac{p^2}{2m} + V(x)$. The case of a particle is only one of the examples. If the systems are discrete and finite (energy levels), the Hamiltonian is a finite-dimensional matrix. In the case of a qubit (or spin- $\frac{1}{2}$ system), the Hamiltonian is a 2 by 2 matrix.

The eigenvalue E_i of \mathcal{H} is the energy of the i th eigenstate $|E_i\rangle$,

$$\mathcal{H}|E_i\rangle = E_i|E_i\rangle. \quad (29)$$

The Hamiltonian in the energy bases $|E_i\rangle$ is diagonal

$$\mathcal{H} = \begin{pmatrix} E_1 & 0 & 0 & 0 \\ 0 & E_2 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & E_N \end{pmatrix}. \quad (30)$$

The solution of the time-dependent Schrödinger's equation (Eq. (28)) is

$$|\psi(t)\rangle = \sum_i \alpha_i e^{-i\frac{E_i}{\hbar}t} |E_i\rangle, \quad (31)$$

where α_i are the coefficients of the initial state in terms of $|E_i\rangle$.

Postulate 3: Measurement

Quantum measurement (collapse). A measure makes a system $|\psi\rangle$ collapse into some state $|\psi_i\rangle$. The possible outcome states $|\psi_i\rangle$ depend on the measurements. For example, if we measure the position of a particle, the outcome states are $|x\rangle$ with $-\infty < x < \infty$. A measurement is described by a set of operators $\{M_m\}$, where m denotes all the possible outcome states. After a measurement, the state becomes

$$\frac{M_m|\psi\rangle}{\sqrt{\langle\psi|M_m^\dagger M_m|\psi\rangle}} \quad (32)$$

with the probability

$$p(m) = \langle\psi|M_m^\dagger M_m|\psi\rangle. \quad (33)$$

The completeness theorem requires that

$$\sum_m M_m^\dagger M_m = \mathbb{1}. \quad (34)$$

For example, the measurement operator on a qubit are

$$M_0 = |0\rangle\langle 0| \quad (35)$$

$$M_1 = |1\rangle\langle 1| \quad (36)$$

Exercise 3: Qubit Measurement

The initial qubit state is $\frac{1}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle$.

1. What are the two possible states after a measurement of $\{M_0, M_1\}$?
2. What are the probabilities to be the above two states, respectively?

Heisenberg uncertainty principle

Postulate 4: Hermiticity

Any physical observables are Hermitian operators. For example, in the position basis, the position and momentum operators are

$$\hat{x} = x \quad (37)$$

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} \quad (38)$$

Let A be the physical observable operator. The expectation value of A of a state $|\psi\rangle$ is

$$\langle A \rangle = \langle \psi | A | \psi \rangle. \quad (39)$$

The state $|p\rangle$ is the eigenvector of the momentum operator \hat{p} ,

$$\hat{p}|p\rangle = p|p\rangle, \quad (40)$$

and for the position operator \hat{x} ,

$$\hat{x}|x\rangle = x|x\rangle. \quad (41)$$

Note that the eigenvectors of a Hermitian operator form a complete set of bases of the space.

The eigenvectors $|A_i\rangle$ of A forms a complete set of bases of the state space. The eigenstates are orthogonal and normal,

$$\langle A_j | A_i \rangle = \delta_{ij}. \quad (42)$$

That is, any state $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_i \alpha_i |A_i\rangle. \quad (43)$$

The completeness implies that the identity $\mathbb{1}$ is,

$$\mathbb{1} = \sum_i |A_i\rangle \langle A_i| \quad (44)$$

The standard deviation of A is $\sigma(A)$,

$$\sigma(A) \equiv \sqrt{\langle A \rangle^2 - \langle A^2 \rangle}. \quad (45)$$

Two operators A and B are compatible if their commutator $[A, B] \equiv AB - BA = 0$. Otherwise, they are incompatible. If

$$[A, B] = c \quad (46)$$

and c is a number, the general uncertainty principle reads

$$\sigma(A)\sigma(B) \geq \frac{|\langle \psi | [A, B] | \psi \rangle|}{2} = \frac{|c|}{2}. \quad (47)$$

Exercise 4: Uncertainty Principle

Prove the Heisenberg uncertainty principle, Eq. (47). Hint: use the Cauchy-Schwarz inequality.

$$\langle \psi | \psi \rangle \langle \phi | \phi \rangle \geq |\langle \psi | \phi \rangle|^2, \quad (48)$$

where $|\psi\rangle$ and $|\phi\rangle$ are two states.

