# Quantum Mechanics

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# III. Quantum Dynamics

## 3.1 Time Evolution and Schrödinger Equation

In quantum mechanics, time is just a parameter, not an operator like position.

### 3.1.1 Time-Evolution Operator

**Time-evolution operator:** $\mathscr{U}(t,t_0)$ evolves a state ket $|\alpha\rangle$ at time $t_0$ to a new state ket at a later time $t > t_0$:

$$|\alpha,t_0;t\rangle = \mathscr{U}(t,t_0)|\alpha,t_0\rangle . \tag{3.1}$$

Expanding the state kets in terms of the eigenkets of an observable $A$:

$$|\alpha,t_0\rangle = \sum_{a'} c_{a'}(t_0)|a'\rangle \tag{3.2}$$

and

$$|\alpha,t_0;t\rangle = \sum_{a'} c_{a'}(t_0)|a'\rangle , \tag{3.3}$$

Then the probability conservation requirement leads to

$$\sum_{a'} |c_{a'}(t_0)|^2 = \sum_{a'} |c_{a'}(t)|^2 . \tag{3.4}$$

The basic properties of the time-evolution operator:

(1) Unitarity:

$$\mathscr{U}^\dagger(t,t_0)\mathscr{U}(t,t_0) = 1 . \tag{3.5}$$

(2) Composition:

$$\mathscr{U}(t_2,t_0) = \mathscr{U}(t_2,t_1)\mathscr{U}(t_1,t_0) \quad (t_2 > t_1 > t_0) . \tag{3.6}$$

(3) Continuity: The infinitesimal time-evolution operator $\mathscr{U}(t_0 + \mathrm{d}t, t_0)$ satisfies

$$\lim_{\mathrm{d}t\to 0} \mathscr{U}(t_0 + \mathrm{d}t, t_0) = 1 . \tag{3.7}$$

Similar to the positional translation operator, we assert that the above requirements can all be satisfies by setting

$$\mathscr{U}(t_0 + \mathrm{d}t, t_0) = 1 - i\Omega \mathrm{d}t , \tag{3.8}$$

where $\Omega$, with the dimension of frequency or inverse time, is a Hermitian operator,

$$\Omega^{\dagger}=\Omega . \tag{3.9}$$

By borrowing from classical mechanics that the Hamiltonian is the generator of time evolution, $\Omega$ can be related to the Hamiltonian operator $H$ by

$$\Omega=\frac{H}{\hbar} . \tag{3.10}$$

Putting the above equation into Eq. (3.8), we obtain

$$\mathscr{U}\left(t_0+\mathrm{d}t, t_0\right)=1-\frac{iH\mathrm{d}t}{\hbar} . \tag{3.11}$$

### 3.1.2 The Schrödinger Equation

From Eq. (3.6), we can get

$$\mathscr{U}\left(t+\mathrm{d}t, t_0\right)=\mathscr{U}\left(t+\mathrm{d}t, t\right)\mathscr{U}\left(t, t_0\right)=\left(1-\frac{iH\mathrm{d}t}{\hbar}\right)\mathscr{U}\left(t, t_0\right), \tag{3.12}$$

which is

$$\mathscr{U}\left(t+\mathrm{d}t, t_0\right)-\mathscr{U}\left(t, t_0\right)=-i\frac{H}{\hbar}\mathrm{d}t\mathscr{U}\left(t, t_0\right), \tag{3.13}$$

whose differential equation form is the **Schrödinger equation for the time-evolution operator**:

$$i\hbar\frac{\partial}{\partial t}\mathscr{U}\left(t, t_0\right)=H\mathscr{U}\left(t, t_0\right) . \tag{3.14}$$

Multiplying both sides by $\left|\alpha, t_0\right\rangle$ on the right, we obtain

$$i\hbar\frac{\partial}{\partial t}\mathscr{U}\left(t, t_0\right)\left|\alpha, t_0\right\rangle=H\mathscr{U}\left(t, t_0\right)\left|\alpha, t_0\right\rangle . \tag{3.15}$$

By applying Eq. (3.1), the above equation becomes

$$i\hbar\frac{\partial}{\partial t}\left|\alpha, t_0; t\right\rangle=H\left|\alpha, t_0; t\right\rangle, \tag{3.16}$$

which is the **Schrödinger equation for a state ket**.

Considering the time dependency of *H* operator, there are three cases for the solution to Eq. (3.15):

(1) *H* is time independent. By Taylor expansion, we may easily verify that

$$\mathscr{U}\left(t, t_0\right)=\exp\left[\frac{-iH\left(t-t_0\right)}{\hbar}\right]. \tag{3.17}$$

(2) *H* is time dependent but the *H* at different times commute. The following solution can be verified by replacing $H\left(t-t_0\right)$ in (1) by $\int_{t_0}^{t}\mathrm{d}t' H\left(t'\right)$:

$$\mathscr{U}\left(t, t_0\right)=\exp\left[\frac{-i}{\hbar}\int_{t_0}^{t}\mathrm{d}t' H\left(t'\right)\right]. \tag{3.18}$$

(3) *H* is time dependent but the *H* at different times do not commute. The following solution, know as the **Dyson series**, will be proved in a later chapter:

$$\mathscr{U}\left(t, t_0\right)=1+\sum_{n=1}^{\infty}\left(-\frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\cdots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n H\left(t_1\right)H\left(t_2\right)\cdots H\left(t_n\right)\right). \tag{3.19}$$

### 3.1.3 Energy Eigenkets

If an observable A commutes with the Hamiltonian operator $H$:

$$[A,H]=0\,, \tag{3.20}$$

The eigenkets of $A$ are also the **energy eigenkets** of $H$, whose eigenvalues are denoted by $E_{a'}$ :

$$H\left|a'\right\rangle = E_{a'}\left|a'\right\rangle. \tag{3.21}$$

Taking $t_0=0$ for simplicity, we can expand the time-evolution operator in terms of $\left|a'\right\rangle\left\langle a'\right|$ :

$$\exp\left(-\frac{iHt}{\hbar}\right)=\sum_{a'}\sum_{a''}\left|a''\right\rangle\left\langle a''\right|\exp\left(-\frac{iHt}{\hbar}\right)\left|a'\right\rangle\left\langle a'\right|\,, \tag{3.22}$$

which enables to solve any initial-value problem once the expansion of the initial ket in terms of $\left\{\left|a'\right\rangle\right\}$ is known. That is, if

$$\left|\alpha,t_0=0\right\rangle=\sum_{a'}\left|a'\right\rangle\left\langle a'\middle|\alpha\right\rangle=\sum_{a'}c_{a'}\left|a'\right\rangle, \tag{3.23}$$

We then have

$$\left|\alpha,t_0=0;t\right\rangle=\exp\left(-\frac{iHt}{\hbar}\right)\left|\alpha,t_0=0\right\rangle=\sum_{a'}\left|a'\right\rangle c_{a'}\exp\left(-\frac{iE_{a'}t}{\hbar}\right). \tag{3.24}$$

So the expansion coefficient changes with time as

$$c_{a'}(t)=c_{a'}(0)\exp\left(-\frac{iE_{a'}t}{\hbar}\right). \tag{3.25}$$

A special case is that the initial state is an eigenket itself:

$$\left|\alpha,t_0=0\right\rangle=\left|a'\right\rangle, \tag{3.26}$$

then

$$\left|\alpha,t_0=0;t\right\rangle=\left|a'\right\rangle\exp\left(-\frac{iE_{a'}t}{\hbar}\right), \tag{3.27}$$

which means that if the system is initially at a simultaneous eigenstate of $A$ and $H$, it remains so at all times.

If there are multiple mutually compatible observables all also commute with $H$:

$$\begin{gathered}[A,B]=[B,C]=[A,C]=\cdots=0\\ [A,H]=[B,H]=[C,H]=\cdots=0\end{gathered}, \tag{3.28}$$

then the time-evolution operator is

$$\exp\left(-\frac{iHt}{\hbar}\right)=\sum_{K'}\left|K'\right\rangle\exp\left(-\frac{iE_{K'}t}{\hbar}\right)\left\langle K'\right|, \tag{3.29}$$

where

$$\left|K'\right\rangle=\left|a',b',c',\cdots\right\rangle. \tag{3.30}$$

### 3.1.4 Time Dependence of Expectation Values

The expectation value of another observable $B$ unnecessarily commutable with either $A$ or $H$ is given by

$$\begin{aligned}\langle B\rangle &= \left(\langle a'|\mathscr{U}^{\dagger}(t,0)\right)\cdot B\cdot\left(\mathscr{U}(t,0)|a'\rangle\right)\\ &= \langle a'|\exp\left(\frac{iE_{a'}t}{\hbar}\right)B\exp\left(-\frac{iE_{a'}t}{\hbar}\right)|a'\rangle \quad ,\\ &= \langle a'|B|a'\rangle\end{aligned} \tag{3.31}$$

which is independent of time. Therefore, an energy eigenstate is referred to as a **stationary state**.

If initially we have

$$|\alpha, t_0 = 0\rangle = \sum_{a'} c_{a'}|a'\rangle\,, \tag{3.32}$$

the expectation value with respect to a superposition of energy eigenstates, or a **nonstationary state** can be computed as

$$\begin{aligned}\langle B\rangle &= \left[\sum_{a'} c_{a'}^{*}\langle a'|\exp\left(\frac{iE_{a'}t}{\hbar}\right)\right]\cdot B\cdot\left[\sum_{a''} c_{a''}\exp\left(-\frac{iE_{a''}t}{\hbar}\right)|a''\rangle\right]\\ &= \sum_{a'}\sum_{a''} c_{a'}^{*}c_{a''}\langle a'|B|a''\rangle\exp\left[-\frac{i\left(E_{a''}-E_{a'}\right)t}{\hbar}\right]\end{aligned}, \tag{3.33}$$

which means that the expectation value consists of oscillating terms whose angular frequencies are determined by **N. Bohr's frequency condition**

$$\omega_{a''a'} = \frac{\left(E_{a''}-E_{a'}\right)}{\hbar}\,. \tag{3.34}$$

### 3.1.5 Correlation Amplitude and the Energy-Time Uncertainty Relation

**Correlation amplitude**:

$$C(t) = \langle \alpha, t_0 = 0|\alpha, t_0 = 0; t\rangle = \langle\alpha|\mathscr{U}(t,0)|\alpha\rangle\,, \tag{3.35}$$

which quantitatively measures the "resemblance" of the state kets at different times.

When the initial ket is an energy eigenket, then

$$C(t) = \langle a', t_0 = 0|a', t_0 = 0; t\rangle = \exp\left(-\frac{iE_{a'}t}{\hbar}\right), \tag{3.36}$$

indicating that the modulus of the correlation amplitude for a stationary state is unity at all times.

When the initial ket is represented by a superposition of the energy eigenkets, then

$$C(t) = \left(\sum_{a'} c_{a'}^{*}\langle a'|\right)\left[\sum_{a''} c_{a''}\exp\left(-\frac{iE_{a''}t}{\hbar}\right)|a''\rangle\right] = \sum_{a'}|c_{a'}|^2\exp\left(-\frac{iE_{a'}t}{\hbar}\right), \tag{3.37}$$

which decreases in magnitude with time due to a strong cancellation among different terms.

Let us suppose that the state ket can be regarded as a superposition of so many energy eigenkets with similar energies that we can regard them as exhibiting a quasi-continuous spectrum, then the sum in Eq. (3.37) can be replaced by the integral

$$\sum_{a'} \to \int \mathrm{d}E\,\rho(E), \quad c_{a'} \to g(E)\big|_{E=E_{a'}} \tag{3.38}$$

to get

$$C(t) = \int \mathrm{d}E\,|g(E)|^2\,\rho(E)\exp\left(-\frac{iEt}{\hbar}\right), \tag{3.39}$$

subject to the normalization condition

$$\int \mathrm{d}E\,|g(E)|^2\,\rho(E) = 1\,, \tag{3.40}$$

where $\rho(E)$ is the density of energy eigenstates.

In a realistic physical situation, $|g(E)|^2 \rho(E)$ may be peaked around $E = E_0$ with width $\Delta E \sim |E - E_0|$, then Eq. (3.39) can be written as

$$C(t) = \exp\left(-\frac{iE_0 t}{\hbar}\right)\int \mathrm{d}E |g(E)|^2 \rho(E) \exp\left(-\frac{i(E-E_0)t}{\hbar}\right), \tag{3.41}$$

whose modulus starts becoming appreciably different from 1 when

$$t \simeq \frac{\hbar}{\Delta E}, \tag{3.42}$$

Which leads to the **Energy-time uncertainty relation**:

$$\Delta t \Delta E \simeq \hbar . \tag{3.43}$$

However, it is of a very different nature from the uncertainty relation between two incompatible observables introduced before.

