

Particle moving along a line:

$$\begin{array}{cccc} x(t), & \dot{x}(t), & \ddot{x}(t), & V(x) \\ \text{position} & v & a & \text{potential} \end{array}$$

Kinetic energy: $\frac{1}{2}mv^2 = \frac{1}{2}m\dot{x}^2$ ①

Potential energy: $V(x)$ ②

Total energy $E = ① + ② = \frac{1}{2}m\dot{x}^2 + V(x)$

$V(x) = -ma = -m\ddot{x}$

Momentum: $p = mv = m\dot{x} \Rightarrow$ Kinetic energy: $\frac{p^2}{2m}$ ③

Potential energy: $V(x)$ ④

Total energy: $E = ③ + ④ = \frac{p^2}{2m} + V(x)$

Hamiltonian function: $H(x, p) = \frac{p^2}{2m} + V(x)$

$$\frac{\partial H(x, p)}{\partial p} = \frac{2p}{2m} = \frac{p}{m} = \dot{x}$$

$$-\frac{\partial H(x, p)}{\partial x} = -\frac{\partial}{\partial x} \left(\frac{p^2}{2m} + V(x) \right) = -V'(x) = m\ddot{x} = \dot{p}$$

TDSE

$$\left\{ \begin{array}{l} i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{H} \psi(x, t) \\ \hat{H} \psi(x) = E \psi(x) \\ i\hbar \frac{\partial \psi(x, t)}{\partial t} = \int_0^t E dt \end{array} \right.$$

$$\begin{aligned} i\hbar \frac{\partial \psi(x, t)}{\partial t} &= E t \cdot \frac{d}{dt} \\ \frac{\partial \psi(x, t)}{\partial t} &= \frac{E t}{i\hbar} = -\frac{iEt}{\hbar} \\ \psi(x, t) &= \exp\left(-\frac{iEt}{\hbar}\right) \end{aligned}$$

$$\psi(x, 0) = \psi(x) = \psi$$

$$\psi(x, t) = \exp\left(-\frac{iEt}{\hbar}\right) \cdot \psi(x)$$

Wavefunction: $\psi(x)$ State of the particle

Probability density: $|\psi(x)|^2 \left(\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \right)$

Mean value: $\bar{x} = \int_{-\infty}^{\infty} x \rho(x) dx = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx$

Uncertainty in position (variance): $(\Delta x)^2 = \overline{(x - \bar{x})^2} = \overline{(x^2 - 2x\bar{x} + \bar{x}^2)} = \bar{x}^2 - \bar{x}^2$

Hilbert Space

Two wavefunctions $\psi_1(x), \psi_2(x)$ from Hilbert space

$$\psi_3(x) = C_1 \psi_1(x) + C_2 \psi_2(x) \quad (\text{linear combination})$$

Quantum state $\psi_3(x)$ is a superposition of state $\psi_1(x)$ and $\psi_2(x)$, with weights C_1 and C_2 .

$$|\psi_3(x)|^2 = |C_1 \psi_1(x) + C_2 \psi_2(x)|^2 = |C_1|^2 |\psi_1(x)|^2 + |C_2|^2 |\psi_2(x)|^2 + \underbrace{C_1^* C_2 \psi_1^*(x) \psi_2(x) + C_2^* C_1 \psi_2^*(x) \psi_1(x)}_{\text{Interference}}$$

复数模平方的展开: $|A+B|^2 = |A|^2 + |B|^2 + A^*B + B^*A$

Interference (如果 $\langle \psi_1(x) | \psi_2(x) \rangle = 0$

orthonormal, 干涉项抵消)

Operator

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

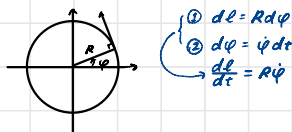
$$\hat{p}^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$$

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad \left(\hat{H} \psi(x) = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) \psi(x) \right)$$