The most classical example of the uncertainty principle is about x and p ,

$$[x, p] = i\hbar. \quad (49)$$

The uncertainty principle reads

$$\sigma(x)\sigma(p) \geq \frac{\hbar}{2}. \quad (50)$$

4 Quantum Dynamics: Schrödinger, Interaction, Heisenberg Pictures

In the experiments, we are interested in the dynamics of a observable A , more specifically, the expectation

$$\langle A(t) \rangle = \langle \psi(t) | A | \psi(t) \rangle \quad (51)$$

There are three main pictures to interpret and solve the problem.

4.1 Schrödinger Picture

Consider that the observable operator A is static and the states $|\psi(t)\rangle$ is evolving.

$$|\psi(t)\rangle \equiv |\psi(t)\rangle_S = e^{-\frac{i\mathcal{H}t}{\hbar}} |\psi(0)\rangle \quad (52)$$

The expectation value in this picture is

$$\langle A(t) \rangle = \langle \psi(t) | A | \psi(t) \rangle \quad (53)$$

4.2 Heisenberg Picture

Consider that the observable operator $A(t)$ is dynamic and the states $|\psi(t)\rangle$ is static.

$$A_h \equiv A(t) = e^{\frac{i\mathcal{H}t}{\hbar}} A e^{-\frac{i\mathcal{H}t}{\hbar}}, \quad (54)$$

and the expectation value is

$$\langle A(t) \rangle = \langle \psi(0) | A_h | \psi(0) \rangle. \quad (55)$$

The evolution of A_h follows the Heisenberg's equation,

$$i\hbar \frac{\partial A_h}{\partial t} = [A_h, \mathcal{H}]. \quad (56)$$

Exercise 5: Proof of the Heisenberg's equation

Let $U(t) = e^{-\frac{i\mathcal{H}t}{\hbar}}$ so that $A_h = U^\dagger A U$. Differentiating A_h with respect to t gives

$$\frac{\partial A_h}{\partial t} = \frac{\partial U^\dagger}{\partial t} A U + U^\dagger A \frac{\partial U}{\partial t} \quad (57)$$

First, show that the derivative of $U(t)$ is

$$i\hbar \frac{\partial}{\partial t} U(t) = \mathcal{H} U(t). \quad (58)$$

Use the two above equations to prove the Heisenberg's equation.

4.3 Interaction Picture

When the Hamiltonian includes two terms: one is the original Hamiltonian \mathcal{H}_0 and the interaction with the external system $V(t)$, it is convenient to use the interaction picture, where both

the states and the operator are evolving. The total Hamiltonian is $\mathcal{H} = \mathcal{H}_0 + V(t)$. The state $|\psi\rangle_I$ is

$$|\psi\rangle_I = e^{i\frac{\mathcal{H}_0 t}{\hbar}} |\psi(t)\rangle_S, \quad (59)$$

and the operator A_I is

$$A_I = e^{i\frac{\mathcal{H}_0 t}{\hbar}} A e^{-i\frac{\mathcal{H}_0 t}{\hbar}}, \quad (60)$$

The Schrödinger equation becomes

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle_I = V_I(t) |\psi\rangle_I, \quad (61)$$

$$V_I(t) \equiv e^{i\frac{\mathcal{H}_0 t}{\hbar}} V(t) e^{-i\frac{\mathcal{H}_0 t}{\hbar}}. \quad (62)$$

Note that the solution to Eq. (61) is not $|\psi(t)\rangle_I = e^{-i\frac{\mathcal{H}_I}{\hbar} t} |\psi(0)\rangle_I$ because the $V_I(t)$ is time-dependent. The solution to Eq. (61) is

$$|\psi(t)\rangle_I = U_I(t, t_0) |\psi(t_0)\rangle_I \quad (63)$$

$$U_I(t, t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^t V_I(t') U_I(t', t_0) dt' \quad (64)$$

