Lecture Notes on Quantum Mechanics

Xueyu Wang(Pollack Wang)

September 1, 2024

Contents

Conventions

- In view of the lack of quality of the author, this review handout is for reference only, please contact the author in time if there are any errors $\boxed{\text{(QQ Mail:1446507095@qq.com or Google Mail:xueyuwang615@gmail.com)}}$.
- The content of this handout is made by the author, please contact the author for reprinting, and any means of protecting the rights of reasonable and legal copyright will be taken to deal with it without permission.

1 Basic Knowledge Points

(1)If an object can absorb all the radiation projected on it without reflection, this object is called an **absolute black body**, or **black body** for short.

(2)The energy unit hv is called **energy quantum**, h is Planck's constant, and its value is $h = 6.62606896(33)x10^{-34}J\mathring{u}s$.

(3)Electromagnetic radiation not only appears in the form of particles with energy hv when it is emitted and absorbed, but also moves in space at a speed c in this form. This particle is called a **light quantum or photon**.

(4)The photoelectric effect is that when light shines on a metal, electrons escape from the metal. This electron is called a **photoelectron**.

(5)Any phenomenon in which h plays an important role can be called a **quantum phenomenon**.

(6)Light has the dual properties of particles and waves, and this property is called **wave-particle duality**.

(7)In order to determine the possible orbits of electron motion, Bohr proposed the quantization condition: in quantum theory, angular momentum must be an integer multiple of h.

(8)de Broglie formula

$$\begin{aligned} E &= h\nu = \hbar\omega, \\ \boldsymbol{p} &= \frac{h}{\lambda}\boldsymbol{n} = \hbar\boldsymbol{k}. \end{aligned} \tag{1}$$

(9)A function represents the wave that describes a particle, and this function is called a **wave function**. It is a complex number.

(10)**Statistical interpretation of wave function:** The intensity of the wave function at a point in space (the square of the absolute value of the amplitude) is proportional to the probability of finding the particle at that point. According to this interpretation, the wave describing the particle is a probability wave.

(11)The wave function should generally satisfy three conditions in the entire region where the variable changes: **finiteness, continuity, and measurable single value**. These three conditions are called **the standard conditions of the wave function**.

(12)Energy has a definite value, so this state is called a **steady state**.

(13)The particle is bound inside the potential well. The state described by the wave function that is zero at infinity is usually called a **bound state**. Generally speaking, the energy levels to which the bound state belongs are discrete.

(14)The lowest energy state of a system is called the **ground state**.

(15)The phenomenon that particles can still penetrate a potential barrier when their energy E is less than the potential barrier height is called **tunneling**.

(16)This normalization method of confining particles in a three-dimensional box and adding periodic boundary conditions is called **box normalization**.

(17)If two operators $\hat{F}$ and $\hat{G}$ have a set of common eigenfunctions ϕ_n, and ϕ_n forms a complete system, then operators $\hat{F}$ and $\hat{G}$ commute.

(18)The operation of changing the sign of all coordinate variables of a function $(x \to -x)$ is called spatial inversion. This operation is represented by the operator $\hat{P}$:

$$\hat{P}\Psi(x,t) = \Psi(-x,t), \tag{2}$$

We call $\hat{P}$ the **parity operator**.

(19)The specific representation of states and mechanical quantities in quantum mechanics is called **representation**.

2 Some Mathematical Background

$|\psi\rangle$ and $\langle\mathit{\Psi}|$
$\langle\mathit{\Psi}|\psi\rangle$.

Definition 2.1. Euler equation

An equation of the form:

$$x^n y^{(n)} + P_1 x^{n-1} y^{(n-1)} + \cdots + P_{n-1} x y' + P_n y = f(x) \tag{3}$$

(where $P_1, P_2, \cdots, P_n$is a constant), is known as **Euler's equation**.
Here, we might as well make $x = e^t$,then

$$\frac{dy}{dx} = \frac{dy}{dt} \cdot \frac{dt}{dx} = \frac{1}{x} \cdot \frac{dy}{dt} \tag{4}$$

$$\begin{aligned} \frac{d^2y}{dx^2} &= \frac{d\frac{dy}{dx}}{dx} = \frac{d(\frac{1}{x}\frac{dy}{dt})}{dx} = \frac{-\frac{1}{x^2} \cdot \frac{dy}{dt}dx + \frac{1}{x} \cdot d(\frac{dy}{dt})}{dx} = -\frac{1}{x^2}\frac{dy}{dt} + \frac{1}{x} \cdot \frac{d(\frac{dy}{dt})}{dt} \cdot \frac{dt}{dx} = -\frac{1}{x^2}\frac{dy}{dt} \\ &+ \frac{1}{x^2}\frac{d^2y}{dt^2} = \frac{1}{x^2}(\frac{d^2y}{dt^2} - \frac{dy}{dt}) \end{aligned} \tag{5}$$

$$\frac{d^3y}{dx^3} = \frac{1}{x^3}\left(\frac{d^3y}{dt^3} - 3\frac{d^2y}{dt^2} + 2\frac{dy}{dt}\right) \tag{6}$$

If the notation D is used at this point to denote the operation of derivation from t, i.e., $\frac{d}{dt}$ denotes.
So we can get

$$\begin{aligned} xy' &= Dy, \\ x^2y'' &= D(D-1)y, \\ x^3y''' &= D(D-1)(D-2)y \end{aligned} \tag{7}$$

Generally,

$$x^k y^{(k)} = D(D-1)(D-2)\cdots(D-k+1)y \tag{8}$$

Theorem 2.2. Euler's formula

$$e^{ix} = \cos x + i\sin x \tag{9}$$

$$e^{-ix} = \cos x - i\sin x \tag{10}$$

2.3 Prove

$$\boxed{\int_0^\infty x^{2n}e^{-ax^2}dx = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n+1}a^n}\sqrt{\frac{\pi}{a}}} \tag{11}$$

2.4 Prove

$$\boxed{\int_0^\infty e^{-ax^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}} \tag{12}$$

Proof.

$$\begin{aligned} \left[\int_{-\infty}^{\infty} e^{-x^2}dx\right]^2 &= \int_{-\infty}^{\infty} e^{-x^2}dx \int_{-\infty}^{\infty} e^{-y^2}dy \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-(x^2+y^2)}dxdy = \int_0^{2\pi}\int_0^\infty e^{r^2}rdrd\theta \\ &= -\frac{1}{2}\int_0^{2\pi}\int_0^\infty e^{-r^2}(-2rdr)d\theta = [\sqrt{\pi}]^2 \end{aligned} \tag{13}$$

Taking the square root of both sides, we have

$$\int_{-\infty}^{\infty} e^{-x^2}dx = \sqrt{\pi} \tag{14}$$

$$\int_{-\infty}^{\infty} e^{-ax^2}dx = \frac{1}{\sqrt{a}}\int_{-\infty}^{\infty} e^{y^2}dy = \frac{\sqrt{\pi}}{\sqrt{a}} \quad (y = \sqrt{a}x) \tag{15}$$

Consider an even function

$$\therefore \int_0^\infty e^{-ax^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{a}} \tag{16}$$

Q.E.D.

😎

2.5 Prove

$$\boxed{\int_{-\infty}^{\infty}\cos(bx)e^{-a^2x^2}dx = \frac{\sqrt{\pi}}{a}e^{-\frac{b^2}{4a^2}}} \tag{17}$$

2.6 Prove

$$\boxed{\int_0^\infty x^n e^{-ax}dx = \frac{n!}{a^{n+1}}} \tag{18}$$

Proof. Look at a special case

$$
\begin{aligned}
\int_0^\infty e^{-ax}x^2dx &= -\frac{1}{a}\int_0^\infty x^2de^{-ax} = -\frac{1}{a}(x^2e^{-ax}\Big|_0^\infty - 2\int_0^\infty e^{-ax}xdx) \\
&= \frac{2}{a}\int_0^\infty e^{-ax}xdx = \frac{2}{a}\cdot(-\frac{1}{a})\int_0^\infty xde^{-ax} \\
&= -\frac{2}{a^2}(x\cdot e^{-ax}\Big|_0^\infty - \int_0^\infty e^{-ax}dx) = \frac{2}{a^2}\int_0^\infty e^{-ax}dx \\
&= -\frac{2}{a^3}\int_0^\infty de^{-ax} = -\frac{2}{a^3}e^{-ax}\Big|_0^\infty = \boxed{\frac{2}{a^3}}
\end{aligned} \tag{19}
$$

Q.E.D.

😎

3 Reference Solution to The Exercises

3.1 Exercise 1:Textbook(P11)

1.2

Proof. .
As can be seen from the title, this is a non-relativistic case.

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} = \boxed{7.09\times 10^{-10}m} \tag{20}$$

However, it should be noted that

$$E = 3eV = 3\times 1.60\times 10^{-19}J$$

😎

3.2 Exercise 2:Textbook(P39,P44-45)

Definition 3.1. Examples

Suppose the width of the one-dimensional infinite square potential well is a. Find the momentum distribution of the particle in the ground state.

Proof.

$$\begin{cases} -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi(x), \quad 0<x<a. \\ \psi(0)=0, \quad \psi(a)=0. \end{cases} \tag{21}$$

$$\psi''(x)+k^2\psi(x)=0, \quad where\ k\equiv\sqrt{2mE/\hbar}. \tag{22}$$

$$\Rightarrow \psi(x) = A\sin(kx+\delta) \tag{23}$$

According to the boundary conditions

$$\psi(0)=0, \quad \psi(0)=A\sin\delta=0, \tag{24}$$

$$\psi(a)=A\sin(ka)=0 \tag{25}$$

$$\Rightarrow \delta=0. \quad \psi(x)=A\sin kx. \tag{26}$$

$$\Rightarrow ka=n\pi, \quad k_n=n\pi/a, \quad n=1,2,\cdots. \tag{27}$$

Therefore, the solution to the Schrödinger equation is (normalized)

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right), & 0<x<a, \\ 0, & x<0, x>a, \end{cases} \tag{28}$$

$$E_n = \frac{\hbar^2k_n^2}{2m} = \frac{1}{2m}\left(\frac{n\pi\hbar}{a}\right)^2, \quad n=1,2,\cdots. \tag{29}$$

The ground state wave function is

$$\psi_1(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) \tag{30}$$

The momentum eigenfunction can be expanded

$$\psi_1(x) = \int C_1(p)\,\psi_p(x)\,\mathrm{d}p, \quad \psi_p(x) = \frac{\mathrm{e}^{\mathrm{i}px/\hbar}}{\sqrt{2\pi\hbar}}, \tag{31}$$

$$\begin{aligned} C_1(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px}\mathrm{d}x \\ &= -\frac{1}{\sqrt{2\pi\hbar}}\sqrt{\frac{2}{a}}\frac{1}{2}\left[\frac{\mathrm{e}^{\mathrm{i}\left(\frac{\pi}{a}-\frac{p}{\hbar}\right)a}-1}{\frac{\pi}{a}-\frac{p}{\hbar}} + \frac{\mathrm{e}^{-\mathrm{i}\left(\frac{\pi}{a}+\frac{p}{\hbar}\right)a}-1}{\frac{\pi}{a}+\frac{p}{\hbar}}\right]. \end{aligned} \tag{32}$$

Finally, the momentum distribution of the ground state particle is $|C_1(p)|^2$.