# 3.2 Elementary Solutions to Schrödinger's Wave Equation

### 3.2.1 Time-Dependent Wave Equation

For a wave function

$$\psi(\mathbf{x}', t) = \langle \mathbf{x}' | \alpha, t_0; t \rangle, \tag{3.44}$$

by applying $\langle \mathbf{x}' |$ to Eq. (3.16), we obtain

$$i\hbar \frac{\partial}{\partial t} \langle \mathbf{x}' | \alpha, t_0; t \rangle = \langle \mathbf{x}' | H | \alpha, t_0; t \rangle, \tag{3.45}$$

where the Hamiltonian is postulated to have the same form as in the classical mechanics:

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}). \tag{3.46}$$

Therefore, we have the **time-dependent Schrödinger's wave equation**

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{x}', t) = -\frac{\hbar^2}{2m}\nabla'^2 \psi(\mathbf{x}', t) + V(\mathbf{x}')\psi(\mathbf{x}', t). \tag{3.47}$$

The quantum mechanics based on this wave equation is known as **wave mechanics**.

### 3.2.2 Time-Independent Wave Equation

As shown in Eq. (3.25), the time evolution of a stationary state can be express as

$$\psi(\mathbf{x}', t) = \langle \mathbf{x}' | a', t_0; t \rangle = \langle \mathbf{x}' | a' \rangle \exp\left(-\frac{iE_{a'} t}{\hbar}\right). \tag{3.48}$$

Substituting it into Eq. (3.47), we have

$$-\frac{\hbar^2}{2m}\nabla'^2 \langle \mathbf{x}' | a' \rangle + V(\mathbf{x}') \langle \mathbf{x}' | a' \rangle = E_{a'} \langle \mathbf{x}' | a' \rangle . \tag{3.49}$$

Because we may always choose the observable $A$ to be that function of the observables $\mathbf{x}$ and $\mathbf{p}$

which coincides with $H$ itself, we may therefor simplify the above equation to be the **time-independent Schrödinger's wave equation**

$$-\frac{\hbar^2}{2m}\nabla'^2 u_E\left(\mathbf{x}'\right)+V\left(\mathbf{x}'\right)u_E\left(\mathbf{x}'\right)=Eu_E\left(\mathbf{x}'\right). \tag{3.50}$$

To solve this equation, some boundary condition has to be imposed. Suppose we seek a solution with

$$E<\lim_{|\mathbf{x}'|\to\infty}V\left(\mathbf{x}'\right), \tag{3.51}$$

whose appropriate boundary condition to be used is

$$u_E\left(\mathbf{x}'\right)\to 0 \quad \text{as} \quad \left|\mathbf{x}'\right|\to\infty . \tag{3.52}$$

Because Eq. (3.50) with this boundary condition allows nontrivial solutions only for a discrete set of $E$, it yields the *quantization of energy levels*.

### 3.2.3 Interpretations of the Wave Function

**Probability density:**

$$\rho\left(\mathbf{x}',t\right)=\left|\psi\left(\mathbf{x}',t\right)\right|^2=\left|\left\langle\mathbf{x}'\middle|\alpha,t_0;t\right\rangle\right|^2. \tag{3.53}$$

Below we use $\mathbf{x}$ for $\mathbf{x}'$ because the position operator will not appear. From Eq. (3.47), we may obtain the **continuity equation**

$$\frac{\partial\rho}{\partial t}+\nabla\cdot\mathbf{j}=0 \tag{3.54}$$

when the potential $V$ is real, where the **probability flux**

$$\begin{aligned}\mathbf{j}\left(\mathbf{x},t\right)&=-\left(\frac{i\hbar}{2m}\right)\left[\psi^*\nabla\psi-\left(\nabla\psi^*\right)\psi\right]\\&=\left(\frac{\hbar}{m}\right)\mathrm{Im}\left(\psi^*\nabla\psi\right)\end{aligned}. \tag{3.55}$$

Taking the integration of the above equation for the whole space, we obtain

$$\int \mathrm{d}^3x\,\mathbf{j}\left(\mathbf{x},t\right)=\frac{\left\langle\mathbf{p}\right\rangle_t}{m}, \tag{3.56}$$

where $\left\langle\mathbf{p}\right\rangle_t$ is the expectation value of the momentum operator at time $t$. If we write the wave function as

$$\psi\left(\mathbf{x},t\right)=\sqrt{\rho\left(\mathbf{x},t\right)}\exp\left[\frac{iS\left(\mathbf{x},t\right)}{\hbar}\right] \tag{3.57}$$

with $S$ real and $\rho>0$, we then have

$$\psi^*\nabla\psi=\sqrt{\rho}\nabla\sqrt{\rho}+\left(\frac{i}{\hbar}\right)\rho\nabla S . \tag{3.58}$$

By putting the above equation into Eq. (3.55), we obtain

$$\mathbf{j}=\frac{\rho\nabla S}{m}, \tag{3.59}$$

which means that the *spatial variation of the phase* of the wave function characterizes the probability flux. For a plane wave, which is a momentum eigenfunction,

$$\psi(\mathbf{x},t) \propto \exp\left(\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x} - i\frac{Et}{\hbar}\right), \tag{3.60}$$

where **p** stands for the eigenvalue of the momentum operator.

We may define a kind of "velocity"

$$\mathbf{v} = \frac{\nabla S}{m} \tag{3.61}$$

to rewrite Eq. (3.54) to be

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0\,, \tag{3.62}$$

just as in fluid dynamics.

### 3.2.4 The Classical Limit

By substituting Eq. (3.57) into both sides of Eq. (3.47), we obtain

$$\begin{aligned} &-\frac{\hbar^2}{2m}\left[\nabla^2\sqrt{\rho} + \frac{2i}{\hbar}\left(\nabla\sqrt{\rho}\right)\cdot\nabla S - \frac{1}{\hbar^2}\sqrt{\rho}\left|\nabla S\right|^2 + \frac{i}{\hbar}\sqrt{\rho}\nabla^2 S\right] + \sqrt{\rho}V \\ &= i\hbar\left[\frac{\partial\sqrt{\rho}}{\partial t} + \frac{i}{\hbar}\sqrt{\rho}\frac{\partial S}{\partial t}\right] \end{aligned}. \tag{3.63}$$

Assuming $\hbar$ is so small that

$$\hbar\left|\nabla^2 S\right| \ll \left|\nabla S\right|^2, \tag{3.64}$$

Eq. (3.63) is then approximated to be the **Hamilton-Jacobi equation** in classical mechanics:

$$\frac{1}{2m}\left|\nabla S(\mathbf{x},t)\right|^2 + V(\mathbf{x}) + \frac{\partial S(\mathbf{x},t)}{\partial t} = 0 \tag{3.65}$$

where $S(\mathbf{x},t)$ stands for Hamilton's principal function.

### 3.2.5 Free Particle in Three Dimensions

A free particle has the potential operator $V(\mathbf{x}) = 0$, so Eq. (3.50) becomes

$$\nabla^2 u_E(\mathbf{x}) = -\frac{2mE}{\hbar^2}u_E(\mathbf{x}). \tag{3.66}$$

Define the **wave vector**

$$\mathbf{k}^2 = k_x^2 + k_y^2 + k_z^2 = \frac{2mE}{\hbar^2} = \frac{\mathbf{p}^2}{\hbar^2} \tag{3.67}$$

that is,

$$\mathbf{p} = \hbar\mathbf{k}\,. \tag{3.68}$$

Eq. (3.66) can be solved by the technique known as "separation of variables". Writing

$$u_E(\mathbf{x}) = u_x(x)u_y(y)u_z(z), \tag{3.69}$$

Eq. (3.66) becomes

$$\left(\frac{1}{u_x}\frac{\mathrm{d}^2 u_x}{\mathrm{d}x^2} + k_x^2\right) + \left(\frac{1}{u_y}\frac{\mathrm{d}^2 u_y}{\mathrm{d}y^2} + k_y^2\right) + \left(\frac{1}{u_z}\frac{\mathrm{d}^2 u_z}{\mathrm{d}z^2} + k_z^2\right) = 0\,, \tag{3.70}$$

whose solution in each dimension is $u_w(w) = c_w \exp(ik_w w)$ for $w = x, y, z$. Therefore, the total solution is

$$u_E(\mathbf{x}) = C \exp(i\mathbf{k}\cdot\mathbf{x}), \tag{3.71}$$

where $C = c_x c_y c_z$ can be normalized by a cubic "big box" with the periodic boundary condition (PBC) whose side length $L \to \infty$. With the PBC, we have

$$k_x = \frac{2\pi}{L} n_x, \quad k_y = \frac{2\pi}{L} n_y, \quad k_z = \frac{2\pi}{L} n_z, \tag{3.72}$$

and the normalization criterion becomes

$$1 = \int_0^L \mathrm{d}x \int_0^L \mathrm{d}y \int_0^L \mathrm{d}z u_E^*(x) u_E(x) = L^3 |C|^2. \tag{3.73}$$

The above equation tells us that $C = 1/L^{3/2}$, so

$$u_E(\mathbf{x}) = \frac{1}{L^{3/2}} \exp(i\mathbf{k}\cdot\mathbf{x}). \tag{3.74}$$

The energy eigenvalue is

$$E = \frac{\mathbf{p}^2}{2m} = \frac{\hbar^2 \mathbf{k}^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 \left(n_x^2 + n_y^2 + n_z^2\right). \tag{3.75}$$

Considering a spherical shell in $\mathbf{k}$ space with radius $|\mathbf{k}| = \frac{2\pi}{L}|\mathbf{n}|$ and thickness $\mathrm{d}|\mathbf{k}| = \frac{2\pi}{L}\mathrm{d}|\mathbf{n}|$, all states within this shell have the same energy $E = \frac{\hbar^2 \mathbf{k}^2}{2m}$. Then the density of states

$$\frac{\mathrm{d}N}{\mathrm{d}E} = \frac{4\pi \mathbf{n}^2 \mathrm{d}|\mathbf{n}|}{\hbar^2 |\mathbf{k}| \mathrm{d}|\mathbf{k}| / m} = \frac{4\pi m}{\hbar^2}\left(\frac{L}{2\pi}\right)^3 |\mathbf{k}| = \sqrt{\frac{m^3 E}{2}} \frac{L^3}{\pi^2 \hbar^3}. \tag{3.76}$$

With the "big box" normalization, Eq. (3.60) for the free particle becomes

$$\psi(\mathbf{x}, t) = \frac{1}{L^{3/2}} \exp\left(\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x} - i\frac{Et}{\hbar}\right), \tag{3.77}$$

and according to Eq. (3.55), we have

$$\mathbf{j}(\mathbf{x}, t) = \frac{\hbar}{m} \mathrm{Im}\left(\psi^* \nabla \psi\right) = \frac{\hbar \mathbf{k}}{m L^3} = \mathbf{v}\rho, \tag{3.78}$$

where $\rho = 1/L^3$ is the probability density.

### 3.2.6 Time Evolution of Wave Packets

The superposition of plane waves leads to the wave-packet description, whose density is non-zero in a limited space. In the one-dimensional case, the wave functions in the position and momentum spaces are connected by a Fourier transform:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(k) \exp(ikx) \mathrm{d}k, \tag{3.79}$$

whose inverse transform is

$$\psi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) \exp(-ikx) \mathrm{d}x. \tag{3.80}$$

For instance, the Gaussian wave packet

$$\psi(x) = \exp\left(-\frac{1}{2}a^2x^2\right), \tag{3.81}$$

whose probability distribution is

$$\left|\psi(x)\right|^2 = \exp\left(-a^2x^2\right). \tag{3.82}$$

The width in the position space is approximately

$$\Delta x \sim 1/a. \tag{3.83}$$

The corresponding wave packet in the momentum is just the Fourier transform of Eq. (3.81):

$$\psi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}a^2x^2 - ikx\right)\mathrm{d}x = \frac{1}{\alpha}\exp\left(-\frac{k^2}{2a^2}\right), \tag{3.84}$$

which is also a Gaussian distribution with a width of

$$\Delta k \sim a. \tag{3.85}$$

Therefore, we have

$$\Delta x \cdot \Delta k \sim 1, \tag{3.86}$$

which is true for all kinds of wave packets.

A plane wave evolving with time

$$\psi_k(x,t) = \exp\left[i(kx - \omega t)\right] \tag{3.87}$$

has the phase velocity

$$u = \omega / k. \tag{3.88}$$

For the electromagnetic wave in vacuum,

$$\omega = ck = 2\pi c / \lambda. \tag{3.89}$$

So

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \psi(k)\exp\left[ik(x - ct)\right]\mathrm{d}k. \tag{3.90}$$

The group velocity is also $c$, the same as the phase velocity. Therefore, the shape of the wave packet does not change.