The Heisenberg's equation becomes

$$i\hbar \frac{\partial A_I}{\partial t} = [A_I, \mathcal{H}_0]. \quad (65)$$

5 Harmonic Oscillators

The Hamiltonian of a simple harmonic oscillator is

$$\mathcal{H} = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}, \quad (66)$$

where $\omega = \sqrt{k/m}$ and k is the spring constant. We define the creation operator a^\dagger and the annihilation operator a ,

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{ip}{m\omega} \right), \quad (67)$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{ip}{m\omega} \right). \quad (68)$$

Exercise 6: Commutation Relation

Show that

$$[a, a^\dagger] = 1. \quad (69)$$

Use the relation $[x, p] = i\hbar$.

The Hamiltonian is rewritten as

$$\mathcal{H} = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) \quad (70)$$

$$= \hbar\omega \left(N + \frac{1}{2} \right) \quad (71)$$

where $N = a^\dagger a$ is the number operator. The eigenvector of N is $|n\rangle$

$$N|n\rangle = n|n\rangle, \quad (72)$$

where n is the eigenvalue. The number states are orthonormal

$$\langle m|n\rangle = \delta_{mn}. \quad (73)$$

Important identities are

$$[N, a] = -a, \quad (74)$$

$$[N, a^\dagger] = a^\dagger, \quad (75)$$

As a result, we have

$$N a^\dagger |n\rangle = (a^\dagger N + a^\dagger) |n\rangle = (n+1) a^\dagger |n\rangle, \quad (76)$$

$$N a |n\rangle = (a N - a) |n\rangle = (n-1) a |n\rangle, \quad (77)$$

These equations imply that

$$a |n\rangle = c_- |n-1\rangle, \quad (78)$$

$$a^\dagger |n\rangle = c_+ |n+1\rangle, \quad (79)$$

The constants c_- and c_+ can be fixed by noting that

$$\langle n|a^* a|n\rangle = n = |c_-|^2, \quad (80)$$

$$\langle n|a a^*|n\rangle = n+1 = |c_+|^2. \quad (81)$$

Taking c_- and c_+ to be positive by convention, $c_- = \sqrt{n}$ and $c_+ = \sqrt{n+1}$. We have the important relations which explain the names, creation and annihilation,

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad (82)$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \quad (83)$$

Note 1: Representation in the number basis

The number n is the number of the energy quanta. The smallest number of n is $n = 0$. The physical meaning of $|n\rangle$ is a state containing n energy quanta. Thus, $|n\rangle$ is called the **number state**. The energy of a harmonic oscillator is

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad (84)$$

The $\frac{1}{2}\hbar\omega$ is interpreted as the vacuum energy since it exists even when $n = 0$. Applying a creation operator on the $|n\rangle$, the state $|n\rangle$ becomes $\sqrt{n+1}|n+1\rangle$, that is, the a^\dagger will create one single quantum to the original state. Similarly, the a will annihilate one energy quantum from the system. We can also prove that

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle. \quad (85)$$

The position operator x and momentum operator p can be expressed as

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \quad (86)$$

$$p = i\sqrt{\frac{m\omega\hbar}{2}}(-a + a^\dagger) \quad (87)$$

5.1 Number States in the Position Bases

As the familiar wave function $\psi(x)$, we can express the $|n\rangle$ in the x bases. The wavefunctions are $\psi(x) \equiv \langle x|n\rangle$. Let's solve the ground states first $\psi_0(x)$. We start with

$$a|0\rangle = 0 \quad (88)$$

$$\Rightarrow \langle x|a|0\rangle = 0 \quad (89)$$

$$\Rightarrow \sqrt{\frac{m\omega}{2\hbar}} \left\langle x \left| x + \frac{ip}{m\omega} \right| 0 \right\rangle = 0 \quad (90)$$

$$\Rightarrow \left(x + \frac{\hbar}{m\omega} \frac{\partial}{\partial x} \right) \psi_0(x) = 0 \quad (91)$$

$$\Rightarrow \psi_0(x) = \frac{1}{\pi^{1/4} \sqrt{x_0}} e^{-\frac{1}{2} \left(\frac{x}{x_0} \right)^2}, \quad (92)$$