😎

Proposition 3.2. Infinitely deep square well

One-dimensional symmetric infinite deep square potential well

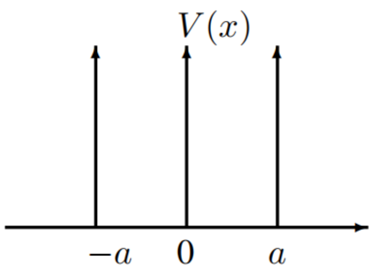

Figure 1: Schematic diagram of a one-dimensional symmetric infinite deep square potential well

The potential of a one-dimensional symmetric infinite-depth square potential well is expressed as

$$V(x) = \begin{cases} \infty & |x| > a \\ 0 & |x| < a \end{cases} \tag{33}$$

Now find the wave function of the particle in the potential well.
(1) Outside the well ($|x| > a$), the particle will not escape the infinitely deep "well", that is, $\psi = 0$.
(2) Inside the well ($|x| < a$), $V(x) = 0$, and the steady-state Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi \quad \Longrightarrow \quad \frac{d^2}{dx^2}\psi + \frac{2mE}{\hbar^2}\psi = 0 \tag{34}$$

Let $k^2 = \frac{2mE}{\hbar^2}$, then

$$\frac{d^2}{dx^2}\psi + k^2\psi = 0 \tag{35}$$

This is a standard second-order homogeneous linear equation with constant coefficients. Its solutions have three equivalent forms

$$\psi = A\cos kx + B\sin kx \tag{36}$$

$$\psi = Ce^{ikx} + C'e^{-ikx} \tag{37}$$

$$\psi = D\sin(kx+\delta) \tag{38}$$

Using boundary conditions

$$\begin{cases} A\sin ka + B\cos ka = 0 \\ -A\sin ka + B\cos ka = 0 \end{cases} \tag{39}$$

$$\Rightarrow \begin{cases} A\sin ka = 0 \\ B\cos ka = 0 \end{cases} \tag{40}$$

A and B cannot be zero at the same time, otherwise $\psi = 0$, that is, ψ is zero everywhere, which is physically meaningless, and the solution is

$$\begin{aligned} &(i) \quad A = 0, \quad \cos ka = 0 \quad \Longrightarrow \quad ka = n\frac{\pi}{2}, \quad k = \frac{n\pi}{2a}(n\,is\,an\,odd\,number) \\ &(ii) \quad B = 0, \quad \sin ka = 0 \quad \Longrightarrow \quad ka = n\frac{\pi}{2}, \quad k = \frac{n\pi}{2a}(n\,is\,an\,even\,number) \end{aligned} \tag{41}$$

Since $k^2 = \frac{2mE}{\hbar^2}$, we have

$$\frac{2mE}{\hbar^2}a^2 = \frac{n^2\pi^2}{4} \tag{42}$$

That is

$$E_n = \frac{n^2\pi^2\hbar^2}{8ma^2} \tag{43}$$

The obtained wave function is

$$\psi_n = \begin{cases} B\cos\frac{n\pi}{2a}x, & n\,is\,an\,odd\,number, \quad |x|<a \\ 0 & |x|>a \end{cases}, \quad \psi_n = \begin{cases} A\sin\frac{n\pi}{2a}x, & n\,is\,an\,even\,number, |x|<a \\ 0 & |x|>a \end{cases} \tag{44}$$

Combining the two formulas,

$$\psi_n = \begin{cases} D\sin\frac{n\pi}{2a}(x+a) & |x|<a \\ 0 & |x|>a \end{cases} \tag{45}$$

Wave function normalization

$$\begin{aligned} 1 &= \int \psi^*\psi d\tau = \int_{-a}^{a} D^2\sin^2\frac{n\pi}{2a}(x+a)dx = D^2\int_{-a}^{a}\left[\frac{1}{2}x - \frac{1}{2}\cos\frac{n\pi}{a}(x+a)\right]dx \\ &= D^2\left[\frac{1}{2}x\Big|_{-a}^{a} - \frac{1}{2}\frac{a}{n\pi}\sin\frac{n\pi}{a}(x+a)|_{-a}^{a}\right] = D^2a \end{aligned} \tag{46}$$

$$\Rightarrow D = \frac{1}{\sqrt{a}} \tag{47}$$

The normalized wave function is

$$\psi_n = \begin{cases} \frac{1}{\sqrt{a}}\sin\frac{n\pi}{2a}(x+a) & |x|<a \\ 0 & |x|>a \end{cases} \tag{48}$$

Q.E.D.

Proposition 3.3. Asymmetric potential well

Asymmetric one-dimensional infinite depth square potential well

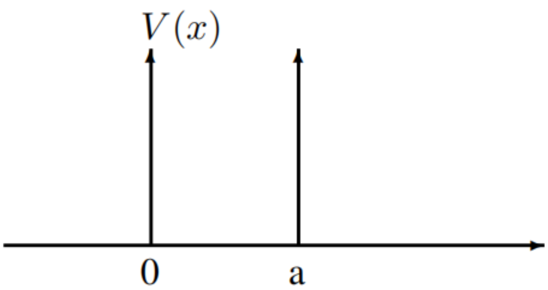

Figure 2: Schematic diagram of a asymmetric one-dimensional infinite depth square potential well

$$V(x) = \begin{cases} 0 & 0<x<a \\ \infty & x\leqslant 0, x\geqslant a \end{cases} \tag{49}$$

(1) Outside the potential well, $\psi = 0$;
(2) Inside the potential well ($0<x<a$), the Schrödinger equation is

$$\frac{d^2}{dx^2}\psi + \frac{2mE}{\hbar^2}\psi = 0 \tag{50}$$

Let$k = \sqrt{\frac{2mE}{\hbar^2}}$, then the solution can be expressed as
According to the boundary conditions, continuity (wave function must be: continuous, finite, single value), we have

$$\begin{cases} \psi(0) = 0 & \Longrightarrow A\sin\delta = 0 \longrightarrow \delta = 0, A\neq 0\,(Otherwise\,it's\,meaningless.) \\ \psi(a) = 0 & \Longrightarrow \sin ka = 0 \longrightarrow ka = n\pi, n = 1,2,3,\cdots \end{cases} \tag{51}$$

Then

$$E = E_n = \frac{\hbar^2\pi^2n^2}{2ma^2} \tag{52}$$

$$\psi_n(x) = A\sin\frac{n\pi x}{a} \tag{53}$$

where $n = 1, 2, 3, \cdots$. Normalize the wave function

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} \tag{54}$$

Q.E.D.

Proposition 3.4. δ potential barrier

Assume there is a one-dimensional δ potential barrier at $x = a$

$$U(x) = A\delta(x-a)(A > 0)$$

A particle with energy E is incident from the left. Find the transmission coefficient.

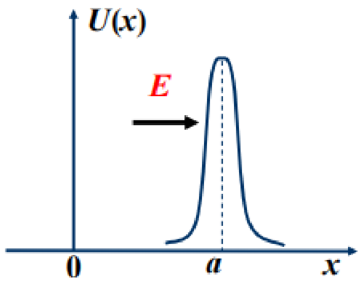

Figure 3: Schematic diagram of a one-dimensional delta barrier

Proof.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + A\delta(x-a)\psi(x) = E\psi(x) \tag{55}$$

Obviously, $\frac{d^2\psi(x)}{dx^2}$ diverges at $x = a$. Integrating the equation in the interval $[a-\varepsilon, a+\varepsilon]$, we have

$$-\frac{\hbar^2}{2m}[\psi'(a+\varepsilon) - \psi'(a-\varepsilon)] + A\psi(a) = E\int_{a-\varepsilon}^{a+\varepsilon}\psi(x)dx \xrightarrow{\varepsilon\to 0} 0 \tag{56}$$

The transition condition can be obtained

$$\boxed{\psi'(a+\varepsilon) - \psi'(a-\varepsilon) = \frac{2mA}{\hbar^2}\psi(a)} \tag{57}$$

It can be seen that $\psi'(x)$ is not continuous. However, in this problem, the particle probability is continuous, so $\psi(x)$ is continuous. The wave function can be expressed as

$$\psi(x) = \begin{cases} e^{ik(x-a)} + Re^{-ik(x-a)}, & x < a \\ Se^{ik(x-a)}, & x > a \end{cases} \tag{58}$$

where the wave vector $k = \frac{\sqrt{2mE}}{\hbar}$.
Substituting the wave function into the transition condition, we have

$$\boxed{ik(S - 1 + R) = \frac{2mA}{\hbar^2}S} \tag{59}$$

At $x = a$, according to the continuity of the wave function, we have

$$\boxed{1 + R = S} \tag{60}$$

Eliminating R, the transmission coefficient is

$$T = |S|^2 = \frac{1}{(1 + \frac{m^2A^2}{\hbar^4k^2})} = \frac{1}{(1 + \frac{mA^2}{2\hbar^2E})} \tag{61}$$

Q.E.D.

Remark. It is easy to prove that $J(x)$ is continuous at $x = a$.
Firstly

$$
\begin{aligned}
&\psi(a-\varepsilon)=1+R=S \\
&\psi(a+\varepsilon)=S \\
&\psi'(a-\varepsilon)=ik(1-R)=ikS-\frac{2mA}{\hbar^2}S \\
&\psi'(a+\varepsilon)=ikS
\end{aligned} \tag{62}
$$

According to the probability flow density formula, for the one-dimensional case,

$$
J_x=\frac{i\hbar}{2m}\left(\psi(x)\frac{d\psi(x)^*}{dx}-\psi(x)^*\frac{d\psi(x)}{dx}\right) \tag{63}
$$

When $x<a$

$$
\begin{aligned}
J_x(a-\varepsilon)&=\frac{i\hbar}{2m}\left[S\cdot\left(ikS-\frac{2mA}{\hbar^2}S\right)^*-S^*\cdot\left(ikS-\frac{2mA}{\hbar^2}S\right)\right] \\
&=\frac{i\hbar}{2m}|S|^2\left(-ik-\frac{2mA}{\hbar^2}-ik+\frac{2mA}{\hbar^2}\right) \\
&=\frac{i\hbar}{2m}|S|^2(-2ik) \\
&=\frac{\hbar k}{m}|S|^2
\end{aligned} \tag{64}
$$

When $x>a$

$$
\begin{aligned}
J_x(a+\varepsilon)&=\frac{i\hbar}{2m}\left[S\cdot(ikS)^*-S^*\cdot ikS\right] \\
&=\frac{i\hbar}{2m}|S|^2\,(-2ik) \\
&=\frac{\hbar k}{m}|S|^2
\end{aligned} \tag{65}
$$

It can be seen that the probability flow density $J(x)$ is continuous at $x=a$.