For the electromagnetic wave in a dispersive medium,

$$\omega = 2\pi c / \lambda n(\lambda). \tag{3.91}$$

So

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \psi(k)\exp\left[i\left(kx - \omega(k)t\right)\right]\mathrm{d}k. \tag{3.92}$$

The center of the wave packet can be determined by

$$\frac{\partial\left(kx - \omega(k)t\right)}{\partial k} = 0, \tag{3.93}$$

which leads to

$$x_\mathrm{c} = \left(\frac{\mathrm{d}\omega}{\mathrm{d}k}\right)t, \tag{3.94}$$

so the group velocity of the wave packet is

$$v_\mathrm{g} = \frac{\mathrm{d}x_\mathrm{c}}{\mathrm{d}t} = \frac{\mathrm{d}\omega}{\mathrm{d}k}. \tag{3.95}$$

For the non-relativistic de Broglie wave,

$$\omega = \hbar k^2 / 2m \, . \tag{3.96}$$

Its phase velocity is

$$u = \omega / k \, , \tag{3.97}$$

different from its group velocity

$$v_{\mathrm{g}} = \mathrm{d}\omega / \mathrm{d}k = \hbar k / m = 2u \, . \tag{3.98}$$

The time-evolution of the wave packet depends on the formulation of $\omega(k)$. Supposing $\psi(k)$ sharply distributes around $k_0$, we may then do the Taylor expansion:

$$\begin{aligned} \omega(k) &= \omega(k_0) + \left(\frac{\mathrm{d}\omega}{\mathrm{d}k}\right)_{k_0}(k-k_0) + \frac{1}{2}\left(\frac{\mathrm{d}^2\omega}{\mathrm{d}k^2}\right)_{k_0}(k-k_0)^2 + \cdots \\ &\approx \omega_0 + v_{\mathrm{g}}(k-k_0) + \frac{1}{2}\beta(k-k_0)^2 \end{aligned} , \tag{3.99}$$

where $\beta \equiv \left(\frac{\mathrm{d}^2\omega}{\mathrm{d}k^2}\right)_{k_0}$. Putting this into Eq. (3.92), we have

$$\begin{aligned} \psi(x,t) &\approx \frac{\exp(-i\omega_0 t)}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(k) \exp\left[i\left(kx - v_{\mathrm{g}}(k-k_0)t - \frac{1}{2}\beta(k-k_0)^2 t\right)\right]\mathrm{d}k \\ &= \exp\left[i(k_0 x - \omega_0 t)\right] \int_{-\infty}^{\infty} \psi(\xi + k_0) \exp\left[i\left(\xi(x - v_{\mathrm{g}}t) - \frac{1}{2}\beta\xi^2 t\right)\right]\mathrm{d}\xi \end{aligned} , \tag{3.100}$$

where $\xi \equiv k - k_0$.

Let us again look into the example of the Gaussian wave packet. For Eq. (3.84), $k_0 = 0$, so

$$\begin{aligned} \psi(x,t) &= \frac{\exp(-i\omega_0 t)}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left[ik(x - v_{\mathrm{g}}t) - \frac{k^2}{2}\left(i\beta t + 1/a^2\right)\right]\mathrm{d}k \\ &\approx \exp(-i\omega_0 t) \frac{a}{\sqrt{1 + i\beta a^2 t}} \exp\left[-\frac{(x - v_{\mathrm{g}}t)^2 a^2}{2(1 + i\beta a^2 t)}\right] \end{aligned} . \tag{3.101}$$

The probability density is

$$|\psi(x,t)|^2 = \frac{a^2}{\sqrt{1 + \beta^2 a^4 t^2}} \exp\left[-\frac{(x - v_{\mathrm{g}}t)^2 a^2}{(1 + \beta^2 a^4 t^2)}\right]. \tag{3.102}$$

So the wave-packet width in the position space is

$$\Delta x \approx \frac{\sqrt{1 + \beta^2 a^4 t^2}}{a} \, . \tag{3.103}$$

If we prepare the wave packet to have the width of $\Delta x_0 = 1/a$, then at time $t$, the width becomes

$$\Delta x \approx \Delta x_0 \sqrt{1 + \beta^2 t^2 / (\Delta x_0)^4} \, . \tag{3.104}$$

Therefore, when $t \ll \Delta x_0^2 / \beta$, the width of the wave packet keeps roughly unchanged. However, it expands significantly after $t > \Delta x_0^2 / \beta$.

For a de Broglie wave, because

$$\omega = \hbar k^2 / 2m$$
$$\beta = \frac{\mathrm{d}^2\omega}{\mathrm{d}k^2} = \frac{\hbar}{m} \neq 0 , \tag{3.105}$$

its width in the position space expands with time.

### 3.2.7 The Rigid-Wall Potential

The rigid-wall potential is

$$V(x) = \begin{cases} \infty, & |x| > a \\ 0, & |x| < a \end{cases} . \tag{3.106}$$

The Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + V(x)\psi(x) = E\psi(x) . \tag{3.107}$$

We divide the whole space into three regions: (1) $x < -a, \quad V \to \infty$; (2) $-a < x < a, \quad V = 0$; (3) $x > a, \quad V \to \infty$. In the first region, the solution of the above equation is

$$\psi_1(x) = C_1 \exp\left(\sqrt{2m(V-E)}x/\hbar\right) + C_2 \exp\left(-\sqrt{2m(V-E)}x/\hbar\right). \tag{3.108}$$

The first term in Eq. (3.108) tends to 0 because *x* is negative, while $C_2$ must be zero, otherwise the second term diverges. Therefore, the wave function in the first region $\psi_1 = 0$. It is the same as in region 3 with $\psi_3 = 0$. In the second region, the solution of Eq. (3.107) is

$$\psi_2(x) = C_1 \exp(ikx) + C_2 \exp(-ikx) = A_1 \sin(kx + \delta) \tag{3.109}$$

if $k = \sqrt{2mE}/\hbar > 0$ and

$$\psi_2(x) = A_2 x + B \tag{3.110}$$

if $k = 0$.

Because the wave function should be continuous in the whole region, it is required that

$$\psi_2(-a) = \psi_1(-a), \quad \psi_2(a) = \psi_3(a). \tag{3.111}$$

With this boundary condition, the solution of Eq. (3.110) is $\psi_2 = 0$, which is unphysical; the solution of Eq. (3.109) leads to

$$\begin{aligned} A\sin(-ka+\delta) &= 0 \\ A\sin(ka+\delta) &= 0 \end{aligned} . \tag{3.112}$$

The meaningful solution should have $A \neq 0$, so

$$\begin{aligned} -ka + \delta &= n_1 \pi \\ ka + \delta &= n_2 \pi \end{aligned}, \tag{3.113}$$

where $n_1, n_2$ are integer numbers. We thus have

$$2ka = (n_2 - n_1)\pi = n\pi \tag{3.114}$$

and

$$\delta = \frac{(n_1 + n_2)}{2}\pi = \frac{n'}{2}\pi \tag{3.115}$$

The energy eigenvalues are then

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{8ma^2}, \tag{3.116}$$

where $n = 1, 2, 3, \cdots$. The corresponding eigenfunctions are

$$\begin{aligned} \phi_n(x) &= A\sin\left[\left(\frac{n\pi}{2a}\right)x + \frac{n'}{2}\pi\right] = A\sin\left[\left(\frac{n\pi}{2a}\right)(x+a) + n'\pi\right] \\ &= \pm A\sin\left[n\pi\left(\frac{x+a}{2a}\right)\right] \end{aligned}. \tag{3.117}$$

The minus sign does not matter because the phase-factor difference is meaningless for a wave function. The normalization requirement

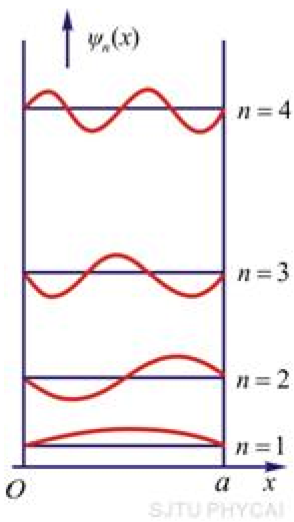
$$\int_{-a}^{a} \phi_n^*(x)\phi_n(x) = 1 \tag{3.118}$$

leads to

$$A = \frac{1}{\sqrt{a}}. \tag{3.119}$$

Therefore, the eigenfunction is

$$\phi_n(x) = \begin{cases} \dfrac{1}{\sqrt{a}}\sin\left[n\pi\left(\dfrac{x+a}{2a}\right)\right], & |x| < a \\ 0, & |x| > a \end{cases}. \tag{3.120}$$



### 3.2.8 The Square-Well Potential

The square-well potential is

$$V(x)=\begin{cases}0, & |x|<a/2\\ V_0, & |x|>a/2\end{cases}, \tag{3.121}$$

where $a$ is the width and $V_0$ is the height. The Schrödinger equation outside the well ($|x|>a/2$) is

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}-\frac{2m}{\hbar^2}(V_0-E)\psi=0. \tag{3.122}$$

Let $k'=\sqrt{2m(V_0-E)/\hbar^2}$, then the solution of Eq. (3.122) should have the form

$$\psi\sim\exp(\pm k'x). \tag{3.123}$$

Considering $\psi(x)\to 0$ when $|x|\to\infty$, the wave function should take the values of

$$\psi(x)=\begin{cases}A\exp(-k'x), & x>a/2\\ B\exp(k'x), & x<-a/2\end{cases}, \tag{3.124}$$

where $A$ and $B$ are two constants to be determined. Inside the well ($|x|<a/2$), the Schrödinger equation becomes

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+\frac{2m}{\hbar^2}E\psi=0. \tag{3.125}$$

Because the potential is spatially symmetric, the solution should be symmetric or antisymmetric. We consider the two cases separately.

(a) Symmetric: Let $k=\sqrt{2mE/\hbar^2}$, the symmetric solution of Eq. (3.125) takes the form

$$\psi(x)\sim\cos(kx). \tag{3.126}$$

The continuity conditions for both $\psi$ and $\psi'$ at $x=\pm\frac{a}{2}$ can be unified as

$$(\ln\psi)'\Big|_{x=\pm\frac{a}{2}}=\frac{\psi'}{\psi}\Big|_{x=\pm\frac{a}{2}}=0, \tag{3.127}$$

namely,

$$\frac{\mathrm{d}}{\mathrm{d}x}\ln\cos(kx)\Big|_{x=\pm\frac{a}{2}}=\frac{\mathrm{d}}{\mathrm{d}x}\ln\exp(-k'x)\Big|_{x=\pm\frac{a}{2}}, \tag{3.128}$$

which leads to

$$k\tan\left(\frac{ka}{2}\right)=k'. \tag{3.129}$$

Let $\xi\equiv ka/2$, $\eta\equiv k'a/2$, the above equation becomes

$$\xi\tan(\xi)=\eta. \tag{3.130}$$

On the other hand, from the definitions of $\xi$ and $\eta$, we have

$$\xi^2+\eta^2=mV_0a^2/2\hbar^2\,, \tag{3.131}$$

which can only be accurately solved numerically.

(b) Antisymmetric: the antisymmetric solution of Eq. (3.125) takes the form

$$\psi(x)\sim\sin(kx)\,. \tag{3.132}$$

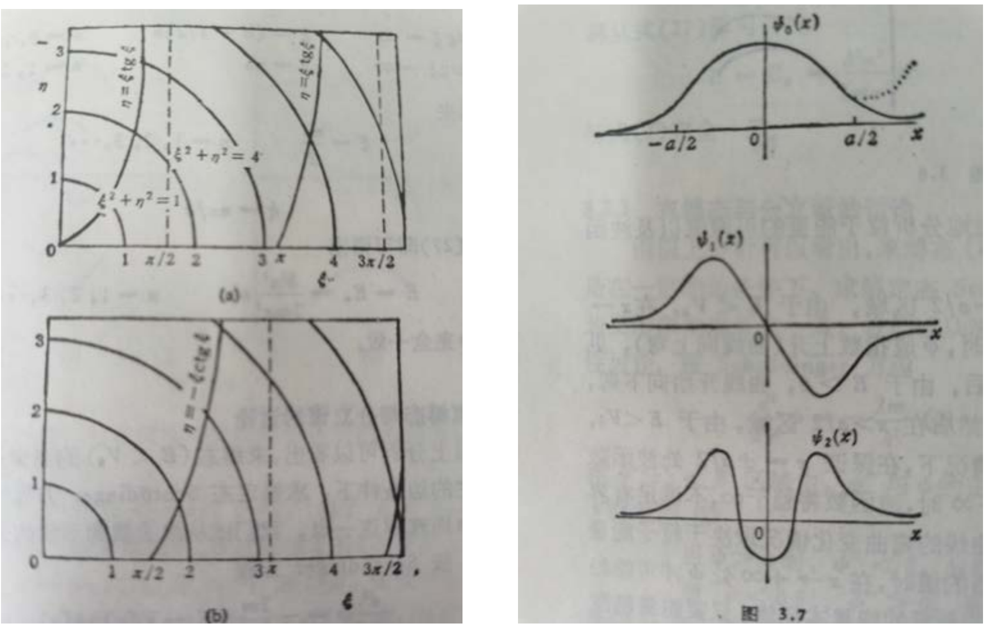
Similarly, according to the continuous requirement of $(\ln\psi)'$ at $x=\pm a$, we have

$$-k\arctan(ka/2)=k'\,, \tag{3.133}$$

which is

$$-\xi\arctan(\xi)=\eta\,. \tag{3.134}$$

From the left panel of the figure below, we can see that the symmetric solution always has a bounded ground state. When $\xi^2+\eta^2=mV_0a^2/2\hbar^2\geq\pi^2$, excited states appear; by contrast, the antisymmetric solution appears only when $\xi^2+\eta^2=mV_0a^2/2\hbar^2\geq\pi^2/4$. The first three eigenstates are plotted in the right panel of the figure below.