where $x_0 = \sqrt{\frac{\hbar}{m\omega}}$

Exercise 7: Uncertainty of the ground state

Show that for the ground state $\psi_0(x)$, the uncertainty relation has a equal sign, that is, the state has the minimum uncertainty,

$$\sigma(x)\sigma(p) = \frac{\hbar}{2}. \quad (93)$$

Using Eqs. (85) and (92), we obtain the expression for $\phi_n(x)$,

$$\psi_n(x) = \left(\frac{1}{\pi^{1/4} \sqrt{2^n n!} x_0^{n+1/2}} \right) \left(x - x_0^2 \frac{\partial}{\partial x} \right)^n e^{-\frac{1}{2} \left(\frac{x}{x_0} \right)^2}. \quad (94)$$

5.2 Dynamics of a Harmonic Oscillator

The Heisenberg's Equations of a and $a^\dagger(t)$ are

$$i\hbar \frac{da^\dagger}{dt} = [a^\dagger, H] = -\hbar\omega a^\dagger, \quad (95)$$

$$i\hbar \frac{da}{dt} = [a, H] = \hbar\omega a, \quad (96)$$

$$(97)$$

whose solutions are

$$a(t) = a(0)e^{-i\omega t}, \quad (98)$$

$$a^\dagger(t) = a^\dagger(0)e^{i\omega t}. \quad (99)$$

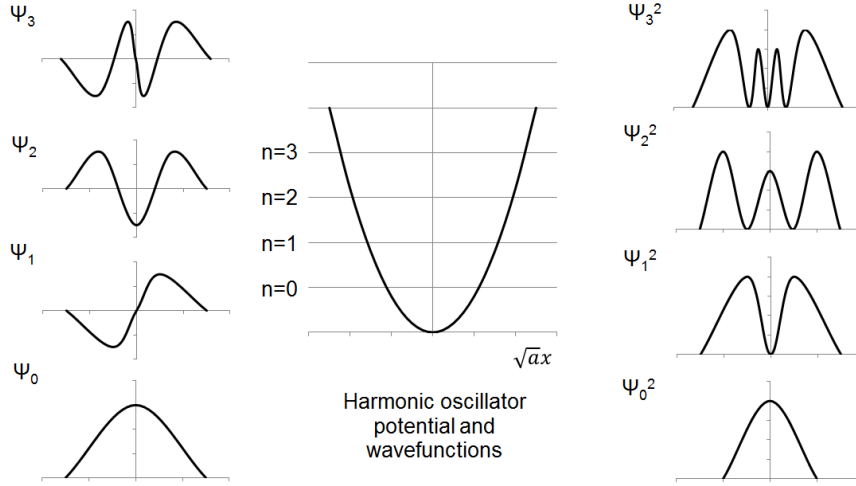


Figure 2: Wavefunction $\psi_n(x)$.

In terms of x and p , Eqs. (98) and (98) read

$$a(t) = x(t) + \frac{ip(t)}{m\omega} = \left(x(0) + \frac{ip(0)}{m\omega} \right) e^{-i\omega t}, \quad (100)$$

$$a^\dagger(t) = x(t) - \frac{ip(t)}{m\omega} = \left(x(0) - \frac{ip(0)}{m\omega} \right) e^{i\omega t}. \quad (101)$$

Solving the equations for $x(t)$ and $p(t)$, we have

$$x(t) = x(0) \cos \omega t + \frac{p(0)}{m\omega} \sin \omega t, \quad (102)$$

$$p(t) = -m\omega x(0) \sin \omega t + p(0) \cos \omega t. \quad (103)$$

Note 2: Heisenberg picture of x and p of a harmonic oscillator

Equations (102) and (103) are exactly the same as the equations of motion derived from the classical mechanics. In contrast, $x(0)$ and $p(0)$ are operators. If we take the number state $|n\rangle$, the expectation value $\langle n|x(t)|n\rangle$ vanishes. We will not observe a expectation value $\langle x(t) \rangle$ obeying the classical motion. It turns out that the state mostly close to a classical state is the coherent state $|\lambda\rangle$, which is the eigenvector of the annihilation operator a ,

$$a|\lambda\rangle = \lambda|\lambda\rangle. \quad (104)$$

We will talk more about the coherent states later.

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