Q.E.D.

Definition 3.5. Be normalized

The normalization constant is independent of time.

Proof. In the following, I will use two methods to prove.
Method I:

$$
\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{+\infty}\left|\Psi(\,x\,,t\,)\right|^2\mathrm{d}x=\int_{-\infty}^{+\infty}\frac{\partial}{\partial t}\left|\Psi(\,x\,,t\,)\right|^2\mathrm{d}x. \tag{66}
$$

(Note that the integral is a function of t only, so the full derivative (d/dt) is used in the first expression, while the product function is a function of both x and t, so the partial derivative $(\partial/\partial t)$ is used in the second expression.)By the rule of derivation

$$
\frac{\partial}{\partial t}\mid\Psi\mid^2=\frac{\partial}{\partial t}(\,\Psi^*\Psi)\;=\Psi^*\frac{\partial\Psi}{\partial t}+\frac{\partial\Psi^*}{\partial t}\Psi. \tag{67}
$$

Schrödinger's equation can be written

$$
\frac{\partial\Psi}{\partial t}=\frac{\mathrm{i}\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2}-\frac{\mathrm{i}}{\hbar}V\Psi \tag{68}
$$

and its conjugate

$$
\frac{\partial\Psi^*}{\partial t}=-\frac{\mathrm{i}\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2}+\frac{\mathrm{i}}{\hbar}V\Psi^* \tag{69}
$$

Therefore

$$
\frac{\partial}{\partial t}\left|\Psi\right|^2=\frac{\mathrm{i}\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2}-\frac{\partial^2\Psi^*}{\partial x^2}\Psi\right)=\frac{\partial}{\partial x}\left[\frac{\mathrm{i}\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)\right] \tag{70}
$$

$$
\Rightarrow\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{+\infty}\mid\Psi(x,t)\mid^2\mathrm{d}x=\frac{\mathrm{i}\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)\bigg|_{-\infty}^{+\infty}. \tag{71}
$$

But as $x\to\pm\infty$,$\Psi(x,t)$ must $\to 0$ - otherwise the wave function is not normalizable.In this way there is

$$
\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{+\infty}\mid\Psi(x,t)\mid^2\mathrm{d}x=0 \tag{72}
$$

Thus the integral is a constant (not dependent on time); if $\boldsymbol{\Psi}$ is normalized at $t=0$, it remains normalized at all subsequent moments.

Q.E.D.

😎

Definition 3.6. Probability flow density

Prove that in the steady state, the probability flow density is independent of time.

Proof. We have two ways to prove this.
Method I

$$\begin{aligned}\Psi(\boldsymbol{r},t) &= \psi(\boldsymbol{r})f(t)\\ &= \psi(\boldsymbol{r})e^{-\frac{i}{\hbar}Et}\end{aligned} \tag{73}$$

$$\begin{aligned}\boldsymbol{J}(\boldsymbol{r},t) &= \frac{i\hbar}{2m}\{\psi(r)e^{-\frac{i}{\hbar}Et}\nabla[\psi^*(r)e^{\frac{i}{\hbar}Et}] - \psi^*(r)e^{\frac{i}{\hbar}Et}\nabla[\psi(r)e^{-\frac{i}{\hbar}Et}]\}\\ &= \frac{i\hbar}{2m}[\psi(r)\nabla\psi^*(r) - \psi^*(r)\nabla\psi(r)] = J(r)\end{aligned} \tag{74}$$

It is easy to see that the above results are independent of time.
Method II
The stationary wave function satisfies the relation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(r,t) = E\Psi(r,t) \tag{75}$$

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi^*(r,t) = -E\Psi^*(r,t) \tag{76}$$

Therefore, there is

$$\begin{aligned}\frac{\partial J}{\partial t} &= \frac{\mathrm{i}\hbar}{2m}\left(\frac{\partial\Psi}{\partial t}\nabla\Psi^* + \Psi\nabla\frac{\partial\Psi^*}{\partial t} - \frac{\partial\Psi^*}{\partial t}\nabla\Psi - \Psi^*\nabla\frac{\partial\Psi}{\partial t}\right)\\ &= \frac{1}{2m}(E\Psi\nabla\Psi^* - E\Psi\nabla\Psi^* + E\Psi^*\nabla\Psi - E\Psi^*\nabla\Psi) = 0\end{aligned} \tag{77}$$

Q.E.D.

😎

3.3 Exercise 3:Textbook(P91)

3.1

$$\psi(x) = \sqrt{\frac{\alpha}{\pi^{\frac{1}{2}}}}\exp\left(-\frac{\alpha^2x^2}{2} - \frac{i}{2}\omega t\right) \tag{78}$$

Proof. .
Normalization:

$$\begin{aligned}&\int_{-\infty}^{+\infty}|\Psi(x)|^2\,dx = \int_{-\infty}^{+\infty}\Psi^*(x)\cdot\Psi(x)dx\\ &= \int_{-\infty}^{+\infty}\sqrt{\frac{\alpha}{\sqrt{\pi}}}e^{-\frac{1}{2}\alpha^2x^2+\frac{i}{2}\omega t}\cdot\sqrt{\frac{\alpha}{\sqrt{\pi}}}e^{-\frac{1}{2}\alpha^2x^2-\frac{i}{2}\omega t}dx\\ &= \frac{\alpha}{\sqrt{\pi}}\int_{-\infty}^{+\infty}e^{-\alpha^2x^2}dx = \frac{\alpha}{\sqrt{\pi}}\cdot\frac{\sqrt{\pi}}{\alpha} = 1.\end{aligned} \tag{79}$$

(1)

$$\begin{aligned}&\overline{U} = \int\psi^*(x)\hat{u}\psi(x)dx = \int_{-\infty}^{+\infty}\sqrt{\frac{\alpha}{\sqrt{x}}}e^{-\frac{1}{2}\alpha^2x^2+\frac{i}{2}\omega t}\cdot\frac{1}{2}mw^2x^2\sqrt{\frac{\alpha}{\sqrt{\pi}}}e^{-\frac{1}{2}\alpha^2x^2-\frac{i}{2}\omega t}dx\\ &= \frac{\alpha}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{1}{2}mw^2x^2e^{-\alpha^2x^2}dx = \frac{\alpha}{\sqrt{\pi}}\cdot\frac{1}{2}mw^2\int_{-\infty}^{+\infty}x^2\cdot e^{-\alpha^2x^2}dx(An\ even\ function)\\ &= \frac{\alpha}{\sqrt{\pi}}\cdot\frac{1}{2}mw^2\cdot 2\times\frac{1}{2^{1+1}(\alpha^2)}\cdot\sqrt{\frac{\pi}{\alpha^2}} = \frac{1}{4}\frac{mw^2}{\alpha^2}(where\ \alpha = \sqrt{\frac{mw}{\hbar}})\\ &= \boxed{\frac{1}{4}\hbar\omega}\end{aligned} \tag{80}$$

(2)
For the ground state energy,$n=0$,$E_0 = (0+\frac{1}{2})\hbar\omega = \frac{1}{2}\hbar\omega$,considering $E_n = \overline{T} + \overline{U}$

$$\therefore \overline{T} = E_0 - \overline{U} = \frac{1}{2}\hbar\omega - \frac{1}{4}\hbar\omega = \boxed{\frac{1}{4}\hbar\omega} \tag{81}$$

You can also use the definition.

$$\hat{T} = \frac{\hat{\overline{P}}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \tag{82}$$

$$\begin{aligned}
\overline{T} &= \int_{-\infty}^{+\infty} \sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-\frac{1}{2}\alpha^2x^2 + \frac{i}{2}wt}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-\frac{1}{2}\alpha^2x^2 - \frac{1}{2}\omega t} dx \\
&= -\frac{\hbar^2}{2m}\frac{\alpha}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-\frac{1}{2}\alpha^2x^2} \cdot (e^{-\frac{1}{2}\alpha^2x^2})'' dx \\
&= \boxed{\frac{1}{4}\hbar\omega}
\end{aligned} \tag{83}$$

Similarly

$$\begin{aligned}
\overline{P} &= \int \psi^*(-i\hbar\frac{d}{dx})\psi dx \\
&= -i\hbar\int_{-\infty}^{+\infty} \sqrt{\frac{\alpha}{\sqrt{x}}} e^{-\frac{1}{2}\alpha^2x^2}\left(\sqrt{\frac{\alpha}{\sqrt{x}}} e^{-\frac{1}{2}\alpha^2x^2}\right)' dx = \boxed{0}
\end{aligned} \tag{84}$$

(3)

One-dimensional case momentum orthogonal normalized system $\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px}$

$$\begin{cases}
\psi(x) = \int_{-\infty}^{+\infty} c_p \cdot \psi_p(x) dp \\
c_p = \int_{-\infty}^{+\infty} \psi(x) \cdot \psi_p^*(x) dx = \int_{-\infty}^{+\infty} \sqrt{\frac{\alpha}{\pi}} e^{-\frac{1}{2}\alpha^2x^2} \times \left(\frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px}\right)^*
\end{cases} \tag{85}$$

$$\begin{aligned}
Original\ formula &= \frac{1}{\sqrt{2\pi\hbar}}\sqrt{\frac{\alpha}{\sqrt{\pi}}}\int_{-\infty}^{+\infty} e^{-\frac{1}{2}\alpha^2x^2}\left[\cos\left(\frac{p}{\hbar}x\right) - i\sin\left(\frac{p}{\hbar}x\right)\right](Euler's\ formula.) \\
&= \frac{1}{\sqrt{2\pi\hbar}}\sqrt{\frac{\alpha}{\sqrt{\pi}}}\int_{-\infty}^{+\infty} e^{-\frac{1}{2}\alpha^2x^2}\cos\left(\frac{p}{\hbar}x\right) dx(Odd\ functions.) \\
&= \sqrt{\frac{1}{\alpha\hbar\sqrt{\pi}}} e^{-\frac{p^2}{2\alpha^2\hbar^2}}
\end{aligned} \tag{86}$$

The probability distribution function of momentum is

$$|c_p|^2 = c_p^* \cdot c_p = \boxed{\frac{1}{\alpha\hbar\sqrt{\pi}} e^{-\frac{p^2}{\alpha^2\hbar^2}}} \tag{87}$$

Q.E.D.