### 3.2.9 The Linear Potential

Given the linear potential

$$V(x)=k|x|\,, \tag{3.135}$$

where $k$ is an arbitrary positive constant. Given a total energy *E*, this potential has a classical turning point at a value $x=a=\dfrac{E}{k}$.

The Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}u_E(x)+k|x|u_E(x)=Eu_E(x)\,. \tag{3.136}$$

By restricting our attention to $x \ge 0$ and putting $y \equiv \frac{x}{\left(\hbar^2/mk\right)^{1/3}}$, $\varepsilon \equiv \frac{E}{E_0}$ into it, we obtain

$$\frac{\mathrm{d}^2 u_E}{\mathrm{d}y^2}-2(y-\varepsilon)u_E(y)=0 \tag{3.137}$$

with $y \ge 0$. Further defining $z \equiv 2^{1/3}(y-\varepsilon)$, the above equation becomes

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}u_E(z)-zu_E(z)=0\,, \tag{3.138}$$

which is the Airy equation with the solution of the Airy function Ai(*z*). It oscillates for negative *z*, and decreases rapidly towards zero for positive values.

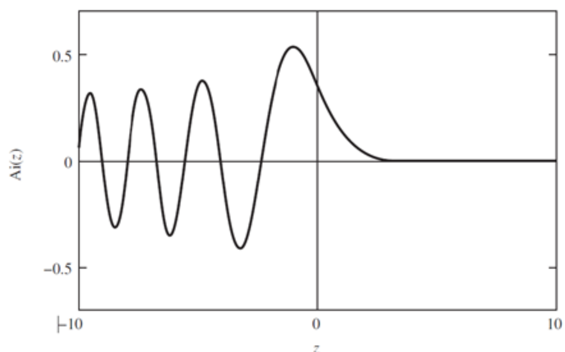
Because $V(-x)=V(x)$, we have two types of solutions, namely $u_E(-x)=\pm u_E(x)$. In either case, $u_E(x)\to 0$ as $x\to\infty$. Furthermore, if $u_E(-x)=-u_E(x)$, we need $u_E(x=0)=0$; if $u_E(-x)=u_E(x)$, we need $u_E'(x=0)=0$. To satisfy these boundary conditions, the energy is quantized as

$$\mathrm{Ai}'(z)=0,\quad z=-1.019,-3.249,-4.820,\cdots\quad \text{(even)} \tag{3.139}$$

and

$$\mathrm{Ai}(z)=0,\quad z=-2.338,-4.088,-5.521,\cdots\quad \text{(odd).} \tag{3.140}$$

The ground-state has an energy $E=\frac{1.019}{2^{1/3}}\left(\frac{\hbar^2k^2}{m}\right)^{1/3}$.




### 3.2.10 The WKB (Semiclassical) Approximation

The WKB Approximation, after G. Wentzel, A. Kramers, and L. Brillouin, is valid in the regions where the wavelength is much shorter than the typical distance over which the potential energy varies. For the linear potential, these regions are far from the classical turning points.

In one dimension, the Schrödinger’s wave equation can be written as

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}u_E(x)+\frac{2m}{\hbar^2}\left(E-V(x)\right)u_E(x)=0\,. \tag{3.141}$$

Define

$$k(x)\equiv\begin{cases}\left[\frac{2m}{\hbar^2}\left(E-V(x)\right)\right]^{1/2}, & E>V(x)\\ -i\left[\frac{2m}{\hbar^2}\left(V(x)-E\right)\right]^{1/2}, & E<V(x)\end{cases}, \tag{3.142}$$

Eq. (3.141) becomes

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}u_E(x)+\left[k(x)\right]^2u_E(x)=0\,. \tag{3.143}$$

If $V$ is independent of $x$, then $k$ is a constant, and $u_E(x)\propto\exp(\pm ikx)$. Consequently, if $V(x)$ varies slowly with $x$, we may try a solution of the form

$$u_E(x)\equiv\exp\left(\frac{iW(x)}{\hbar}\right). \tag{3.144}$$

Eq. (3.143) becomes

$$i\hbar\frac{\mathrm{d}^2W}{\mathrm{d}x^2}-\left(\frac{\mathrm{d}W}{\mathrm{d}x}\right)^2+\hbar^2\left[k(x)\right]^2=0\,. \tag{3.145}$$

Applying the “slowly varying” condition

$$\hbar\left|\frac{\mathrm{d}^2W}{\mathrm{d}x^2}\right|\ll\left|\frac{\mathrm{d}W}{\mathrm{d}x}\right|^2, \tag{3.146}$$

the lowest-order approximation $W_0(x)$ then satisfies

$$\frac{\mathrm{d}}{\mathrm{d}x}W_0(x)=\pm\hbar k(x), \tag{3.147}$$

which leads to the first-order approximation

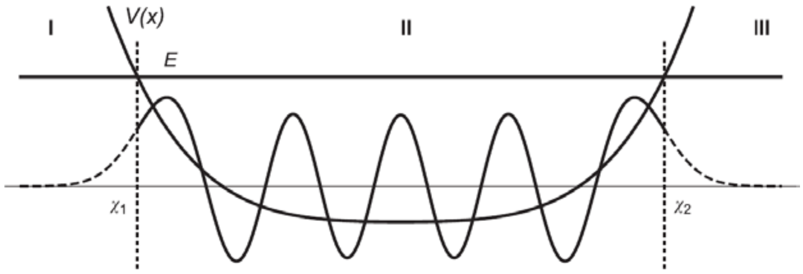
$$\begin{aligned}\left(\frac{\mathrm{d}W_1}{\mathrm{d}x}\right)^2&=\hbar^2\left[k(x)\right]^2+i\hbar\frac{\mathrm{d}^2W_0}{\mathrm{d}x^2}\\&=\hbar^2\left[k(x)\right]^2\pm i\hbar^2\frac{\mathrm{d}}{\mathrm{d}x}k(x)\end{aligned}. \tag{3.148}$$

Because the second term is much smaller than the first due to the “slowly varying” condition,

$$\begin{aligned}W(x)\approx W_1(x)&=\pm\hbar\int^x\mathrm{d}x'\left[k^2(x')\pm ik'(x')\right]^{1/2}\\&\approx\pm\hbar\int^x\mathrm{d}x'k(x')\left[1\pm\frac{i}{2}\frac{k'(x')}{k^2(x')}\right]\\&=\pm\hbar\int^x\mathrm{d}x'k(x')+\frac{i}{2}\hbar\ln\left[k(x)\right]\end{aligned}. \tag{3.149}$$

Therefore, the WKB approximation for the wave function is

$$u_E(x)\approx\exp\left[iW(x)/\hbar\right]=\frac{1}{\sqrt{k(x)}}\exp\left[\pm i\int^x dx'k(x')\right]. \tag{3.150}$$



Schematic diagram for behavior of the wave function $u_E(x)$ in a potential well $V(x)$ with turning points $x_1$ and $x_2$. Note the similarity with Figure 2.3 near the turning points.

The requirement of continuity at both turnover points $x_1, x_2$ for $E-V$ leads to the consistency condition:

$$\int_{x_1}^{x_2} \mathrm{d}x \sqrt{2m\left[E-V(x)\right]} = \left(n+\frac{1}{2}\right)\pi\hbar, \quad n=0,1,2,3,\cdots \tag{3.151}$$

Because condition Eq. (3.146) is the same as Eq. (3.64), the WKB approximation is a "semiclassical" approximation. Moreover, Eq. (3.146) is equivalent to $|k'(x)| \ll |k^2(x)|$, so in terms of the de Broglie wavelength, it amounts to

$$\lambdabar = \frac{\hbar}{\sqrt{2m\left[E-V(x)\right]}} \ll \frac{2\left[E-V(x)\right]}{|\mathrm{d}V/\mathrm{d}x|}. \tag{3.152}$$

In other words, $\lambdabar$ must be small compared with the characteristic distance over which the potential varies appreciably. Thus the semiclassical picture is reliable in the short-wavelength limit.

# 3.3 The Schrödinger Versus Heisenberg Picture

**Schrödinger picture:** State kets evolve with time while observables are time-independent.
**Heisenberg picture:** Observables evolve with time while state kets are time-independent.

### 3.3.1 The Heisenberg Equation of Motion

We introduce the unitary transformation

$$|\alpha\rangle \to U|\alpha\rangle, \tag{3.153}$$

where $U$ may stand for the translation operator $\mathscr{T}(\mathrm{d}\mathbf{x})$ or the time-evolution operator $\mathscr{U}(t,t_0)$, during which **state kets change while operators keep unchanged.** The inner product of a state bra and a state ket remains unchanged:

$$\langle\beta|\alpha\rangle \to \langle\beta|U^\dagger U|\alpha\rangle = \langle\beta|\alpha\rangle, \tag{3.154}$$

but the following changes as

$$\langle\beta|X|\alpha\rangle \to \langle\beta|U^\dagger X U|\alpha\rangle, \tag{3.155}$$

During which **operators change while state kets keep unchanged**. **Both approaches lead to the same result for the expectation value of an operator**.

For simplicity, set $t_0 = 0$, then the time-evolution operator

$$\mathscr{U}(t) \equiv \mathscr{U}(t, t_0 = 0) = \exp\left(-i\frac{Ht}{\hbar}\right). \tag{3.156}$$

Then an observable in the Heisenberg picture is

$$A^{(\mathrm{H})}(t) = \mathscr{U}^{\dagger}(t) A^{(\mathrm{S})} \mathscr{U}(t), \tag{3.157}$$

where the superscripts H and S stand for Heisenberg and Schrödinger, respectively. At $t = 0$,

$$A^{(\mathrm{H})}(0) = A^{(\mathrm{S})}, \tag{3.158}$$

and the state kets also coincide between the two pictures, and do not change in the Heisenberg picture. The expectation value is obviously the same in both pictures.

We now derive the equation of motion in the Heisenberg picture. Assuming $A^{(\mathrm{S})}$ does not depend explicitly on time, by differentiating Eq. (3.157) and using Eq. (3.14), we obtain

$$\begin{aligned}\frac{\mathrm{d}A^{(\mathrm{H})}}{\mathrm{d}t} &= \frac{\partial \mathscr{U}^{\dagger}}{\partial t} A^{(\mathrm{S})} \mathscr{U} + \mathscr{U}^{\dagger} A^{(\mathrm{S})} \frac{\partial \mathscr{U}}{\partial t} \\ &= -\frac{1}{i\hbar} \mathscr{U}^{\dagger} H \mathscr{U} \mathscr{U}^{\dagger} A^{(\mathrm{S})} \mathscr{U} + \frac{1}{i\hbar} \mathscr{U}^{\dagger} A^{(\mathrm{S})} \mathscr{U} \mathscr{U}^{\dagger} H \mathscr{U} \\ &= \frac{1}{i\hbar}\left[A^{(\mathrm{H})}, \mathscr{U}^{\dagger} H \mathscr{U}\right]\end{aligned} . \tag{3.159}$$

According to Eq. (3.156), $\mathscr{U}$ and $H$ commute, so

$$\mathscr{U}^{\dagger} H \mathscr{U} = H . \tag{3.160}$$

Therefore, Eq. (3.159) becomes the **Heisenberg equation of motion**

$$\frac{\mathrm{d}A^{(\mathrm{H})}}{\mathrm{d}t} = \frac{1}{i\hbar}\left[A^{(\mathrm{H})}, H\right]. \tag{3.161}$$

If we apply Dirac's quantization rule reversely

$$\frac{[,]}{i\hbar} \to [,]_{\text{classical}} \tag{3.162}$$

to Eq. (3.161), we immediately obtain its counterpart in classical physics

$$\frac{\mathrm{d}A}{\mathrm{d}t} = [A, H]_{\text{classical}} . \tag{3.163}$$

In general, for a physical system with classical analogues, we assume the Hamiltonian to be of the same form as in classical physics; we merely replace the classical $x_i$ and $p_i$ by the corresponding operators in quantum mechanics. For non-commuting observables, we require $H$ to be Hermitian; for instance, we write the quantum-mechanical analogue of the classical product $xp$ as $\frac{1}{2}(xp + px)$.

If $F$ and $G$ are functions that can be expanded in powers of $p_j$ and $x_i$, respectively, we may have

$$\left[x_i, F(\mathbf{p})\right] = i\hbar \frac{\partial F}{\partial p_i} \tag{3.164}$$

and

$$\left[p_i, G(\mathbf{x})\right] = -i\hbar\frac{\partial G}{\partial x_i}. \tag{3.165}$$

### 3.3.2 Free Particles and Ehrenfest's Theorem

We treat again the free-particle problem with the Heisenberg equation of motion. The Hamiltonian for a free particle of mass $m$ is

$$H = \frac{\mathbf{p}^2}{2m} = \frac{\left(p_x^2 + p_y^2 + p_z^2\right)}{2m}. \tag{3.166}$$

According to Eq. (3.161), we have

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = \frac{1}{i\hbar}\left[p_i, H\right] = 0. \tag{3.167}$$

Therefore, for a free particle, the momentum operator is a constant of the motion. More generally, any operators commuting with the Hamiltonian is a constant of the motion.