L2



Particle moving on a ring:



kinetic energy: $T = \frac{1}{2}mv^2 = \frac{1}{2}m(R\dot{\phi})^2 = \frac{1}{2}mR^2\dot{\phi}^2$

Angular momentum: $L = \vec{r} \times \vec{p}$ ($L_z = mR^2\dot{\phi}$)

Classical Hamiltonian function: $H = T = \frac{L^2}{2mR^2} = \frac{L^2}{2I}$

$\dot{\phi} = \frac{\partial H}{\partial L} = \frac{L}{mR^2} = \dot{\phi}$

$\dot{L} = -\frac{\partial H}{\partial \phi} = 0$ (H 中不显含 ϕ) $\rightarrow$ 守恒量 L 守恒

$\phi(t) = \phi(t_0) + \frac{\dot{\phi}}{mR^2}(t - t_0)$

Eigenvalue problem of the angular momentum operator

$\hat{L}\psi(\phi) = L\psi(\phi)$

$L_k = \hbar k \quad (k \in \mathbb{Z})$

$E_k = \frac{\hbar^2 k^2}{2mR^2} = \frac{L^2}{2mR^2}$

$-i\hbar \frac{\partial}{\partial \phi} \psi(\phi) = L\psi(\phi)$

$-\frac{i\hbar}{L} \frac{\partial \psi(\phi)}{\partial \phi} = \psi(\phi)$

$\frac{\partial \psi(\phi)}{\partial \phi} = -\frac{iL}{\hbar} \psi + A$

$\psi(\phi) = C \exp(-\frac{iL}{\hbar} \phi)$

$\psi(\phi + 2\pi k) = \psi(\phi)$

$C \exp(-\frac{iL}{\hbar} \phi + \frac{2\pi i \hbar k}{L}) = C \exp(-\frac{iL}{\hbar} \phi)$

$\exp(-\frac{2\pi i \hbar k}{L}) = 1 \quad (e^{i2\pi} = \cos(2\pi) + i\sin(2\pi))$

$\cos(-\frac{2\pi \hbar k}{L}) + i\sin(-\frac{2\pi \hbar k}{L}) = 1$

$\frac{2\pi \hbar k}{L} = 2\pi k$
 $L = \hbar k$
 $L_k = \hbar k$

Operator

$\hat{L} = -i\hbar \frac{\partial}{\partial \phi}$

$\hat{H} = -\frac{\hbar^2}{2mR^2} \frac{\partial^2}{\partial \phi^2}$

$\psi(\phi + 2\pi) = \psi(\phi) \quad B.C$

$\int_0^{2\pi} |\psi(\phi)|^2 d\phi = 1$

TISE

$\hat{H}\psi(\phi) = E\psi(\phi)$

$-\frac{\hbar^2}{2mR^2} \frac{\partial^2}{\partial \phi^2} \psi(\phi) = E\psi(\phi)$

$\frac{d^2}{d\phi^2} \psi(\phi) = -k^2 \psi(\phi)$

$(k^2 = -\frac{2mR^2 E}{\hbar^2})$

$\psi_k(\phi) = C \exp(ik\phi)$

Normalized

$\int_0^{2\pi} C^* \exp(-\frac{i}{2} k \phi) d\phi = 1$

$C = \frac{1}{\sqrt{2\pi}}$

$\psi_k(\phi) = \frac{1}{\sqrt{2\pi}} \exp(ik\phi)$

$\hbar^2 \kappa^2 \psi''(\kappa) + \lambda \psi(\kappa) = 0$
 $y(\kappa) = \psi(\phi)$
 $\lambda = \hbar^2 \omega^2 - \frac{\hbar^2}{2mR^2}$
 $T(\phi) = \psi(\phi) = e^{i\phi}$
 $\psi(\phi) = A \exp(i\phi) + B \exp(-i\phi)$
 $\psi(\phi) = A e^{i\phi} + B e^{-i\phi}$
Euler: $e^{i\phi} = \cos(\phi) + i\sin(\phi)$
 $\psi(\phi) = C \cos(k\phi) + D \sin(k\phi)$
 $\psi_k(\phi) = C e^{ik\phi}$