😎

Remark. .
1.Note the use of Euler's formula.
2.Note the characteristics of odd functions in symmetric intervals.

3.2

$$\psi(r,\theta,\varphi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}} \tag{88}$$

Proof. Normalization:

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{+\infty} |\Psi(r)|^2 r^2 \sin\theta dr d\theta d\varphi = 4\pi\int_0^{+\infty} \frac{1}{\pi a^3} e^{-\frac{2r}{a_0}} dr = \frac{4}{a^3}\cdot\frac{2!}{(\frac{2}{a_0})^{2+1}} = 1 \tag{89}$$

(1)

$$\begin{aligned}
\overline{r} &= \int_0^{2\pi}\int_0^{\pi}\int_0^{+\infty} \psi^* r\psi r^2 \sin\theta dr d\theta d\varphi \\
&= \int_0^{2\pi}\int_0^{\pi}\int_0^{+\infty} \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}} r \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}} r^2 \sin\theta dr d\theta d\varphi \\
&= \frac{1}{\pi a_0^3} 4\pi \int_0^{+\infty} e^{-\frac{2r}{a_0}} r^3 dr = \boxed{\frac{3}{2}a_0}
\end{aligned} \tag{90}$$

(2)

$$\begin{aligned}\overline{U} &= \iint d\omega \int_0^{+\infty} \psi^*(r)\frac{-e_s^2}{r}\psi(r)r^2dr \\ &= 4\pi\frac{-e_s^2}{\pi a_0^3}\int_0^{+\infty} e^{-\frac{2r}{a_0}}rdr = \boxed{\frac{e_s^2}{a_0}}\end{aligned} \tag{91}$$

(3)
The probability of an electron appearing in the $r+dr$ shell is

$$\omega(r)dr = \int_0^{\pi}\int_0^{2\pi}[\psi(r,\theta,\varphi)]^2r^2\sin\theta drd\theta d\varphi = \frac{4}{a_0^3}e^{-2r/a_0}r^2dr \tag{92}$$

$$\Rightarrow \omega(r) = \frac{4}{a_0^3}e^{-2r/a_0}r^2 \tag{93}$$

At this time

$$\frac{d\omega(r)}{dr} = \frac{4}{a_0^3}(2-\frac{2}{a_0}r)re^{-2r/a_0} \tag{94}$$

Making

$$\frac{d\omega(r)}{dr} = 0, \Rightarrow r_1 = 0, \quad r_2 = \infty, \quad r_3 = a_0 \tag{95}$$

When $r_1 = 0, r_2 = \infty, \omega(r) = 0$ is the position with the minimum probability.
Further

$$\begin{aligned}\frac{d^2\omega(r)}{dr^2} &= \frac{4}{a_0^3}(2-\frac{8}{a_0}r+\frac{4}{a_0^2}r^2)e^{-2r/a_0} \\ \frac{d^2\omega(r)}{dr^2}\Big|_{r=a_0} &= -\frac{8}{a_0^3}e^{-2} < 0\end{aligned} \tag{96}$$

$\therefore r = a_0$ is the most probable radius.
(4)

$$\hat{T} = \frac{1}{2m}\hat{p}^2 = -\frac{\hbar^2}{2m}\nabla \tag{97}$$

$$(\text{Note:} \boxed{\nabla^2 = \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial}{\partial\varphi^2}\right]})$$

$$\begin{aligned}\overline{T} &= -\frac{\hbar^2}{2m}\int_0^{\pi}\int_0^{2\pi}\int_0^{\infty}\frac{1}{\pi a_0^3}e^{-r/a_0}\nabla^2(e^{-r/a_0})r^2\sin\theta drd\theta d\varphi \\ &= -\frac{\hbar^2}{2m}\int_0^{\pi}\int_0^{2\pi}\int_0^{\infty}\frac{1}{\pi a_0^3}e^{-r/a_0}\frac{1}{r^2}\frac{d}{dr}[r^2\frac{d}{dr}(e^{-r/a_0})]r^2\sin\theta drd\theta d\varphi \\ &= -\frac{4\hbar^2}{2ma_0^3}(-\frac{1}{a_0})\int_0^{\infty}(2r-\frac{r^2}{a_0})e^{-r/a_0}dr \\ &= \frac{4\hbar^2}{2ma_0^4}(2\frac{a_0^2}{4}-\frac{a_0^2}{4}) = \boxed{\frac{\hbar^2}{2ma_0^2}}\end{aligned} \tag{98}$$

(5)

$$
\begin{aligned}
c(p) &= \int \psi_{\vec{p}}^{*}(\vec{r})\psi(r,\theta,\varphi)d\tau \\
&= \frac{1}{(2\pi\hbar)^{3/2}}\int_0^\infty \frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}r^2dr\int_0^\pi e^{-\frac{i}{\hbar}pr\cos\theta}\sin\theta d\theta\int_0^{2\pi}d\varphi \\
&= \frac{2\pi}{(2\pi\hbar)^{3/2}\sqrt{\pi a_0^3}}\int_0^\infty r^2e^{-r/a_0}dr\int_0^\pi e^{-\frac{i}{\hbar}pr\cos\theta}d(-\cos\theta) \\
&= \frac{2\pi}{(2\pi\hbar)^{3/2}\sqrt{\pi a_0^3}}\int_0^\infty r^2e^{-r/a_0}dr\frac{\hbar}{ipr}e^{-\frac{i}{\hbar}pr\cos\theta}\Big|_0^\pi \\
&= \frac{2\pi}{(2\pi\hbar)^{3/2}\sqrt{\pi a_0^3}}\frac{\hbar}{ip}\int_0^\infty re^{-r/a_0}(e^{\frac{i}{\hbar}pr}-e^{-\frac{i}{\hbar}pr})dr \\
&(note: \boxed{\int_0^\infty x^ne^{-ax}dx=\frac{n!}{a^{n+1}}}) \\
&= \frac{2\pi}{(2\pi\hbar)^{3/2}\sqrt{\pi a_0^3}}\frac{\hbar}{ip}[\frac{1}{(\frac{1}{a_0}-\frac{i}{\hbar}p)^2}-\frac{1}{(\frac{1}{a_0}+\frac{i}{\hbar}p)^2}] \\
&= \frac{1}{\sqrt{2a_0^3\hbar^3}ip\pi}\frac{4ip}{a_0\hbar(\frac{1}{a_0^2}+\frac{p^2}{\hbar^2})^2} \\
&= \frac{4}{\sqrt{2a_0^3\hbar^3}\pi a_0}\frac{a_0^4\hbar^4}{(a_0^2p^2+\hbar^2)^2} \\
&= \frac{(2a_0\hbar)^{3/2}\hbar}{\pi(a_0^2p^2+\hbar^2)^2}
\end{aligned} \tag{99}
$$

Momentum Probability Distribution Function

$$
\omega(p)=|c(p)|^2=\boxed{\frac{8a_0^3\hbar^5}{\pi^2(a_0p^2+\hbar^2)^4}} \tag{100}
$$

😎

3.6

$$
\psi(x)=A[\sin^2 kx+\frac{1}{2}\cos kx] \tag{101}
$$

Proof. .

According to Theorem 2.2

Theorem 3.7. Euler's formula

$$
e^{ikx}=\cos kx+i\sin kx \tag{102}
$$

$$
e^{-ikx}=\cos kx-i\sin kx \tag{103}
$$

$$
\begin{aligned}
\psi(x) &= A[\sin^2 kx+\frac{1}{2}\cos kx]=A[\frac{1}{2}(1-\cos 2kx)+\frac{1}{2}\cos kx] \\
&= \frac{A}{2}[1-\cos 2kx+\cos kx](Euler's\ formula) \\
&= \frac{A}{2}[1-\frac{1}{2}(e^{i2kx}-e^{-i2kx})+\frac{1}{2}(e^{ikx}+e^{-ikx})] \\
&= \frac{A\sqrt{2\pi\hbar}}{2}[e^{i0x}-\frac{1}{2}e^{i2kx}-\frac{1}{2}e^{-i2kx}+\frac{1}{2}e^{ikx}+\frac{1}{2}e^{-ikx}]\cdot\frac{1}{\sqrt{2\pi\hbar}}
\end{aligned} \tag{104}
$$

Because the corresponding eigenfunction

$$
\begin{cases}
\varphi_p(x)=\frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\cdot\varphi_k(x)=\frac{e^{ikx}}{\sqrt{2\pi\hbar}} \\
p=\hbar k
\end{cases} \tag{105}
$$

Therefore, the normalization factor is

$$
(\frac{A\sqrt{2\pi\hbar}}{2})^2\cdot[1^2+2\times(\frac{1}{2})^2+2\times|-\frac{1}{2}|^2]=1 \tag{106}
$$

$$
\Rightarrow A=\frac{1}{\sqrt{\pi\hbar}} \tag{107}
$$

$$Original\ formula = \frac{\sqrt{2}}{4}[2e^{i0x} - e^{i2kx} - e^{-i2kx} + e^{ikx} + e^{-ikx}] \cdot \frac{1}{\sqrt{2\pi\hbar}} \tag{108}$$

$$\begin{array}{lccccc} Wave\ vector\ k\ value & 2k & k & 0 & -k & -2k \\ Momentum\ p = \hbar k\ value & 2\hbar k & \hbar k & 0 & -\hbar k & -2\hbar k \\ Kinetic\ energy\ T = \dfrac{p^2}{2m}\ value & \dfrac{(2\hbar k)^2}{2m} & \dfrac{(\hbar k)^2}{2m} & 0 & \dfrac{(-2\hbar k)^2}{2m} & \dfrac{(-\hbar k)^2}{2m} \\ Corresponding\ probability\ w_n = |c_n|^2 & \dfrac{1}{8} \times 1 & \dfrac{1}{8} \times 1 & \dfrac{1}{8} \times 4 & \dfrac{1}{8} \times 1 & \dfrac{1}{8} \times 1 \end{array} \tag{109}$$

$$\therefore \overline{p} = \sum_n w_n p_n = \boxed{0} \tag{110}$$

$$\therefore \overline{T} = \frac{\overline{p}^2}{2m} = \boxed{\frac{5k^2\hbar^2}{8m}} \tag{111}$$

😎

3.9

$$\psi(r, \theta, \varphi) = \frac{1}{2} R_{21}(r) Y_{10}(\theta, \varphi) - \frac{\sqrt{3}}{2} R_{21}(r) Y_{1-1}(\theta, \varphi) \tag{112}$$

Proof. .
Prove normalization:$|\frac{1}{2}|^2 + |-\frac{\sqrt{3}}{2}| = 1$
In this state, the values of the quantum numbers are $n = 2, l = 1, m = 0, -1$.
(1)
The energy of a hydrogen atom has a definite value (with probability 1)

$$\overline{E_2} = E_2 = -\frac{m_e e_s^2}{2n^2\hbar^2} = \boxed{-\frac{m_e}{8\hbar^2}(\frac{e^2}{4\pi\varepsilon_0})^2} \tag{113}$$

(2)
The square of angular momentum has a definite value (with probability 1)

$$\overline{L^2} = L^2 = l(l+1)\hbar^2 = 1 \cdot (1+1)\hbar^2 = \boxed{2\hbar^2} \tag{114}$$

(3)
L_z has possible value:$0, -\hbar$

$$\overline{L_z} = 0 \times \frac{1}{4} - \hbar \times \frac{3}{4} = \boxed{-\frac{3}{4}\hbar} \tag{115}$$

😎

4 Some Common Proofs

4.1 Probability Flow Conservation Law

In quantum mechanics, due to the statistical interpretation of the wave function ψ, $\rho(\vec{r}, t) = \psi^*(\vec{r}, t)\psi(\vec{r}, t)$ represents the probability density at $\vec{r}$ at time t.