On the other hand, by using Eq. (3.164), we have

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \frac{1}{i\hbar}\left[x_i, H\right] = \frac{1}{i\hbar}\frac{1}{2m}i\hbar\frac{\partial}{\partial p_i}\left(\sum_{j=1}^{3} p_j^2\right) = \frac{p_i}{m} = \frac{p_i(0)}{m}, \tag{3.168}$$

whose solution is

$$x_i(t) = x_i(0) + \frac{p_i(0)}{m}t. \tag{3.169}$$

Noe that the commutator of position at different times does not vanish:

$$\left[x_i(t), x_i(0)\right] = \left[\frac{p_i(0)t}{m}, x_i(0)\right] = -i\hbar\frac{t}{m}. \tag{3.170}$$

The corresponding uncertainty relation is

$$\left\langle\left(\Delta x_i\right)^2\right\rangle_t \left\langle\left(\Delta x_i\right)^2\right\rangle_{t=0} \geq \frac{\hbar^2 t^2}{4m^2}. \tag{3.171}$$

This relation implies that even if a free particle is initially well localized, its position becomes more and more uncertain with time.

We now add a potential $V(\mathbf{x})$ to the free-particle Hamiltonian:

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}). \tag{3.172}$$

With Eq. (3.163) and Eq. (3.165), we have

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = \frac{1}{i\hbar}\left[p_i, V(\mathbf{x})\right] = -\frac{\partial}{\partial x_i}V(\mathbf{x}). \tag{3.173}$$

On the other hand, because $x_i$ commutes with $V(\mathbf{x})$, Eq. (3.168) still holds. We use Eq. (3.161) twice to obtain

$$\frac{\mathrm{d}^2 x_i}{\mathrm{d}t^2} = \frac{1}{i\hbar}\left[\frac{\mathrm{d}x_i}{\mathrm{d}t}, H\right] = \frac{1}{i\hbar}\left[\frac{p_i}{m}, H\right] = \frac{1}{m}\frac{\mathrm{d}p_i}{\mathrm{d}t}. \tag{3.174}$$

Combining this equation with Eq. (3.173) and rewriting in the vectorial form, we finally get

$$m\frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = -\nabla V(\mathbf{x}), \tag{3.175}$$

which is the quantum-mechanical analogue of Newton's second law in the Heisenberg picture. By taking the expectation values with the time-invariant Heisenberg state ket, we obtain the **Ehrenfest theorem**

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\mathbf{x}\rangle = \frac{\mathrm{d}\langle\mathbf{p}\rangle}{\mathrm{d}t} = -\langle\nabla V(\mathbf{x})\rangle, \tag{3.176}$$

which is valid in both the Heisenberg and Schrödinger pictures.

### 3.3.3 Base Kets and Transition Amplitudes

In the Schrödinger picture, the eigenvalue function

$$A|a'\rangle = a'|a'\rangle . \tag{3.177}$$

Because $A$ does not change, so the base kets cannot change with time either.

In the Heisenberg picture, $A$ changes with time:

$$A^{(\mathrm{H})}(t) = \mathscr{U}^\dagger A(0)\mathscr{U} . \tag{3.178}$$

Since the two pictures coincide at $t = 0$, combining the above two equations together to get

$$\mathscr{U}^\dagger A(0)\mathscr{U}\mathscr{U}^\dagger|a'\rangle = a'\mathscr{U}^\dagger|a'\rangle, \tag{3.179}$$

which is just an eigenvalue function for $A^{(\mathrm{H})}$:

$$A^{(\mathrm{H})}\left(\mathscr{U}^\dagger|a'\rangle\right) = a'\left(\mathscr{U}^\dagger|a'\rangle\right). \tag{3.180}$$

Therefore, in the Heisenberg picture, the eigenvalues do not change with time, while the base kets move with time as

$$|a',t\rangle_H = \mathscr{U}^\dagger|a'\rangle, \tag{3.181}$$

which satisfies the "wrong-sign Schrödinger equation"

$$i\hbar\frac{\partial}{\partial t}|a',t\rangle_H = -H|a',t\rangle_H . \tag{3.182}$$

The relation between the observables in both pictures is

$$\begin{aligned} A^{(\mathrm{H})}(t) &= \sum_{a'}|a',t\rangle_H\, a'\, {}_H\langle a',t| \\ &= \sum_{a'}\mathscr{U}^\dagger|a'\rangle a'\langle a'|\mathscr{U} \\ &= \mathscr{U}^\dagger A^{(\mathrm{S})}\mathscr{U} \end{aligned} . \tag{3.183}$$

The expansion coefficients of a state ket is the same for both pictures:

$$c_{a'}(t) = \langle a'|\mathscr{U}|\alpha, t_0 = 0\rangle . \tag{3.184}$$

In the Schrödinger picture, the base bra is $\langle a'|$, and the state ket is $\mathscr{U}|\alpha, t_0 = 0\rangle$; while in the Heisenberg picture, the base bra is $\langle a'|\mathscr{U}$, and the state ket is $|\alpha, t_0 = 0\rangle$.

**Transition amplitude:** The probability amplitude for a physical system initially prepared at $t$

= 0 to be in the eigenstate of observable $A$ with eigenvalue $a'$ to be found in an eigenstate of observable $B$ with eigenvalue $b'$, which is

$$\langle b'|\mathscr{U}(t,0)|a'\rangle . \tag{3.185}$$

In the Schrödinger picture, the base bra is $\langle b'|$ and the state ket is $\mathscr{U}|a'\rangle$; while in the Heisenberg picture, the base bra is $\langle b'|\mathscr{U}$, while the state ket is $|a'\rangle$.

To summarize, the differences between the Schrödinger picture and the Heisenberg picture is:

| | Schrödinger picture | Heisenberg picture |
|---|---|---|
| Observable | Stationary | Moving: Eq. (3.157) and Eq. (3.161) |
| State ket | Moving: Eq. (3.1) and Eq. (3.16) | Stationary |
| Base ket | Stationary | Moving oppositely:<br>Eq. (3.181) and Eq. (3.182) |

# 3.4 Simple Harmonic Oscillator

### 3.4.1 Schrödinger's Wave Equation Solution

The Hamiltonian of a one-dimensional oscillator is

$$H=\frac{p^2}{2m}+\frac{m\omega^2x^2}{2}, \tag{3.186}$$

where $\omega=\sqrt{k/m}$ is the angular frequency with $k$ being the spring constant. So the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}u_E(x)+\frac{1}{2}m\omega^2x^2u_E(x)=Eu_E(x), \tag{3.187}$$

which will be solved based on the concept of *generating functions*.

First, put $y\equiv\dfrac{x}{\sqrt{\hbar/m\omega}}$, $\varepsilon\equiv\dfrac{2E}{\hbar\omega}$ into the above equation to obtain

$$\frac{\mathrm{d}^2}{\mathrm{d}y^2}u(y)+\left(\varepsilon-y^2\right)u(y)=0 . \tag{3.188}$$

Considering the solution of the differential equation $w''(y)-y^2w(y)=0$ is $w(y)\propto\exp\left(\pm\dfrac{y^2}{2}\right)$, and the solution must tend to zero when $y\to\pm\infty$ to satisfy the requirement of normalization, we have to choose the solution with the minus sign. Therefore, the solution can be written in the form

$$u(y)=h(y)\exp\left(-\frac{y^2}{2}\right). \tag{3.189}$$

Put Eq. (3.189) into Eq. (3.188), we know $h(y)$ satisfies the differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}y^2}h(y)-2y\frac{d}{dy}h(y)+(\varepsilon-1)h(y)=0 . \tag{3.190}$$

Let us now consider the **Hermite polynormials** $H_n(x)$ defined by its generating function $g(x,t)$ through

$$g(x,t) \equiv \exp\left(-t^2 + 2tx\right) \equiv \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} . \tag{3.191}$$

Taking the derivatives of the above two equations with respect to *x*, we have

$$\begin{aligned} \frac{\partial g}{\partial x} &= 2tg(x,t) = \sum_{n=0}^{\infty} 2H_n(x) \frac{t^{n+1}}{n!} = \sum_{n=0}^{\infty} 2(n+1) H_n(x) \frac{t^{n+1}}{(n+1)!} \\ \frac{\partial g}{\partial x} &= \sum_{n=0}^{\infty} H_n'(x) \frac{t^n}{n!} \end{aligned} . \tag{3.192}$$

Comparing the two derivatives, we get

$$H_n'(x) = 2nH_{n-1}(x) . \tag{3.193}$$

On the other hand, taking the derivatives of Eqs. (3.191) with respect to *t*, we obtain

$$\begin{aligned} \frac{\partial g}{\partial t} &= -2tg(x,t) + 2xg(x,t) \\ &= -\sum_{n=0}^{\infty} 2H_n(x) \frac{t^{n+1}}{n!} + \sum_{n=0}^{\infty} 2xH_n(x) \frac{t^n}{n!} \\ &= -\sum_{n=0}^{\infty} 2nH_{n-1}(x) \frac{t^n}{n!} + \sum_{n=0}^{\infty} 2xH_n(x) \frac{t^n}{n!} \end{aligned} \tag{3.194}$$

and

$$\frac{\partial g}{\partial t} = \sum_{n=0}^{\infty} nH_n(x) \frac{t^{n-1}}{n!} = \sum_{n=0}^{\infty} H_{n+1}(x) \frac{t^n}{n!} . \tag{3.195}$$

Comparing the above two equations, we obtain the recursion relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) , \tag{3.196}$$

which we combine with Eq. (3.193) to find

$$\begin{aligned} H_n''(x) &= 2n \cdot 2(n-1) H_{n-2}(x) \\ &= 2n\left[2xH_{n-1}(x) - H_n(x)\right] \\ &= 2xH_n'(x) - 2nH_n(x) \end{aligned} , \tag{3.197}$$

from which we can build the Hermite polynomials

$$\begin{aligned} &H_0(x) = 1 \\ &H_1(x) = 2x \\ &H_2(x) = 4x^2 - 2 \\ &H_3(x) = 8x^3 - 12x \\ &\cdots \end{aligned} . \tag{3.198}$$

Eq. (3.197) gives the differential equation satisfied by the Hermite polynomials as

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0 , \tag{3.199}$$

where *n* is a nonnegative integer. Comparing with Eq. (3.190), we know

$$u_n(x) = c_n H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)\exp\left(-\frac{m\omega x^2}{2\hbar}\right) \tag{3.200}$$

up to some normalization constant $c_n$, which can be determined from the othogonality relationship given by the generating function

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) \exp\left(-x^2\right) \mathrm{d}x = 2^n n! \sqrt{\pi}\delta_{nm} \tag{3.201}$$

**3.4.2 Annihilation, Creation, and Number Operators**

The importance of the simple harmonic oscillator in quantum mechanics is exhibited by: (1) Any potential well can be approximated by a simple harmonic oscillator; (2) It is an important starting point for much of quantum field theory.

Define the non-Hermitian **annihilation operator**

$$a \equiv \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right) \tag{3.202}$$

and the **creation operator**

$$a^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right), \tag{3.203}$$

which obeys the canonical commutation relation

$$\left[a, a^\dagger\right] = \frac{1}{2\hbar}\left(-i[x, p] + i[p, x]\right) = 1. \tag{3.204}$$

The Hermitian **number operator** can then be defined as

$$N \equiv a^\dagger a = \frac{m\omega}{2\hbar}\left(x^2 + \frac{p^2}{m^2\omega^2}\right) + \frac{i}{2\hbar}[x, p] = \frac{H}{\hbar\omega} - \frac{1}{2}. \tag{3.205}$$

In this way, the Hamiltonian can be expressed as

$$H = \hbar\omega\left(N + \frac{1}{2}\right). \tag{3.206}$$

The eigenfunction of the number operator is

$$N|n\rangle = n|n\rangle, \tag{3.207}$$

so we have

$$H|n\rangle = E_n|n\rangle \tag{3.208}$$

with the energy eigenvalues

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{3.209}$$

Using Eq. (3.204), we have

$$[N, a] = \left[a^\dagger a, a\right] = a^\dagger[a, a] + \left[a^\dagger, a\right]a = -a. \tag{3.210}$$

Similarly, we also have

$$\left[N, a^\dagger\right] = a^\dagger. \tag{3.211}$$

As a result, we have

$$Na^\dagger|n\rangle = \left(\left[N, a^\dagger\right] + a^\dagger N\right)|n\rangle = (n+1)a^\dagger|n\rangle \tag{3.212}$$

and

$$Na|n\rangle = \left(\left[N, a\right] + aN\right)|n\rangle = (n-1)a|n\rangle . \tag{3.213}$$

These relations imply that $a^\dagger|n\rangle$ ( $a|n\rangle$ ) is also an eigenket of $N$ with eigenvalue increased (decreased) by 1, corresponding to the creation (annihilation) of one quantum unit of energy $\hbar\omega$ .