Same

TDSE

波函数随时间的变化规律

$i\hbar \frac{\partial}{\partial t} \psi(t, \phi) = \hat{H}\psi(t, \phi)$

Variable Separation 分离变量

① $\psi(t, \phi) = T(t) \phi(\phi)$

② $i\hbar \frac{\partial}{\partial t} (T(t) \phi(\phi)) = -\frac{\hbar^2}{2mR^2} \frac{\partial^2}{\partial \phi^2} (T(t) \phi(\phi))$

$i\hbar \phi(\phi) \frac{\partial T(t)}{\partial t} = T(t) [-\frac{\hbar^2}{2mR^2} \frac{\partial^2 \phi(\phi)}{\partial \phi^2}]$

$\frac{i\hbar}{T(t)} \frac{\partial T(t)}{\partial t} = -\frac{\hbar^2}{2mR^2} \frac{1}{\phi(\phi)} \frac{\partial^2 \phi(\phi)}{\partial \phi^2} = E$

③ $i\hbar \frac{\partial T(t)}{\partial t} = T(t) E$ (Time 时间)

$\int_0^{T(t)} i\hbar \frac{\partial T(t)}{\partial t} dt = \int_0^E E dt$
 $i\hbar \ln T(t) = Et$
 $T(t) = \exp(-\frac{iEt}{\hbar})$

④ $\frac{\partial^2 \phi(\phi)}{\partial \phi^2} = -\frac{2mR^2 E \phi(\phi)}{\hbar^2}$

$\phi(\phi) = \frac{e^{i\phi}}{\sqrt{2\pi}}$ (或者作 $\psi_k(\phi)$)

$\psi(t, \phi) = e^{-\frac{iEt}{\hbar}} \phi(\phi)$

$E_k = \frac{\hbar^2 k^2}{2mR^2}$

Features of the eigenvalue spectrum, degeneracy

Ground state: $E_k = 0 \quad (k=0), \quad \psi_k(\phi) = \frac{1}{\sqrt{2\pi}}$

Excited state: $E_k = \frac{\hbar^2 k^2}{2mR^2} > 0$

Non-degeneracy: E_0

Doubly degeneracy: $E_k = E_{-k} = \frac{\hbar^2 k^2}{2mR^2}$

$\psi_k(\phi) = \frac{1}{\sqrt{2\pi}} \exp(ik\phi) \Rightarrow \begin{cases} \psi_{k,1}(\phi) = \frac{1}{\sqrt{2\pi}} \cos(k\phi) \\ \psi_{k,2}(\phi) = \frac{1}{\sqrt{2\pi}} \sin(k\phi) \end{cases}$
 $\int_0^{2\pi} \psi_{k,1}^*(\phi) \psi_{k,2}(\phi) d\phi = 0 \rightarrow \text{orthonormal}$

简并性

Standing wave
驻波

Physical meaning of the obtained eigensolutions

$\hat{H}$ = Hamiltonian operator, energy operator

$\hat{L}$ = Angular momentum operator

$$\psi_k(t, \varphi) = \psi_k(\varphi) e^{-\frac{i}{\hbar} E_k t}$$

The ground state: $\psi_0(t, \varphi) = \frac{1}{\sqrt{2\pi}} \rightarrow$ zero energy / zero angular momentum (no motion)

For $k \neq 0$, the stationary state $\psi_k(t, \varphi) = \frac{1}{\sqrt{2\pi}} \exp\left\{ik\left(\varphi - \frac{\hbar k}{2mR^2} t\right)\right\}$

$$\underbrace{e^{-ik\varphi}}_{\text{stationary wave}} \underbrace{\phi(k)}_{\text{time dependent}}$$

$$\frac{1}{\sqrt{2\pi}} \cos(k\varphi) e^{-\frac{i}{\hbar} E_k t}, \quad \frac{1}{\sqrt{2\pi}} \sin(k\varphi) e^{-\frac{i}{\hbar} E_k t}$$