The rate of change of probability density over time is

$$\frac{\partial \rho(\vec{r}, t)}{\partial t} = \psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi \tag{116}$$

From the Schrödinger equation $i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + U(\vec{r})\psi$,we have

$$\begin{cases} \dfrac{\partial \psi}{\partial t} = \dfrac{i\hbar}{2m}\nabla^2\psi + \dfrac{1}{i\hbar}U(\vec{r})\psi \\ \\ \dfrac{\partial \psi^*}{\partial t} = -\dfrac{i\hbar}{2m}\nabla^2\psi^* - \dfrac{1}{i\hbar}U(\vec{r})\psi^* \end{cases} \tag{117}$$

Substituting into (116), we get

$$\begin{cases} \psi^*\dfrac{\partial \psi}{\partial t} = \psi^*\dfrac{i\hbar}{2m}\nabla^2\psi + \psi^*\dfrac{1}{i\hbar}U(\vec{r})\psi \\ \\ \dfrac{\partial \psi^*}{\partial t}\psi = -\psi\dfrac{i\hbar}{2m}\nabla^2\psi^* - \dfrac{1}{i\hbar}U(\vec{r})\psi^*\psi \end{cases} \tag{118}$$

So, there is

$$\frac{\partial \rho}{\partial t}=\frac{i\hbar}{2m}(\psi^*\nabla^2\psi-\psi\nabla^2\psi^*)=\frac{i\hbar}{2m}\nabla\cdot(\psi^*\nabla\psi-\psi\nabla\psi^*) \tag{119}$$

Making

$$\vec{J}=-\frac{i\hbar}{2m}(\psi^*\nabla\psi-\psi\nabla\psi^*)=\frac{i\hbar}{2m}(\psi\nabla\psi^*-\psi^*\nabla\psi) \tag{120}$$

It is called the **probability flow density**. So we have

$$\boxed{\frac{\partial \rho}{\partial t}+\nabla\cdot\vec{J}=0} \tag{121}$$

This is the law of conservation of probability flow. In quantum mechanics, the law of conservation of probability flow is a corollary of the statistical interpretation of the wave function and the Schrödinger equation. The law of conservation of probability flow states that, in non-relativistic quantum mechanics, particles can generally neither be created nor annihilated. The total number of particles in the system is conserved. Particles must appear in all space. This is an inevitable event with a probability of 1.

Furthermore, we have

Mass flow density:$\vec{J}_m=m\vec{J}$

Current density:$\vec{J}_q=q\vec{J}$

Law of conservation of charge

$$\frac{\partial w_q}{\partial t}+\nabla\cdot\vec{J}_q=0 \tag{122}$$

law of conservation of mass

$$\frac{\partial w_m}{\partial t}+\nabla\cdot\vec{J}_m=0 \tag{123}$$

In the steady state, the probability flow density (current density, mass flow density) is independent of time t(Looking at the **Definition 3.1** for proofs).

4.2 Operators

The momentum operator $\hat{\vec{p}}$ is a linear operator.

Proof. .
For any functions u_1, u_2, constants c_1, c_2, we have

$$\hat{\vec{p}}(c_1u_1+c_2u_2)=-i\hbar\nabla\left(c_1u_1+c_2u_2\right)=-i\hbar\nabla\left(c_1u_1\right)-i\hbar\nabla\left(c_2u_2\right)=-i\hbar c_1\nabla\left(u_1\right)-i\hbar c_2\nabla\left(u_2\right)=c_1\hat{\vec{p}}u_1+c_2\hat{\vec{p}}u_2 \tag{124}$$

😎

4.3 Hermitian operators for mechanical quantities

For two arbitrary functions ψ and φ, if the operator $\hat{F}$ satisfies the following equation

$$\int\psi^*\hat{F}\phi dx=\int\left(\hat{F}\psi\right)^*\phi dx \tag{125}$$

Then $\hat{F}$ is called the **Hermitian operator**. Where x represents all relevant variables, and the integration range is the entire region of variation of all variables.

(1)Prove that the eigenvalues of a Hermitian operator are real numbers.

Proof. .
Let λ represent the eigenvalue of $\hat{F}$ and ψ represent the eigenfunction to which it belongs, we have

$$\hat{F}\psi=\lambda\psi \tag{126}$$

By the definition of the Hermitian operator(125),Taking $\psi=\phi$, we have

$$\lambda\int\psi^*\psi dx=\lambda^*\int\psi^*\psi dx \tag{127}$$

$$\therefore\lambda=\lambda^*$$

This means that the eigenvalues of Hermitian operators are real numbers.

Q.E.D.

😎

(2) Verify that the operator representing the mechanical quantity is a Hermitian operator $(\psi,\hat{F}\varphi)=(\hat{F}\psi,\varphi)$**.**

Proof. .
1) Verify that the coordinate operator x is a Hermitian operator.

Since x is a real number, we have

$$\int_{-\infty}^{+\infty} \psi^* x\phi dx = \int_{-\infty}^{\infty} (x\psi)^* \phi dx \tag{128}$$

2) Verify that the momentum operator is a Hermitian operator

$$\begin{aligned}\int_{-\infty}^{\infty} \psi^* \hat{p}_x \phi dx &= -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{d\phi}{dx} dx = -i\hbar \int_{-\infty}^{\infty} \psi^* d\phi = -i\hbar\psi^* \cdot \phi\Big|_{-\infty}^{\infty} + i\hbar \int_{-\infty}^{\infty} \phi d\psi^* \\ &= -i\hbar\psi^* \cdot \phi\Big|_{-\infty}^{\infty} + i\hbar \int_{-\infty}^{\infty} \frac{d\psi^*}{dx} \phi dx = \int_{-\infty}^{\infty} (\hat{p}_x \psi)^* \phi dx\end{aligned} \tag{129}$$

where ψ and φ are equal to zero at $x \to \pm\infty$.

😎

(3)Orthogonality of Eigenfunctions of Hermitian Operators

1)Definition of mutual orthogonality. If two functions ψ_1 and ψ_2 satisfy the relation

$$\int \psi_1^* \psi_2 d\tau = 0 \tag{130}$$

Here, the integral is the integral of the entire space of the change of the variable, so ψ_1 and ψ_2 are said to be orthogonal to each other.

2)Two eigenfunctions of a Hermitian operator belonging to different eigenvalues are mutually orthogonal. Let ϕ_1, ϕ_2,$\cdots$, ϕ_n,$\cdots$ be the eigenfunctions of the Hermitian operator $\hat{F}$, and their eigenvalues λ_1, λ_2,$\cdots$,λ_n,$\cdots$ are all unequal.

Proof. .
Using the eigenvalue equation, let $\hat{F}\phi_k = \lambda_k\phi_k, \hat{F}\phi_l = \lambda_l\phi_l$, and when $k \neq l, \lambda_k \neq \lambda_l$.
Since $\hat{F}$ is a Hermitian operator, the eigenvalue is a real number, that is, $\lambda_k = \lambda_k^*$, so

$$(\hat{F}\phi_k)^* = \lambda_k \phi_k^* \tag{131}$$

Multiply both sides of (131) by ϕ_l and integrate over the entire region of the variable to obtain

$$\int (\hat{F}\phi_k)^* \phi_l d\tau = \lambda_k \int \phi_k^* \phi_l d\tau \tag{132}$$

Multiply both sides of (131) by ϕ_k^* and integrate over the entire region of the variable to obtain

$$\int \phi_k^* (\hat{F}\phi_l) d\tau = \lambda_l \int \phi_k^* \phi_l d\tau \tag{133}$$

According to the definition of Hermitian operator, we have

$$\int \phi_k^* (\hat{F}\phi_l) d\tau = \int (\hat{F}\phi_k)^* \phi_l d\tau \tag{134}$$

$$\Rightarrow \lambda_k \int \phi_k^* \phi_l d\tau = \lambda_l \int \phi_k^* \phi_l d\tau \tag{135}$$

Since $\lambda_k \neq \lambda_l$, we have

$$\int \phi_k^* \phi_l d\tau = 0 \tag{136}$$

Q.E.D.

😎

4.4 The Commutation Relation

As anticipated,there's an extra term,involving $(x\hat{p} - \hat{p}x)$. We call this the **commutator** of x and $\hat{p}$;it is a measure of how badly they fail to commute.In general,the commutator of operators $\hat{A}$ and $\hat{B}$ is

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} \tag{137}$$

Proposition 4.1. Commutator's identities

The commutator has the following properties:

$$
\begin{aligned}
&[\hat{A},\hat{B}] = -[\hat{B},\hat{A}] \\
&[\hat{A},\hat{A}] = 0 \\
&[\hat{A},c] = 0 \\
&[\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}] \\
&[\hat{A},\hat{B}\hat{C}] = \hat{B}[\hat{A},\hat{C}] + [\hat{A},\hat{B}]\hat{C} \\
&[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B} \\
&[\hat{A},\hat{B}]^\dagger = [\hat{B}^\dagger,\hat{A}^\dagger] \\
&\Big[\hat{A},[\hat{B},\hat{C}]\Big] + \Big[\hat{B},[\hat{C},\hat{A}]\Big] + \Big[\hat{C},[\hat{A},\hat{B}]\Big] = 0
\end{aligned}
\tag{138}
$$

where c is a constant.