Eq. (3.213) implies that

$$a|n\rangle = c|n-1\rangle , \tag{3.214}$$

where $c$ is a normalization constant. Note that

$$\langle n|a^\dagger a|n\rangle = \langle n|N|n\rangle = n = |c|^2 , \tag{3.215}$$

So by taking $c$ to be real and positive by convention, we finally obtain

$$a|n\rangle = \sqrt{n}|n-1\rangle \tag{3.216}$$

and

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle . \tag{3.217}$$

By repeatedly applying the annihilation operator $a$ to Eq. (3.216), we obtain

$$\begin{aligned} a^2|n\rangle &= \sqrt{n(n-1)}|n-2\rangle \\ a^3|n\rangle &= \sqrt{n(n-1)(n-2)}|n-3\rangle \\ &\vdots \end{aligned} \tag{3.218}$$

until the ground state $n=0$ , whose energy, according to Eq. (3.209), is

$$E_0 = \frac{1}{2}\hbar\omega . \tag{3.219}$$

By successively applying the creation operator $a^\dagger$ to the ground state $|0\rangle$, we have

$$|n\rangle = \left[\frac{\left(a^\dagger\right)^n}{\sqrt{n!}}\right]|0\rangle \tag{3.220}$$

with corresponding eigenvalues of

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0,1,2,3,\cdots . \tag{3.221}$$

From Eq. (3.216) and Eq. (3.217), we obtain the matrix elements

$$\langle n'|a|n\rangle = \sqrt{n}\delta_{n',n-1}, \quad \langle n'|a^\dagger|n\rangle = \sqrt{n+1}\delta_{n',n+1} . \tag{3.222}$$

Together with

$$x = \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^\dagger\right), \quad p = i\sqrt{\frac{m\hbar\omega}{2}}\left(-a + a^\dagger\right), \tag{3.223}$$

we get the matrix elements of the $x$ and $p$ operators:

$$
\begin{aligned}
\langle n'|x|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right) \\
\langle n'|p|n\rangle &= i\sqrt{\frac{m\hbar\omega}{2}}\left(-\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right)
\end{aligned} . \tag{3.224}
$$

Neither $x$ nor $p$ is diagonal in the $N$-representation because they do not commute with $N$.

The energy eigenfunctions in position space can also be obtained by the operator method. In the $x$-representation, because $a|0\rangle = 0$, we have

$$
\langle x'|a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\langle x'|\left(x + \frac{ip}{m\omega}\right)|0\rangle = 0 . \tag{3.225}
$$

Using $\langle x'|p|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle$, the above equation becomes

$$
\left(x' + x_0^2\frac{\mathrm{d}}{\mathrm{d}x'}\right)\langle x'|0\rangle = 0 , \tag{3.226}
$$

where $x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$. The normalized solution is

$$
\langle x'|0\rangle = \frac{1}{\pi^{1/4}\sqrt{x_0}}\exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right]. \tag{3.227}
$$

The energy eigenfunctions for excited states are

$$
\begin{aligned}
\langle x'|1\rangle &= \langle x'|a^\dagger|0\rangle = \frac{1}{\sqrt{2}x_0}\left(x' - x_0^2\frac{\mathrm{d}}{\mathrm{d}x'}\right)\langle x'|0\rangle \\
\langle x'|2\rangle &= \frac{1}{\sqrt{2}}\langle x'|\left(a^\dagger\right)^2|0\rangle = \frac{1}{\sqrt{2!}}\left(\frac{1}{\sqrt{2}x_0}\right)^2\left(x' - x_0^2\frac{\mathrm{d}}{\mathrm{d}x'}\right)^2\langle x'|0\rangle \\
&\vdots \\
\langle x'|n\rangle &= \left(\frac{1}{\pi^{1/4}\sqrt{2^n n!}}\right)\left(\frac{1}{x_0^{n+1/2}}\right)\left(x' - x_0^2\frac{\mathrm{d}}{\mathrm{d}x'}\right)^n\exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right]
\end{aligned} . \tag{3.228}
$$

Now we look at the expectation values of $x^2$ and $p^2$ for the ground state. Note that

$$
x^2 = \left(\frac{\hbar}{2m\omega}\right)\left(a^2 + a^{+2} + a^+a + aa^+\right), \tag{3.229}
$$

which yields

$$
\langle x^2\rangle = \frac{\hbar}{2m\omega} = \frac{x_0^2}{2} . \tag{3.230}
$$

Likewise,

$$
\langle p^2\rangle = \frac{\hbar m\omega}{2} . \tag{3.231}
$$

The kinetic energy

$$
\left\langle\frac{p^2}{2m}\right\rangle = \frac{\hbar\omega}{4} = \frac{\langle H\rangle}{2} \tag{3.232}
$$

and the potential energy

$$\left\langle \frac{m\omega^2 x^2}{2} \right\rangle = \frac{\hbar\omega}{4} = \frac{\langle H \rangle}{2} \tag{3.233}$$

satisfies the virial theorem.

Because $\langle x \rangle = \langle p \rangle = 0$ , we have

$$\left\langle (\Delta x)^2 \right\rangle = \left\langle x^2 \right\rangle = \frac{\hbar}{2m\omega} \tag{3.234}$$

and

$$\left\langle (\Delta p)^2 \right\rangle = \left\langle p^2 \right\rangle = \frac{\hbar m\omega}{2} , \tag{3.235}$$

which satisfies the minimum uncertainty product form:

$$\left\langle (\Delta x)^2 \right\rangle \left\langle (\Delta p)^2 \right\rangle = \frac{\hbar^2}{4} . \tag{3.236}$$

This is not surprising because the ground-state wave function has a Gaussian shape. In contrast, the uncertainty products for the excited states are larger:

$$\left\langle (\Delta x)^2 \right\rangle \left\langle (\Delta p)^2 \right\rangle = \left( n + \frac{1}{2} \right)^2 \hbar^2 . \tag{3.237}$$

### 3.4.3 Time Development of the Oscillator

In the Heisenberg picture, $x$, $p$, $a$, and $a^\dagger$ are all time-dependent. According to Eq. (3.173) and Eq. (3.168), the Heisenberg equations of motion for $p$ and $x$ are

$$\frac{dp}{dt} = -\frac{\mathrm{d}}{\mathrm{d}x} V(x) = -m\omega^2 x \tag{3.238}$$

and

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{p}{m} . \tag{3.239}$$

This pair of coupled differential equations is equivalent to two uncoupled ones:

$$\frac{\mathrm{d}a}{\mathrm{d}t} = \sqrt{\frac{m\omega}{2\hbar}} \left( \frac{p}{m} - i\omega x \right) = -i\omega a \tag{3.240}$$

and

$$\frac{\mathrm{d}a^\dagger}{\mathrm{d}t} = i\omega a^\dagger , \tag{3.241}$$

whose solutions are

$$a(t) = a(0) \exp(-i\omega t) \tag{3.242}$$

and

$$a^\dagger(t) = a^\dagger(0) \exp(i\omega t) . \tag{3.243}$$

The above two equations can be rewritten in terms of $x$ and $p$ as

$$x(t)+\frac{ip(t)}{m\omega}=x(0)\exp(-i\omega t)+i\left[\frac{p(0)}{m\omega}\right]\exp(-i\omega t) \tag{3.244}$$

and

$$x(t)-\frac{ip(t)}{m\omega}=x(0)\exp(i\omega t)-i\left[\frac{p(0)}{m\omega}\right]\exp(i\omega t). \tag{3.245}$$

Separating the Hermitian and anti-Hermitian parts, we deduce

$$x(t)=x(0)\cos(\omega t)+\left[\frac{p(0)}{m\omega}\right]\sin(\omega t) \tag{3.246}$$

and

$$p(t)=-m\omega x(0)\sin(\omega t)+p(0)\cos(\omega t). \tag{3.247}$$

We see that the *x* and *p* operators “oscillate” just like their classical analogue.

Eq. (3.246) can be reached in an alternative way of utilizing the **Baker-Hausdorff lemma**:

$$\begin{aligned}&\exp(iG\lambda)A\exp(-iG\lambda)=A+i\lambda[G,A]+\left(\frac{i^2\lambda^2}{2!}\right)[G,[G,A]]\\&+\cdots+\left(\frac{i^n\lambda^n}{n!}\right)[G,[G,[G,\cdots[G,A]]]\cdots]+\cdots\end{aligned}, \tag{3.248}$$

where *G* is a Hermitian operator and $\lambda$ is a real parameter. By applying it, we have

$$\begin{aligned}x(t)&=\exp\left(\frac{iHt}{\hbar}\right)x(0)\exp\left(\frac{-iHt}{\hbar}\right)\\&=x(0)+\left(\frac{it}{\hbar}\right)[H,x(0)]+\left(\frac{i^2t^2}{2!\hbar^2}\right)[H,[H,x(0)]]+\cdots\end{aligned}. \tag{3.249}$$

Each term of the right-hand side can be reduced to either *x* or *p* by repeatedly applying

$$[H,x(0)]=-i\frac{\hbar p(0)}{m} \tag{3.250}$$

and

$$[H,p(0)]=i\hbar m\omega^2x(0). \tag{3.251}$$

Therefore, we obtain

$$\begin{aligned}x(t)&=x(0)+\left[\frac{p(0)}{m}\right]t-\left(\frac{1}{2!}\right)t^2\omega^2x(0)-\left(\frac{1}{3!}\right)\frac{t^3\omega^2p(0)}{m}+\cdots\\&=x(0)\cos(\omega t)+\left[\frac{p(0)}{m\omega}\right]\sin(\omega t)\end{aligned}, \tag{3.252}$$

in agreement with Eq. (3.246).

The **coherent state** $\lambda$ defined by

$$a|\lambda\rangle=\lambda|\lambda\rangle \tag{3.253}$$

can bounce back and forth without spreading in shape. It has the following properties:

(1) When it is expressed as a superposition of energy eigenstates

$$|\lambda\rangle = \sum_{n=0}^{\infty} f(n)|n\rangle, \tag{3.254}$$

the distribution of $|f(n)|^2$ is of the Poisson type about some mean value $\bar{n}$:

$$|f(n)|^2 = \left(\frac{\bar{n}^n}{n!}\right)\exp(-\bar{n}). \tag{3.255}$$

(2) It can be obtained by translating the ground state by some finite distance.

(3) It satisfies the minimum uncertainty product relation at all times.

# 3.5 Propagators and Feynman Path Integrals

### 3.5.1 Propagators in Wave Mechanics

We start with

$$\begin{aligned} |\alpha, t_0; t\rangle &= \exp\left[-i\frac{H(t-t_0)}{\hbar}\right]|\alpha, t_0\rangle \\ &= \sum_{a'} |a'\rangle\langle a'|\alpha, t_0\rangle \exp\left[-i\frac{E_{a'}(t-t_0)}{\hbar}\right] \end{aligned}. \tag{3.256}$$

Multiplying both sides by $\langle \mathbf{x}'|$, we have

$$\langle \mathbf{x}'|\alpha, t_0; t\rangle = \sum_{a'} \langle \mathbf{x}'|a'\rangle\langle a'|\alpha, t_0\rangle \exp\left[-i\frac{E_{a'}(t-t_0)}{\hbar}\right], \tag{3.257}$$

which is just the wave function

$$\psi(\mathbf{x}', t) = \sum_{a'} c_{a'}(t_0) u_{a'}(\mathbf{x}') \exp\left[-i\frac{E_{a'}(t-t_0)}{\hbar}\right] \tag{3.258}$$

with $u_{a'}(\mathbf{x}') = \langle \mathbf{x}'|a'\rangle$ standing for the eigenfunction of operator $A$ with eigenvalue $a'$. Because

$$\langle a'|\alpha, t_0\rangle = \int \mathrm{d}^3x' \langle a'|\mathbf{x}'\rangle\langle \mathbf{x}'|\alpha, t_0\rangle, \tag{3.259}$$

namely,

$$c_{a'}(t_0) = \int \mathrm{d}^3x' u_{a'}^*(\mathbf{x}')\psi(\mathbf{x}', t_0), \tag{3.260}$$

Eq. (3.258) can be written as

$$\psi(\mathbf{x}'', t) = \int \mathrm{d}^3x' K(\mathbf{x}'', t; \mathbf{x}', t_0)\psi(\mathbf{x}', t_0), \tag{3.261}$$

where the **propagator**

$$
\begin{aligned}
K\left(\mathbf{x}'',t;\mathbf{x}',t_0\right) &= \sum_{a'}\left\langle \mathbf{x}''\middle|a'\right\rangle\left\langle a'\middle|\mathbf{x}'\right\rangle \exp\left[-i\frac{E_{a'}\left(t-t_0\right)}{\hbar}\right] \\
&= \left\langle \mathbf{x}''\right| \exp\left[-i\frac{H\left(t-t_0\right)}{\hbar}\right]\left|\mathbf{x}'\right\rangle
\end{aligned}, \tag{3.262}
$$

which is simply the Green's function for the time-dependent wave equation satisfying

$$
\left[-\left(\frac{\hbar^2}{2m}\right)\nabla''^2 + V\left(\mathbf{x}''\right) - i\hbar\frac{\partial}{\partial t}\right]K\left(\mathbf{x}'',t;\mathbf{x}',t_0\right) = -i\hbar\delta^3\left(\mathbf{x}''-\mathbf{x}'\right)\delta\left(t-t_0\right) \tag{3.263}
$$

with the boundary condition $K\left(\mathbf{x}'',t;\mathbf{x}',t_0\right)=0$ for $t<t_0$.

For a free particle in one dimension,

$$
\begin{aligned}
p\left|p'\right\rangle &= p'\left|p'\right\rangle \\
H\left|p'\right\rangle &= \frac{p'^2}{2m}\left|p'\right\rangle
\end{aligned}. \tag{3.264}
$$

The propagator

$$
\begin{aligned}
K\left(\mathbf{x}'',t;\mathbf{x}',t_0\right) &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}p' \exp\left[\frac{ip\left(x''-x'\right)}{\hbar} - \frac{ip'^2\left(t-t_0\right)}{2m\hbar}\right] \\
&= \sqrt{\frac{m}{2\pi i\hbar\left(t-t_0\right)}} \exp\left[\frac{im\left(x''-x'\right)^2}{2\hbar\left(t-t_0\right)}\right]
\end{aligned}. \tag{3.265}
$$

For the simple harmonic oscillator, the wave function of an energy eigenstate

$$
\begin{aligned}
u_n\left(x\right)\exp\left(-i\frac{E_n t}{\hbar}\right) &= \frac{1}{2^{n/2}\sqrt{n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right) \\
&\times H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\exp\left[-i\omega\left(n+\frac{1}{2}\right)t\right]
\end{aligned}, \tag{3.266}
$$

so the propagator can be proved to be

$$
\begin{aligned}
K\left(\mathbf{x}'',t;\mathbf{x}',t_0\right) &= \sqrt{\frac{m\omega}{2\pi i\hbar\sin\left[\omega\left(t-t_0\right)\right]}} \\
&\exp\left[\frac{im\omega}{2\hbar\sin\left[\omega\left(t-t_0\right)\right]}\left\{\left(x''^2+x'^2\right)\cos\left[\omega\left(t-t_0\right)\right]-2x''x'\right\}\right]
\end{aligned}. \tag{3.267}
$$

Setting $\mathbf{x}''=\mathbf{x}'$ and $t_0=0$, by integrating over all space, we have

$$
\begin{aligned}
G\left(t\right) &= \int \mathrm{d}^3x' K\left(\mathbf{x}'',t;\mathbf{x}',t_0\right) \\
&= \int \mathrm{d}^3x' \sum_{a'}\left|\left\langle \mathbf{x}'\middle|a'\right\rangle\right|^2 \exp\left(-i\frac{E_{a'}t}{\hbar}\right), \\
&= \sum_{a'}\exp\left(-i\frac{E_{a'}t}{\hbar}\right)
\end{aligned} \tag{3.268}
$$

which is the "sum over states", reminiscent of the partition function in statistical mechanics.

The Laplace-Fourier transform of $G\left(t\right)$ is

$$
\begin{aligned}
\tilde{G}(E) &= -i\int_0^\infty \mathrm{d}t G(t)\exp\left(i\frac{Et}{\hbar}\right)/\hbar \\
&= -i\int_0^\infty \mathrm{d}t\sum_{a'}\exp\left(-i\frac{E_{a'}t}{\hbar}\right)\exp\left(i\frac{Et}{\hbar}\right)/\hbar
\end{aligned}
\quad . \tag{3.269}
$$

In the complex plane, we give $E$ a small positive imaginary part:

$$E \to E + i\varepsilon \tag{3.270}$$

and take the limit $\varepsilon \to 0$ to obtain

$$\tilde{G}(E) = \sum_{a'}\frac{1}{E - E_{a'}}, \tag{3.271}$$

which means that the energy spectrum is simple holes in the complex $E$-plane.

### 3.5.2 Path Integrals as the Sum Over Paths

In the Heisenberg picture, the propagator can be written as

$$
\begin{aligned}
K(\mathbf{x}'',t;\mathbf{x}',t_0) &= \sum_{a'}\langle\mathbf{x}''|a'\rangle\langle a'|\mathbf{x}'\rangle\exp\left[-i\frac{E_{a'}(t-t_0)}{\hbar}\right] \\
&= \sum_{a'}\langle\mathbf{x}''|\exp\left(-i\frac{Ht}{\hbar}\right)|a'\rangle\langle a'|\exp\left(-i\frac{Ht_0}{\hbar}\right)|\mathbf{x}'\rangle \\
&= \langle\mathbf{x}'',t|\mathbf{x}',t_0\rangle
\end{aligned}
\quad , \tag{3.272}
$$

which is the **transition amplitude** for the particle prepared at $t_0$ with position eigenvalue $\mathbf{x}'$ to be found at a later time $t$ at $\mathbf{x}''$.

Because of the completeness condition

$$\int \mathrm{d}^3x''|\mathbf{x}'',t''\rangle\langle\mathbf{x}'',t''| = 1, \tag{3.273}$$

for $t''' > t'' > t'$, we have the **composition property** of the transition amplitude:

$$\langle\mathbf{x}''',t'''|\mathbf{x}',t'\rangle = \int \mathrm{d}^3x''\langle\mathbf{x}''',t'''|\mathbf{x}'',t''\rangle\langle\mathbf{x}'',t''|\mathbf{x}',t'\rangle. \tag{3.274}$$

Obviously, we can this as many times as we wish for an infinitesimal time interval. For a set of $(x_j,t_j),\quad j=1,2,\cdots,N$ with an even time interval of

$$\Delta t \equiv t_j - t_{j-1} = \frac{t_N - t_1}{N-1}, \tag{3.275}$$

we have

$$
\begin{aligned}
\langle x_N,t_N|x_1,t_1\rangle &= \int \mathrm{d}x_{N-1}\int \mathrm{d}x_{N-2}\cdots\int \mathrm{d}x_2\,\langle x_N,t_N|x_{N-1},t_{N-1}\rangle \\
&\times\langle x_{N-1},t_{N-1}|x_{N-2},t_{N-2}\rangle\cdots\langle x_2,t_2|x_1,t_1\rangle
\end{aligned}
\quad , \tag{3.276}
$$

which means that we must sum over all possible paths in the space-time plane between the start and end points, in contrast to the unique path in classical mechanics.

### 3.5.3 Feynman's Formulation

Feynman has attempted a new formulation of quantum mechanics based on the concept of paths with the following considerations: (1) the superposition principle of various alternative paths, (2) the composition property of the transition amplitude, and (3) classical correspondence in the

$\hbar \to 0$ limit.

In classical mechanics, according to Hamilton's principle, the unique path is that minimizing the action, defined as the time integral of the classical Lagrangian:

$$\delta \int_{t_1}^{t_2} \mathrm{d}t L_{\text{classical}}\left(x, \dot{x}\right) = 0 . \tag{3.277}$$

For quantum mechanics, we introduce

$$S\left(n, n-1\right) \equiv \int_{t_{n-1}}^{t_n} \mathrm{d}t L_{\text{classical}}\left(x, \dot{x}\right), \tag{3.278}$$

and the transition from time $t_{n-1}$ to $t_n$ for an infinitesimal $\Delta t$ is *assumed* to be written as

$$\left\langle x_n, t_n \middle| x_{n-1}, t_{n-1} \right\rangle = \frac{1}{w\left(\Delta t\right)} \exp\left[ i \frac{S\left(n, n-1\right)}{\hbar} \right], \tag{3.279}$$

where $w\left(\Delta t\right)$ has the dimension of length. For $\Delta t \to 0$, we can make a straight-line approximation as

$$\begin{aligned} S\left(n, n-1\right) &= \int_{t_{n-1}}^{t_n} \mathrm{d}t \left[ \frac{m\dot{x}^2}{2} - V\left(x\right) \right] \\ &= \Delta t \left[ \frac{m}{2} \left( \frac{x_n - x_{n-1}}{\Delta t} \right)^2 - V\left( \frac{x_n + x_{n-1}}{2} \right) \right] \end{aligned}. \tag{3.280}$$

Because the weight $w\left(\Delta t\right)$ is assumed to be independent of $V\left(x\right)$, we may obtain it through the calculation of the free-particle case. We already know that, in the Heisenberg picture, for a free particle,

$$\left.\left\langle x_n, t_n \middle| x_{n-1}, t_{n-1} \right\rangle\right|_{t_n = t_{n-1}} = \delta\left(x_n - x_{n-1}\right). \tag{3.281}$$

On the other hand, Eq. (3.279) for a free particle becomes

$$\left\langle x_n, t_n \middle| x_{n-1}, t_{n-1} \right\rangle = \frac{1}{w\left(\Delta t\right)} \exp\left[ i \frac{m\left(x_n - x_{n-1}\right)^2}{2\hbar \Delta t} \right]. \tag{3.282}$$

Comparing the above two equations and using the fact that

$$\int_{-\infty}^{\infty} d\xi \exp\left( \frac{im\xi^2}{2\hbar\Delta t} \right) = \sqrt{\frac{2\pi i \hbar \Delta t}{m}} , \tag{3.283}$$

where $\xi \equiv x_N - x_{N-1}$, we determine that

$$w\left(\Delta t\right) = \sqrt{\frac{2\pi i \hbar \Delta t}{m}} . \tag{3.284}$$

For a pair of fixed starting point $\left\langle x_1, t_1 \right\rangle$ and ending point $\left\langle x_N, t_N \right\rangle$, we have

$$\exp\left[ i \frac{S\left(N, 1\right)}{\hbar} \right] = \exp\left[ \frac{i}{\hbar} \sum_{n=2}^{N} S\left(n, n-1\right) \right] = \prod_{n=2}^{N} \exp\left[ i \frac{S\left(n, n-1\right)}{\hbar} \right]. \tag{3.285}$$

According to Eq. (3.276) and Eq. (3.282), by using Eq. (3.285), we have

$$\begin{aligned}\langle x_N, t_N | x_1, t_1\rangle &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N-1}{2}}\int \mathrm{d}x_{N-1}\int \mathrm{d}x_{N-2}\cdots\int \mathrm{d}x_2 \prod_{n=2}^{N}\exp\left[\frac{iS(n,n-1)}{\hbar}\right]\\ &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N-1}{2}}\int \mathrm{d}x_{N-1}\int \mathrm{d}x_{N-2}\cdots\int \mathrm{d}x_2 \exp\left[\frac{iS(N,1)}{\hbar}\right]\end{aligned}, \tag{3.286}$$

whose meaning is the sum over all possible paths.

Define the integral operator

$$\int_{x_1}^{x_N}\mathscr{D}\left[x(t)\right] \equiv \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N-1}{2}}\int \mathrm{d}x_{N-1}\int \mathrm{d}x_{N-2}\cdots\int \mathrm{d}x_2 , \tag{3.287}$$

Eq. (3.286) can be written as

$$\langle x_N, t_N | x_1, t_1\rangle = \int_{x_1}^{x_N}\mathscr{D}\left[x(t)\right]\exp\left[i\int_{t_1}^{t_N}\mathrm{d}t\frac{L_{\text{classical}}(x,\dot{x})}{\hbar}\right], \tag{3.288}$$

which is known as **Feynman's path integral**.

Below we show that Feynman's formulation is completely equivalent to Schrödinger's wave mechanics.

In the limit $\Delta t \to 0$, we have

$$\begin{aligned}\langle x_N, t_N | x_1, t_1\rangle &= \int \mathrm{d}x_{N-1}\langle x_N, t_N | x_{N-1}, t_{N-1}\rangle\langle x_{N-1}, t_{N-1} | x_1, t_1\rangle\\ &= \int \mathrm{d}x_{N-1}\sqrt{\frac{m}{2\pi i\hbar\Delta t}}\exp\left[\frac{im}{2\hbar}\frac{(x_N - x_{N-1})^2}{\Delta t} - \frac{iV\Delta t}{\hbar}\right]\langle x_{N-1}, t_{N-1} | x_1, t_1\rangle\end{aligned}. \tag{3.289}$$

Letting $x_N \to x$ and $t_N \to t + \Delta t$, we obtain

$$\langle x, t+\Delta t | x_1, t_1\rangle = \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\int_{-\infty}^{\infty}\mathrm{d}\xi\exp\left(\frac{im\xi^2}{2\hbar\Delta t} - \frac{iV\Delta t}{\hbar}\right)\langle x-\xi, t | x_1, t_1\rangle . \tag{3.290}$$

By expanding $\langle x-\xi, t | x_1, t_1\rangle$ in powers of $\xi$ as well as $\langle x, t+\Delta t | x_1, t_1\rangle$ and $\exp(-iV\Delta t/\hbar)$ in powers of $\Delta t$, the above equation becomes

$$\begin{aligned}&\langle x, t | x_1, t_1\rangle + \Delta t\frac{\partial}{\partial t}\langle x, t | x_1, t_1\rangle = \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\int_{-\infty}^{\infty}\mathrm{d}\xi\exp\left(\frac{im\xi^2}{2\hbar\Delta t}\right)\left(1 - \frac{iV\Delta t}{\hbar} + \cdots\right)\\ &\times\left(\langle x, t | x_1, t_1\rangle + \frac{\xi^2}{2}\frac{\partial^2}{\partial x^2}\langle x, t | x_1, t_1\rangle + \cdots\right)\end{aligned}, \tag{3.291}$$

where a linear term of $\xi$ is dropped because it vanishes when integrated with respect to $\xi$. Using

$$\int_{-\infty}^{\infty}\mathrm{d}\xi\xi^2\exp\left(\frac{im\xi^2}{2\hbar\Delta t}\right) = \sqrt{2\pi}\left(\frac{i\hbar\Delta t}{m}\right)^{3/2} \tag{3.292}$$

and applying Eq. (3.283), we obtain

$$\Delta t \frac{\partial}{\partial t}\langle x,t|x_1,t_1\rangle = \frac{i\hbar\Delta t}{2m}\frac{\partial^2}{\partial x^2}\langle x,t|x_1,t_1\rangle - i\frac{\Delta t}{\hbar}V\langle x,t|x_1,t_1\rangle, \tag{3.293}$$

which shows that $\langle x,t|x_1,t_1\rangle$ satisfies the time-dependent Schrödinger wave equation

$$i\hbar\frac{\partial}{\partial t}\langle x,t|x_1,t_1\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\langle x,t|x_1,t_1\rangle + V\langle x,t|x_1,t_1\rangle. \tag{3.294}$$