Mechanical quantities are all functions of coordinates and momentum, and the commutator relationship between position and momentum can be used to derive commutator relationships between other mechanical quantities. Therefore, the commutator equation of position and momentum is called the **basic commutator equation**.

Prove:

$$[x,\hat{p}_x] = x\hat{p}_x - \hat{p}_x x = i\hbar \tag{139}$$

Proof.
Acting the commutator relation on the wave function, we have

$$[x,\hat{p}_x]\psi = x\hat{p}_x\psi - \hat{p}_x x\psi \tag{140}$$

Considering the momentum operator, $\boxed{\hat{p}_x = -i\hbar\nabla = -i\hbar\frac{\partial}{\partial x}}$

$$x\hat{p}_x\psi = -i\hbar x\frac{\partial}{\partial x}\psi \tag{141}$$

$$\hat{p}_x x\psi = -i\hbar\frac{\partial}{\partial x}(x\psi) = -i\hbar\left(\psi + x\frac{\partial}{\partial x}\psi\right) \tag{142}$$

$$\stackrel{(18)-(19)}{\Longrightarrow} (x\hat{p}_x - \hat{p}_x x)\psi = i\hbar\psi \tag{143}$$

Q.E.D.

😎

Remark. .
1.This lovely and ubiquitous formula is known as the **canonical commutation relation**.
2.**Ditto.**

$$[x,\hat{p}_y] = x\hat{p}_y - \hat{p}_y x = 0$$

4.5 Heisenberg's Uncertainty Principle

Proof of the **Generalized Uncertainty Principle**.

Proof.
For any observable A, we have

$$\sigma_A^2 = \left\langle \left(\hat{A} - \langle A\rangle\right)\Psi \middle| \left(\hat{A} - \langle A\rangle\right)\Psi \right\rangle = \langle f|f\rangle \tag{144}$$

where $f \equiv \left(\hat{A} - \langle A\rangle\right)\Psi$.Likewise, for any other observable, B,

$$\sigma_B^2 = \langle g|g\rangle\,, where \quad g \equiv (B - \langle B\rangle)\,\Psi.$$

Therefore (invoking the **Schwarz inequality**)

$$\sigma_A^2\sigma_B^2 = \langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2\,. \tag{145}$$

Now, for any complex number z,

$$|z|^2 = [\mathrm{Re}\,(z)]^2 + [\mathrm{Im}\,(z)]^2 \geq [\mathrm{Im}\,(z)]^2 = \left[\frac{1}{2i}(z - z^*)\right]^2. \tag{146}$$

Therefore, letting $z = \langle f|g\rangle$,

$$\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\left[\langle f|g\rangle - \langle g|f\rangle\right]\right)^2. \tag{147}$$

But (exploiting the hermiticity of $\left(\hat{A}-(A)\right)$,in the first line)

$$\begin{aligned}\langle f|g\rangle &= \left\langle\left(\hat{A}-\langle A\rangle\right)\Psi\middle|\left(\hat{B}-\langle B\rangle\right)\Psi\right\rangle = \langle\Psi|\left(\hat{A}-\langle A\rangle\right)\left(\hat{B}-\langle B\rangle\right)\Psi\rangle \\ &= |\Psi|\left(\hat{A}\hat{B}-\hat{A}\langle B\rangle-\hat{B}\langle A\rangle+\langle A\rangle\langle B\rangle\right)\Psi \\ &= \left\langle\Psi\middle|\hat{A}\hat{B}\Psi\right\rangle - \langle B\rangle\left\langle\Psi\middle|\hat{A}\Psi\right\rangle\rangle - \langle A\rangle\left\langle\Psi\middle|\hat{B}\Psi\right\rangle + \langle A\rangle\langle B\rangle\left\langle\Psi|\Psi\right\rangle \\ &= \left\langle\hat{A}\hat{B}\right\rangle - \langle B\rangle\langle A\rangle - \langle A\rangle\langle B\rangle + \langle A\rangle\langle B\rangle \\ &= \left\langle\hat{A}\hat{B}\right\rangle - \langle A\rangle\langle B\rangle\end{aligned} \tag{148}$$

(Remember, (A) and (B) are numbers, not operators, so you can write them in either order.Similarly,

$$\langle g|f\rangle = \langle\hat{B}\hat{A}\rangle - \langle A\rangle\langle B\rangle, \tag{149}$$

so

$$\langle f|g\rangle - \langle g|f\rangle = \langle\hat{A}\hat{B}\rangle - \langle\hat{B}\hat{A}\rangle = \langle[\hat{A},\hat{B}]\rangle, \tag{150}$$

where

$$\left[\hat{A},\hat{B}\right] \equiv \hat{A}\hat{B}-\hat{B}\hat{A} \tag{151}$$

is the commutator of the two operators .Conclusion:

$$\boxed{\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right)^2.} \tag{152}$$

Q.E.D.

😎

When the system is in the $\hat{L}_z$ eigenstate

$$\overline{(\Delta L_x)^2}\cdot\overline{(\Delta L_y)^2} \geq \frac{\hbar^2}{4}\overline{L_z}^2 = \frac{\hbar^2}{4}(m\hbar)^2 = \frac{1}{4}m^2\hbar^4 \tag{153}$$

Using the uncertainty relation, it is proved that: in the $\hat{L}_z$ eigenstate Y_{lm},$\langle L_x\rangle = \langle L_y\rangle = 0$.

Proof.

$$\because [\hat{L}_y,\hat{L}_z] = i\hbar\hat{L}_x \quad \therefore \overline{(\Delta L_y)^2}\bullet\overline{(\Delta L_z)^2} \geq \frac{\hbar^2}{4}\overline{L_x}^2 \tag{154}$$

Since the measured mechanical quantity $\hat{L}_z$ has a definite value in the $\hat{L}_z$ eigenstate Y_{lm}, the mean square deviation of $\hat{L}_z$ must be zero, that is,

$$\overline{(\Delta L_z)^2} = 0 \tag{155}$$

From the uncertainty relation, we know that

$$\overline{(\Delta L_y)^2}\bullet 0 \geq \frac{\hbar^2}{4}\overline{L_x}^2 \Rightarrow 0 \geq \frac{\hbar^2}{4}\overline{L_x}^2 \tag{156}$$

$$\therefore \overline{L_x} = 0, \textbf{Ditto.}\overline{L_y} = 0 \tag{157}$$

Q.E.D.

😎

4.6 Conserved quantity

Definition of conserved quantity: The time-independent mechanical quantity $\hat{F}$ commutes with the system's Hamiltonian H, that is,

$$\frac{d\overline{F}}{dt} = \frac{\overline{\partial F}}{\partial t} + \frac{1}{ih}\overline{[\hat{F},\hat{H}]} \tag{158}$$

$\hat{F}$ is called a conserved quantity. As the name suggests, a conserved quantity does not change and is independent of time.

From this, we can derive the law of conservation of momentum, the law of conservation of angular momentum, and the law of conservation of energy.

4.7 Angular Momentum

Mechanical quantities are represented by operators in quantum mechanics, then the operator representation of angular momentum in quantum mechanics is

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} \tag{159}$$

The following are all expressed in rectangular coordinates.
Naturally, we have

$$\hat{\vec{r}} = x\vec{i} + y\vec{j} + z\vec{k} \tag{160}$$

$$\hat{\vec{p}} = -i\hbar\nabla = p_x\vec{i} + p_y\vec{j} + p_z\vec{z} = -i\hbar\left(\vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}\right) \tag{161}$$

Then,

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x & y & z \\ \hat{p}_x & \hat{p}_y & \hat{p}_z \end{vmatrix} = (yp_z - zp_y)\vec{i} + (zp_x - xp_z)\vec{j} + (xp_y - yp_x)\vec{k} \tag{162}$$

The three components of the angular momentum operator in the rectangular coordinate system are

$$\begin{aligned} \hat{L}_x &= yp_z - zp_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ \hat{L}_y &= zp_x - xp_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ \hat{L}_z &= xp_y - yp_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{aligned} \tag{163}$$

4.8 Angular Momentum Operator Commutator Relation

Proposition 4.2. The angular momentum commutator's identities

The three components of the angular momentum operator in the rectangular coordinate system are

$$\begin{aligned} [\hat{L}_\alpha, x_\beta] &= \varepsilon_{\alpha\beta\gamma} i\hbar x_\gamma \\ [\hat{L}_\alpha, p_\beta] &= \varepsilon_{\alpha\beta\gamma} i\hbar p_\gamma \\ [\hat{L}_\alpha, \hat{L}_\beta] &= \varepsilon_{\alpha\beta\gamma} i\hbar l_\gamma \\ [\hat{L}_\alpha, r^2] &= 0 \\ [\hat{L}_\alpha, p^2] &= 0 \\ [\hat{L}_\alpha, \hat{L}^2] &= 0 \\ \vec{L} \times \vec{L} &= i\hbar\vec{L} \end{aligned} \tag{164}$$

Among them, (x, y, z) is denoted as (x_1, x_2, x_3); $(\hat{L}_x, \hat{L}_y, \hat{L}_z)$ is denoted as $(\hat{L}_1, \hat{L}_2, \hat{L}_3)$.

1.Prove:

$$[\hat{L}_x, x] = 0 \tag{165}$$

Proof.

$$[\hat{L}_x, x] = \hat{L}_x x - x\hat{L}_x = (y\hat{p}_z x - z\hat{p}_y x) - (xy\hat{p}_z - xz\hat{p}_y) = 0 \tag{166}$$

Q.E.D.

😎

2.Prove:

$$[\hat{L}_x, y] = i\hbar z \tag{167}$$

Proof.

$$[\hat{L}_x, y] = \hat{L}_x y - y\hat{L}_x = (y\hat{p}_z y - z\hat{p}_y y) - (yy\hat{p}_z - yz\hat{p}_y) = z(y\hat{p}_y - \hat{p}_y y) = i\hbar z \tag{168}$$

Q.E.D.

😎

Remark. .
The proof using the properties of commutative form is more intuitive and concise.

$$[\hat{L}_x, x] = [yp_z - zp_y, x] = [yp_z, x] - [zp_y, x] = y[p_z, x] + [y, x]p_z - z[p_y, x] - [z, x]p_y = 0 \tag{169}$$

$$[\hat{L}_x, y] = [yp_z - zp_y, y] = [yp_z, y] - [zp_y, y] = y[p_z, y] + [y, y]p_z - z[p_y, y] - [z, y]p_y = i\hbar z \tag{170}$$

Ditto.

$$\begin{aligned} &[\hat{L}_x, x] = 0; \quad [\hat{L}_x, y] = i\hbar z; \quad [\hat{L}_x, z] = -i\hbar y \\ &[\hat{L}_y, x] = -i\hbar z; \quad [\hat{L}_y, y] = 0; \quad [\hat{L}_y, z] = i\hbar x \\ &[\hat{L}_z, x] = i\hbar y; \quad [\hat{L}_x, y] = -i\hbar x; \quad [\hat{L}_z, z] = 0. \end{aligned} \tag{171}$$

Also

$$[\hat{L}_x, \hat{p}_x] = [yp_z - zp_y, p_x] = [yp_z, p_x] - [zp_y, p_x] = y[p_z, p_x] + [y, p_x]p_z - z[p_y, p_x] - [z, p_x]p_y = 0 \tag{172}$$

$$[\hat{L}_x, \hat{p}_y] = [yp_z - zp_y, p_y] = [yp_z, p_y] - [zp_y, p_y] = y[p_z, p_y] + [y, p_y]p_z - z[p_y, p_y] - [z, p_y]p_y = i\hbar p_z \tag{173}$$

Q.E.D.

3.Prove:

$$[\hat{L}_\alpha, \hat{L}_\beta] = \varepsilon_{\alpha\beta\gamma} i\hbar \hat{L}_\gamma \tag{174}$$

Proof. .
Trivial.

$$[\hat{L}_x, \hat{L}_x] = \hat{L}_x\hat{L}_x - \hat{L}_x\hat{L}_x = 0 \tag{175}$$

Then

$$\begin{aligned} [\hat{L}_x, \hat{L}_y] &= \hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x \\ &= (y\hat{p}_z - z\hat{p}_y)(z\hat{p}_x - x\hat{p}_z) - (z\hat{p}_x - x\hat{p}_z)(y\hat{p}_z - z\hat{p}_y) \\ &= yp_zzp_x - yp_zxp_z - zp_yzp_x + zp_yxp_z - zp_xyp_z + zp_xzp_y + xp_zyp_z - xp_zzp_y \\ &= p_zzyp_x + zp_zxp_y - zp_zyp_x - p_zzxp_y \\ &= (zp_z - p_zz)(xp_y - yp_x) \\ &= i\hbar\hat{L}_z \end{aligned} \tag{176}$$

Q.E.D.

😎

Remark. .
For the above proof, we can also

$$\begin{aligned} [\hat{L}_x, \hat{L}_x] &= 0 \\ [\hat{L}_x, \hat{L}_y] &= [\hat{L}_x, zp_x - xp_z] = [\hat{L}_x, zp_x] - [\hat{L}_x, xp_z] \\ &= z[\hat{L}_x, p_x] + [\hat{L}_x, z]p_x - x[\hat{L}_x, p_z] - [\hat{L}_x, x]p_z \\ &= -i\hbar yp_x + i\hbar xp_y = i\hbar\hat{L}_z \end{aligned} \tag{177}$$

Q.E.D.

Ditto.

$$\begin{aligned} &[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \quad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x \quad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y \\ &[\hat{L}_x, \hat{L}_x] = [\hat{L}_y, \hat{L}_y] = [\hat{L}_z, \hat{L}_z] = 0 \end{aligned} \tag{178}$$

It can also be expressed as:

$$\vec{L} \times \vec{L} = i\hbar\vec{L} \tag{179}$$

Proof.

$$\begin{aligned} \vec{L} \times \vec{L} &= (L_yL_z - L_zL_y)\vec{i} + (L_zL_x - L_xL_z)\vec{j} + (L_xL_y - L_yL_x)\vec{k} \\ &= [L_y, L_z]\vec{i} + [L_z, L_y]\vec{j} + [L_x, L_y]\vec{k} \\ &= i\hbar L_x\vec{i} + i\hbar L_y\vec{j} + i\hbar L_z\vec{k} \\ &= i\hbar\vec{L} \end{aligned} \tag{180}$$

Q.E.D.

4.Prove

The commutation relationship between the components of angular momentum, operators $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ and position square $\vec{r}^2$:

$$[\hat{L}_\alpha, r^2] = 0 \tag{181}$$

Proof.

$$\begin{aligned}
&[\hat{L}_x, r^2] = [\hat{L}_x, x^2 + y^2 + z^2] = [\hat{L}_x, x^2] + [\hat{L}_x, y^2] + [\hat{L}_x, z^2] \\
&[\hat{L}_x, x^2] = x[\hat{L}_x, x] + [\hat{L}_x, x]x = 0 \\
&[\hat{L}_x, y^2] = y[\hat{L}_x, y] + [\hat{L}_x, y]y = i\hbar z + i\hbar zy = 2i\hbar yz \\
&[\hat{L}_x, z^2] = z[\hat{L}_x, z] + [\hat{L}_x, z]z = -i\hbar zy - i\hbar yz = -2i\hbar yz \\
&[\hat{L}_x, r^2] = 0
\end{aligned} \tag{182}$$

Ditto.

$$[\hat{L}_y, r^2] = 0 \quad [\hat{L}_z, r^2] = 0 \tag{183}$$

Q.E.D.

😎

5.Prove

The commutation relation between the momentum component operators $\hat{L}_x, \hat{L}_y, \hat{L}_z$ and the square of angular momentum p^2 is:

$$[\hat{L}_\alpha, \hat{p}^2] = 0 \tag{184}$$

Proof.

$$\begin{aligned}
&[\hat{L}_x, p^2] = [\hat{L}_x, p_x^2 + p_y^2 + p_z^2] = [\hat{L}_x, p_x^2] + [\hat{L}_x, p_y^2] + [\hat{L}_x, p_z^2] \\
&[\hat{L}_x, p_x^2] = p_x[\hat{L}_x, p_x] + [\hat{L}_x, p_x]p_x = 0 \\
&[\hat{L}_x, p_y^2] = p_y[\hat{L}_x, p_y] + [\hat{L}_x, p_y]p_y = i\hbar p_y p_z + i\hbar p_z p_y = 2i\hbar p_y p_z \\
&[\hat{L}_x, p_z^2] = p_z[\hat{L}_x, p_z] + [\hat{L}_x, p_z]p_z = -i\hbar p_z p_y - i\hbar p_y p_z = -2i\hbar p_y p_z \\
&[\hat{L}_x, p^2] = 0
\end{aligned} \tag{185}$$

Ditto.

$$[\hat{L}_y, p^2] = 0 \quad [\hat{L}_z, p^2] = 0 \tag{186}$$

This is formally identical to the proof of $[\hat{L}_\alpha, r^2] = 0$.

Q.E.D.

😎

6.Prove

The commutation relation between the angular momentum components $\hat{L}_x$,$\hat{L}_y$,$\hat{L}_z$ and the angular momentum square operator $\hat{L}^2$ is:

$$[\hat{L}_\alpha, \hat{L}^2] = 0 \quad (\alpha = x, y, z) \tag{187}$$

Proof.

$$\begin{aligned}
&[\hat{L}_x, \hat{L}^2] = [\hat{L}_x, \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2] = [\hat{L}_x, \hat{L}_x^2] + [\hat{L}_x, \hat{L}_y^2] + [\hat{L}_x, \hat{L}_z^2] \\
&[\hat{L}_x, \hat{L}_x^2] = 0 \\
&[\hat{L}_x, \hat{L}_y^2] = \hat{L}_y[\hat{L}_x, \hat{L}_y] + [\hat{L}_x, \hat{L}_y]\hat{L}_y = i\hbar \hat{L}_y \hat{L}_z + i\hbar \hat{L}_z \hat{L}_y \\
&[\hat{L}_x, \hat{L}_z^2] = \hat{L}_z[\hat{L}_x, \hat{L}_z] + [\hat{L}_x, \hat{L}_z]\hat{L}_z = -i\hbar \hat{L}_z \hat{L}_y - i\hbar \hat{L}_y \hat{L}_z \\
&[\hat{L}_x, \hat{L}^2] = 0
\end{aligned} \tag{188}$$

Ditto.

$$[\hat{L}_y, \hat{L}^2] = 0 \quad [\hat{L}_z, \hat{L}^2] = 0 \tag{189}$$

Q.E.D.

😎

4.9 The Eigenvalue

1.The Eigenvalue of $\hat{L}_z$

The expression of the angular momentum z component $\hat{L}_z$ in spherical coordinates is

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi} \tag{190}$$

Then the **eigenvalue equation** of $\hat{L}_z$ is

$$\hat{L}_z\psi(\varphi) = \lambda\psi(\varphi) \tag{191}$$

In order to correspond, λ is used to represent the eigenvalue, which is a real number;$\psi(\varphi)$ is the eigenfunction. So, we have

$$-i\hbar\frac{\partial}{\partial\varphi}\psi = \lambda\psi \quad \Longrightarrow \quad \frac{\psi'}{\psi} = \frac{i\lambda}{\hbar} \tag{192}$$

Integrate both sides simultaneously

$$\ln\psi = \frac{i\lambda}{\hbar}\varphi \quad \Longrightarrow \quad \psi(\varphi) = C\exp\left(\frac{i\lambda\varphi}{\hbar}\right) \tag{193}$$

Using **periodic boundary conditions**

$$\psi(\varphi) = \psi(\varphi + 2\pi) \tag{194}$$

$$\exp\left(\frac{i\lambda\varphi}{\hbar}\right) = \exp\left(\frac{i\lambda\varphi}{\hbar}\right)\exp\left(\frac{i2\pi\lambda}{\hbar}\right) \quad \Longrightarrow \quad \exp\left(\frac{i2\pi\lambda}{\hbar}\right) = 1 \tag{195}$$

Then

$$\frac{2\pi\lambda}{\hbar} = m2\pi, \quad m = 0, \pm1, \pm2, \ldots \tag{196}$$

That is, the eigenvalue of $\hat{L}_z$ is

$$\boxed{\lambda = L_z = m\hbar, \quad (m = 0, \pm1, \pm2, \cdots)} \tag{197}$$

Normalize the eigenfunction

$$\int_0^{2\pi}\psi^*\psi d\varphi = C^2 2\pi = 1 \quad \Longrightarrow \quad C = \frac{1}{\sqrt{2\pi}} \tag{198}$$

Therefore, the eigenvalue equation of $\hat{L}_z$ is

$$\hat{L}_z\psi(\varphi) = m\hbar\psi(\varphi) \tag{199}$$

The eigenfunction of $\hat{L}_z$ is

$$\psi_m(\varphi) = \frac{1}{\sqrt{2\pi}}e^{im\varphi} \tag{200}$$

The corresponding eigenvalues are $m\hbar, m = 0, \pm1, \pm2, \cdots$. It is easy to prove that the eigenfunction $\psi_m(\varphi)$ is orthogonal, that is,

$$\int_0^{2\pi}\psi_m^*(\varphi)\psi_n(\varphi)d\varphi = \frac{1}{2\pi}\int_0^{2\pi}e^{-im\varphi}e^{in\varphi}d\varphi = \delta_{mn} \tag{201}$$

2.The Eigenvalue of $\hat{L}^2$ According to the properties and observation rules of **Legendre polynomials**, the proof is rather complicated and will be omitted here.