# 3.6 Potentials and Gauge Transformations

### 3.6.1 Zero Point of the Potential Energy

Let $|\alpha,t_0;t\rangle$ be a state ket in the presence of potential $V(\mathbf{x})$, and $|\widetilde{\alpha,t_0;t}\rangle$ corresponds to $\tilde{V}(\mathbf{x}) = V(\mathbf{x}) + V_0$, where $V_0$ is a constant potential, and they are the same at $t=0$. According to Eq. (3.1) and Eq. (3.17),

$$\begin{aligned}|\widetilde{\alpha,t_0;t}\rangle &= \exp\left[-i\left(\frac{\mathbf{p}^2}{2m}+V(x)+V_0\right)\frac{(t-t_0)}{\hbar}\right]|\alpha,t_0\rangle \\ &= \exp\left[-i\frac{V_0(t-t_0)}{\hbar}\right]|\alpha,t_0;t\rangle\end{aligned}. \tag{3.295}$$

Therefore, the existence of $V_0$ does not affect the expect values of observables, but causes a phase difference that can be detected in experiment. This pure quantum-mechanical effect is different from the meaningless zero point of the potential energy in classical mechanics.

This is an example of **gauge transformations**. The change of the zero-point energy of the potential

$$V(\mathbf{x}) \to V(\mathbf{x}) + V_0 \tag{3.296}$$

must be accompanied by a change in the state ket

$$|\alpha,t_0;t\rangle \to \exp\left[-i\frac{V_0(t-t_0)}{\hbar}\right]|\alpha,t_0;t\rangle, \tag{3.297}$$

and thus the wave function

$$\psi(\mathbf{x}',t) \to \exp\left[-i\frac{V_0(t-t_0)}{\hbar}\right]\psi(\mathbf{x}',t). \tag{3.298}$$

If $V_0$ is spatially uniform but changes with time, the transformation in Eq. (3.297) becomes

$$|\alpha,t_0;t\rangle \to \exp\left[-i\int_{t_0}^{t}\mathrm{d}t'\frac{V_0 t'}{\hbar}\right]|\alpha,t_0;t\rangle. \tag{3.299}$$

### 3.6.2 Kinematic Momentum in Electromagnetism

The Hamiltonian for a particle of electric charge $e$ subjected to the electromagnetic field is

$$H=\frac{1}{2m}\left(\mathbf{p}-\frac{e\mathbf{A}}{c}\right)^2+e\phi=\frac{1}{2m}\left(p^2-\frac{e}{c}(\mathbf{p}\cdot\mathbf{A}+\mathbf{A}\cdot\mathbf{p})+\left(\frac{e}{c}\right)^2\mathbf{A}^2\right)+e\phi\,, \tag{3.300}$$

and the electric field $\mathbf{E}=-\nabla\phi$ and the magnetic field $\mathbf{B}=\nabla\times\mathbf{A}$. So

$$\frac{\mathrm{d}x_i}{\mathrm{d}t}=\frac{[x_i,H]}{i\hbar}=\frac{p_i-eA_i/c}{m}\,. \tag{3.301}$$

The **p** here is called **canonical momentum**, as distinguished from **kinematical** (or mechanical) **momentum**

$$\Pi\equiv m\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}=\mathbf{p}-\frac{e\mathbf{A}}{c}\,. \tag{3.302}$$

Although $[p_i,p_j]=0$, we have

$$[\Pi_i,\Pi_j]=\frac{i\hbar e}{c}\varepsilon_{ijk}B_k\,. \tag{3.303}$$

Rewriting the Hamiltonian as

$$H=\frac{\Pi^2}{2m}+e\phi \tag{3.304}$$

and using the fundamental commutation relation, we can derive the quantum-mechanical version of the **Lorentz force** as

$$m\frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2}=\frac{\mathrm{d}\Pi}{\mathrm{d}t}=e\left[\mathbf{E}+\frac{1}{2c}\left(\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}\times\mathbf{B}-\mathbf{B}\times\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}\right)\right], \tag{3.305}$$

which is Ehrenfest's theorem written in the Heisenberg picture for the charged particle in an electromagnetic field.

We now study Schrödinger's wave equation with $\phi$ and **A**. Because

$$\begin{aligned}&\langle\mathbf{x}'|\left[\mathbf{p}-\frac{e\mathbf{A}(\mathbf{x})}{c}\right]^2|\alpha,t_0;t\rangle=\left[-i\hbar\nabla'-\frac{e\mathbf{A}(\mathbf{x}')}{c}\right]\langle\mathbf{x}'|\left[\mathbf{p}-\frac{e\mathbf{A}(\mathbf{x})}{c}\right]|\alpha,t_0;t\rangle\\&=\left[-i\hbar\nabla'-\frac{e\mathbf{A}(\mathbf{x}')}{c}\right]\cdot\left[-i\hbar\nabla'-\frac{e\mathbf{A}(\mathbf{x}')}{c}\right]\langle\mathbf{x}'|\alpha,t_0;t\rangle\end{aligned}\,, \tag{3.306}$$

we have Schrödinger's wave equation

$$\begin{aligned}&\frac{1}{2m}\left[-i\hbar\nabla'-\frac{e\mathbf{A}(\mathbf{x}')}{c}\right]\cdot\left[-i\hbar\nabla'-\frac{e\mathbf{A}(\mathbf{x}')}{c}\right]\langle\mathbf{x}'|\alpha,t_0;t\rangle+e\phi(\mathbf{x}')\langle\mathbf{x}'|\alpha,t_0;t\rangle\\&=i\hbar\frac{\partial}{\partial t}\langle\mathbf{x}'|\alpha,t_0;t\rangle\end{aligned}\,. \tag{3.307}$$

From this equation we readily obtain the continuity equation

$$\frac{\partial\rho}{\partial t}+\nabla'\cdot\mathbf{j}=0\,, \tag{3.308}$$

where the probability density is still $\rho\equiv|\psi|^2=|\langle\mathbf{x}'|\alpha,t_0;t\rangle|^2$, but the probability flux

$$\mathbf{j}=\frac{\hbar}{m}\mathrm{Im}\left(\psi^*\nabla'\psi\right)-\frac{e}{mc}\mathbf{A}|\psi|^2\,. \tag{3.309}$$

Using Eq. (3.57), the flux can be rewritten as

$$\mathbf{j}=\frac{\rho}{m}\left(\nabla S-\frac{e\mathbf{A}}{c}\right), \tag{3.310}$$

different from the usual form of Eq. (3.59). The space integral of $\mathbf{j}$ is proportional to the expectation value of kinematical momentum:

$$\int \mathbf{j}\mathrm{d}^3x'=\frac{\langle \mathbf{p}-e\mathbf{A}/c\rangle}{m}=\frac{\langle \Pi\rangle}{m}. \tag{3.311}$$

### 3.6.3 Gauge Transformations in Electromagnetism

If we do the time-independent gauge transformation

$$\tilde{\phi}\to\phi,\quad \tilde{A}\to A+\nabla\Lambda, \tag{3.312}$$

and the state kets before and after the gauge transformation are $|\alpha\rangle$ and $|\tilde{\alpha}\rangle$, respectively. As in classical mechanics, $\langle\mathbf{x}\rangle$ and $\langle\Pi\rangle$ are expected not to change, whereas $\langle\mathbf{p}\rangle$ is expected to change. Therefore, along with normalization, the basic requirements are

$$\langle\alpha|\alpha\rangle=\langle\tilde{\alpha}|\tilde{\alpha}\rangle, \tag{3.313}$$

$$\langle\alpha|\mathbf{x}|\alpha\rangle=\langle\tilde{\alpha}|\mathbf{x}|\tilde{\alpha}\rangle, \tag{3.314}$$

and

$$\mathrm{a}\langle\alpha|\mathbf{p}-\frac{e\mathbf{A}}{c}|\alpha\rangle=\langle\tilde{\alpha}|\mathbf{p}-\frac{e\tilde{\mathbf{A}}}{c}|\tilde{\alpha}\rangle. \tag{3.315}$$

We must construct an operator $\mathscr{G}$ to relate the two state kets:

$$|\tilde{\alpha}\rangle=\mathscr{G}|\alpha\rangle \tag{3.316}$$

to satisfy the above requirements. Eqs. (3.314) and (3.315) are satisfied if

$$\mathscr{G}^{\dagger}\mathbf{x}\mathscr{G}=\mathbf{x} \tag{3.317}$$

and

$$\mathscr{G}^{\dagger}\left(\mathbf{p}-\frac{e\mathbf{A}}{c}-\frac{e\nabla\Lambda}{c}\right)\mathscr{G}=\mathbf{p}-\frac{e\mathbf{A}}{c}. \tag{3.318}$$

Below we will show that

$$\mathscr{G}=\exp\left[i\frac{e\Lambda(\mathbf{x})}{\hbar c}\right] \tag{3.319}$$

will do the job. First, the normalization requirement of Eq. (3.313) is obviously satisfied. Second, Eq. (3.317) is satisfied because $\mathbf{x}$ commutes with any function of $\mathbf{x}$. Finally, by using Eq. (3.165), we get

$$
\begin{aligned}
&\exp\left[-i\frac{e\Lambda(\mathbf{x})}{\hbar c}\right]\mathbf{p}\exp\left[i\frac{e\Lambda(\mathbf{x})}{\hbar c}\right]=\exp\left[-i\frac{e\Lambda(\mathbf{x})}{\hbar c}\right]\left[\mathbf{p},\exp\left[i\frac{e\Lambda(\mathbf{x})}{\hbar c}\right]\right]+\mathbf{p}\\
&=-\exp\left[-i\frac{e\Lambda(\mathbf{x})}{\hbar c}\right]i\hbar\nabla\exp\left[i\frac{e\Lambda(\mathbf{x})}{\hbar c}\right]+\mathbf{p}\\
&=\mathbf{p}+\frac{e\nabla\Lambda}{c}
\end{aligned}
\quad, \tag{3.320}
$$

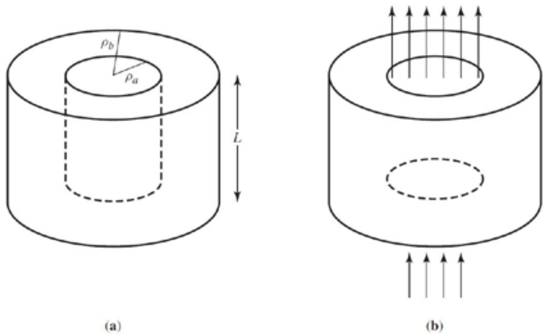
which demonstrates that Eq. (3.315) is also satisfied.

The probability flux relation is also gauge invariant if

$$
\rho\to\rho,\quad S\to S+\frac{e\Lambda}{c}\,. \tag{3.321}
$$

### 3.6.4 The Aharonov-Bohm Effect

The Aharonov-Bohm effect shows that the vector potential has detectable consequences in quantum mechanics.




Hollow cylindrical shell (a) without a magnetic field, (b) with a uniform magnetic field.

A uniform magnetic field $\mathbf{B}=B\hat{\mathbf{z}}$ is applied inside the cylinder. The corresponding vector potential to generate **B** is

$$
\mathbf{A}=\left(\frac{B\rho_a^2}{2\rho}\right)\hat{\boldsymbol{\phi}}\,, \tag{3.322}
$$

where $\hat{\boldsymbol{\phi}}$ is the unit vector in the direction of increasing azimuthal angle. In the Schrödinger equation, the gradient in cylindrical coordinates is expressed as:

$$
\boldsymbol{\nabla}=\hat{\boldsymbol{\rho}}\frac{\partial}{\partial\rho}+\hat{\mathbf{z}}\frac{\partial}{\partial z}+\hat{\boldsymbol{\phi}}\frac{1}{\rho}\frac{\partial}{\partial\phi}\,. \tag{3.323}
$$

For this problem, the gradient $\boldsymbol{\nabla}$ should be replaced by $\boldsymbol{\nabla}-(ie/\hbar c)\mathbf{A}$, which can be accomplished in Eq. (3.323) by

$$
\frac{\partial}{\partial\phi}\to\frac{\partial}{\partial\phi}-\frac{ie}{\hbar c}\frac{B\rho_a^2}{2}\,. \tag{3.324}
$$

This replacement allows the particle in the shell can also feel the influence of the vector potential.