The spherical harmonics $Y_{lm}(\theta,\varphi)$ are the common eigenfunctions of the squared angular momentum operator $\hat{L}^2$ and the z-component angular momentum operator $\hat{L}_z$.

$$\begin{gathered}\boxed{\hat{L}^2Y_{lm}(\theta,\varphi) = l(l+1)\hbar^2Y_{lm}(\theta,\varphi)}\\ \boxed{\hat{L}_zY_{lm}(\theta,\varphi) = m\hbar Y_{lm}(\theta,\varphi)}\end{gathered} \tag{202}$$

The eigenvalues are $l(l+1)m\hbar$ and $m\hbar$.Because l represents the magnitude of angular momentum, it is called the angular quantum number, and m is called the magnetic quantum number because it is related to the magnetic moment properties of the system. The value of l is $l = 0, 1, 2, \cdots$ and for a value of l, the value of m is $m = 0, \pm1, \pm2, \cdots, \pm l$, and can take $(2l{+}1)$ values. Therefore, corresponding to an eigenvalue $l(l{+}1)m\hbar$ of $\hat{L}^2$, there are $(2l{+}1)$ different eigenfunctions $Y_{lm}(\theta,\varphi)$ due to different m. We call the situation where there is more than one eigenfunction corresponding to an eigenvalue "**degeneracy**", and the number of eigenfunctions corresponding to the same eigenvalue is called "degeneracy". The eigenvalues of $\hat{L}^2$ are $(2l+1)$ degree degenerate. According to the customary notation in spectroscopy, the state with $l = 0$ is called the s(sharp) state, and the states with $l = 1, 2, 3, \cdots$ are called the p(principal), d (diffuse), f(fundamental), ... states, respectively. Particles in these states are referred to as $s, p, d, f, \cdots$ particles,respectively.

5 Quantum Mechanics Quiz Questions(2023)

5.1 Fill in the Blanks

1.The momentum of a free particle is a constant of motion, which is **the law of conservation of momentum** in quantum mechanics.

2.If two operators have a common set of eigenfunctions φ_n, and φ_n form a complete system, then the two operators must **commute**.

3.The potential energy of a one-dimensional linear oscillator is $U(y)=\frac{1}{2}m\omega^2y^2$, the energy obtained by solving the steady-state Schrödinger equation is $\boxed{E_n=(n+\frac{1}{2})\hbar\omega, n=0,1,2,\cdots}$, and the ground state energy is $\boxed{\frac{1}{2}\hbar\omega}$.

4.In quantum mechanics, **wave functions** are used to describe the state of microscopic systems.

5.Given $[\hat{C},\hat{D}]=-i\hat{F}$, d and b are constants, then $\boxed{[\hat{C}-d,\hat{D}+b]=-i\hat{F}}$

6.The phenomenon that particles can still penetrate a potential barrier when their **energy E is less than the potential barrier height** is called the tunnel effect.

7.The expression of the law of conservation of mass in quantum mechanics is $\boxed{\frac{\partial w_m}{\partial t}+\nabla\cdot\vec{J}_m=0}$.

8.Let $\hat{P}$ be the parity operator, x, y be the spatial coordinates, and t be the time coordinate, then we have $\boxed{\hat{P}\psi(-x,y,t)=\psi(x,-y,t)}$.

9. The wave function should usually meet three conditions in the entire region where the variable changes, namely, **finiteness, continuity and measurable single value**. These three conditions are called standard conditions of the wave function.

10. The normalization method of confining particles in **a three-dimensional box** and adding **periodic boundary conditions** is called box normalization.

11.It is known that the wave function of the hydrogen atom is $\psi(r,\theta,\varphi)=Ce^{-r/a_0}$(C is a constant), then the expected value of r is $\boxed{\frac{3}{2}a_0}$.

Proof.

$$\begin{aligned}\langle r\rangle &= \int\psi^* r\psi\ d\tau=\int(Ce^{-r/a_0})r(Ce^{-r/a_0})r^2\sin\theta drd\theta d\varphi\\ &= C^2\int_0^\infty\int_0^\pi\int_0^{2\pi}r^3e^{-2r/a_0}\sin\theta d\varphi d\theta dr\\ &= C^2\left(\frac{3a_0^4}{8}\right)\cdot 2\cdot 2\pi=C^2\cdot\frac{3a_0^4}{2}\cdot\pi\end{aligned}\tag{203}$$

Next, we need to determine the constant C. The wave function must be normalized, that is:

$$\int|\psi|^2d\tau=1=C^2\int_0^\infty\int_0^\pi\int_0^{2\pi}e^{-2r/a_0}r^2\sin\theta d\varphi d\theta dr=C^2\left(\frac{a_0^3}{4}\right)\cdot 2\cdot 2\pi=C^2\cdot\frac{a_0^3}{2}\cdot\pi\tag{204}$$

$$\Rightarrow C^2=\frac{1}{\pi a_0^3}\tag{205}$$

$$\therefore\langle r\rangle=\frac{1}{\pi a_0^3}\cdot\frac{3a_0^4}{2}\cdot\pi=\boxed{\frac{3a_0}{2}}\tag{206}$$

😎

Proposition 5.1. Gamma function

The gamma function is defined as

$$\Gamma(x)=\int_0^\infty \mathrm{e}^{-t}t^{x-1}\mathrm{d}t\quad(x>0)\tag{207}$$

Its basic nature is

$$\Gamma(x+1)=x\Gamma(x)\tag{208}$$

This formula can be proved by the integration by parts formula as follows

$$\begin{aligned}\Gamma(x+1)&=\int_0^\infty\mathrm{e}^{-t}t^x\mathrm{d}t=-\int_0^\infty t^x\mathrm{d}\left(\mathrm{e}^{-t}\right)\\ &=-\left[t^x\mathrm{e}^{-t}\right]_{t=0}^\infty+x\int_0^\infty\mathrm{e}^{-t}t^{x-1}\mathrm{d}t=x\Gamma(x)\end{aligned}\tag{209}$$

Easy to obtain

$$\Gamma(1)=\int_0^{\infty} \mathrm{e}^{-t}\mathrm{d}t=1 \tag{210}$$

Furthermore, we can deduce from the basic properties that

$$\Gamma(2)=1\cdot\Gamma(1)=1,\quad \Gamma(3)=2\cdot\Gamma(2)=2!,\quad \Gamma(4)=3\cdot\Gamma(3)=3!,\cdots \tag{211}$$

Continue to recursively get

$$\Gamma(n+1)=n!\quad (n=0,1,2,\cdots) \tag{212}$$

It should be noted that the gamma function is not defined when the independent variable is zero or a negative integer, which means

$$\Gamma(-n)\to\infty\quad (n=0,1,2,\cdots) \tag{213}$$

12.The phenomenon of **electron diffraction** can prove the existence of de Broglie waves.

13.The de Broglie wavelength of a free electron with a mass of $9.11\times10^{-31}kg$ and a kinetic energy of 8 eV is 0.434 nm.

$$\lambda=\frac{h}{p}=\frac{h}{\sqrt{2mE}}=\boxed{4.341\times10^{-10}m} \tag{214}$$

Remark. .
$\boxed{8eV=8\times1.60\times10^{-19}J}$

Proposition 5.2. Degeneracy

When the spin is not considered, when the particle moves in the Coulomb field, the bound state energy level can be expressed as E_n, and its degeneracy is $\boxed{n^2}$. If the spin of the particle is considered to be s, the degeneracy of E_n, is $\boxed{(2s+1)n^2}$.

5.2 Short Answer Questions

Proposition 5.3. Write down the statistical interpretation of the wave function proposed by Born.

Answer: The intensity of the wave function at a point in space (the square of the absolute value of the amplitude) is proportional to the probability of finding the particle at that point.

Proposition 5.4. Write down the principle of superposition of states in quantum mechanics.

Answer:

Proposition 5.5. Representation.

Answer:The specific representation of states and mechanical quantities in quantum mechanics is called representation.

5.3 Variational method

Proposition 5.6. Variational method

The particle moves in an infinite potential well $(-a<x<a)$, and the test wave function is

$$\psi(x)=\begin{cases} N(a^2-x^2)(a^2-\lambda x^2), & |x|<a\\ 0, & |x|\geq a\end{cases} \tag{215}$$

As an approximation to its ground state wave function, find the approximate energy level.

Proof. .
(1)Find the normalization factor N

$$\int_{-a}^{a}|\psi(x)|^2dx=\int_{-a}^{a}N^2(x^2-a^2)^2(a^2-\lambda^2x^2)^2dx=1 \tag{216}$$

$$\Rightarrow N^2=\frac{31.5}{16(\lambda^2-6\lambda+21)a^9} \tag{217}$$

(2)Find $\overline{H}(\lambda)$

$$\overline{H} = \int_{-a}^{a} \psi^* \hat{H} \psi(x) = \frac{3}{4} \frac{11\lambda^2 - 14\lambda + 35}{\lambda^2 - 6\lambda + 21} \frac{\hbar^2}{ma^2} \tag{218}$$

(note:Infinitely deep potential well $\boxed{\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + 0}$)

(3)

$$\begin{cases} \dfrac{d\overline{H}(\lambda)}{d\lambda} = 0 \\ \dfrac{d^2\overline{H}(\lambda)}{d\lambda^2}\Big|_{\lambda} < 0 \end{cases} \tag{219}$$

$$\Rightarrow \lambda_{min} = \lambda_0 \tag{220}$$

(4)Determine $\lambda_0 \to \overline{H}(\lambda_0)$ as the lowest energy (ground state) $\psi(x, \lambda)$, which is the ground state wave function.

Q.E.D.

😎

References

[1] Litskevich, M., Hossain, M.S., Zhang, SB. et al. Boundary modes of a charge density wave state in a topological material. Nat. Phys. (2024). https://doi.org/10.1038/s41567-024-02469-1

Dear readers, if you find any problems and questions, please feel free to contact me, I would appreciate it.

Have fun! 😎