Perinent angular probability: $\frac{1}{2\pi} \cos^2(k\varphi), \quad \frac{1}{2\pi} \sin^2(k\varphi)$

Experimental relevance (spectroscopy)

$$E_{k \text{ initial}} - E_{k \text{ final}} = \frac{2\pi\hbar c}{\lambda}$$

λ = wavelength of absorbed light

General Quantum state

$$\psi(\varphi) = \sum_{k=-\infty}^{k=\infty} C_k \psi_k(\varphi) \quad (\psi_k(\varphi) = \frac{1}{\sqrt{2\pi}} e^{ik\varphi})$$

$$C_k = \int_0^{2\pi} d\varphi \psi_k^*(\varphi) \psi(\varphi)$$

simple matter to prove that: $\int_0^{2\pi} d\varphi |\psi(\varphi)|^2 = \sum_{k=-\infty}^{k=\infty} |C_k|^2 = 1$

$$\psi(\varphi) = \frac{1}{\sqrt{2\pi}} \sum_{k=-\infty}^{k=\infty} C_k e^{ik\varphi}$$

$$\psi(t, \varphi) = \sum_{k=-\infty}^{k=\infty} C_k \psi_k(\varphi)$$

$$\psi(t, \varphi) = \sum_{k=-\infty}^{k=\infty} C_k \psi_k(\varphi) e^{-\frac{i}{\hbar} E_k (t - t_0)}$$

Quantum measurement: Particle on a ring as an example

$$\psi(\varphi) = \sum_{k=-\infty}^{+\infty} C_k \psi_k(\varphi) \quad C_k = \phi(L_k) = \int_0^{2\pi} d\varphi \psi_k^*(\varphi) \psi(\varphi)$$

$$|\psi|^2 = \int_0^{2\pi} d\varphi \psi^*(\varphi) \psi(\varphi) = \sum_{k \in \mathbb{Z}} |\phi(L_k)|^2$$

Detector measuring the energy

$$p(E_0) = |C_0|^2 = |\phi(L_0)|^2$$

$$p(E_k) = |C_{-k}|^2 + |C_k|^2 = |\phi(L_{-k})|^2 + |\phi(L_k)|^2 \quad (k > 0)$$

Assuming unit normalization, $\sum_{k \in \mathbb{Z}} |C_k|^2 = \sum_{k \in \mathbb{Z}} |\phi(L_k)|^2 = 1$

$$C_0 \psi_0(\varphi) = \phi(L_0) \psi(\varphi)$$

$$C_{-k} \psi_{-k}(\varphi) + C_k \psi_k(\varphi) = \phi(L_{-k}) \psi_{-k}(\varphi) + \phi(L_k) \psi_k(\varphi)$$

The passage (jump) due to measurement is called again
wavefunction collapse

Detector measuring the position

$$p(\varphi_1 \leq \varphi \leq \varphi_2) = \int_{\varphi_1}^{\varphi_2} |\psi(\varphi)|^2 d\varphi = \sum_{k \in \mathbb{Z}} |C_k|^2 = \sum_{k \in \mathbb{Z}} |\phi(L_k)|^2 = 1 \quad (\text{Normalization})$$

$$p(L_{k_1} \leq L \leq L_{k_2}) = \sum_{L_{k_1} \leq L \leq L_{k_2}} |\phi(L_k)|^2$$

Particle moving along a line

Assume $R \rightarrow \infty$ (Radius be infinite) $\Rightarrow \begin{cases} x = R\varphi \\ p = \frac{\hbar}{R} \end{cases}$ angular momentum

$|\psi(x)|^2$ probability density for position x

$|\phi(p)|^2$ probability density for momentum p

$$\frac{\hat{L}}{R} = -i\hbar \frac{\partial}{\partial R\varphi} = -i\hbar \frac{\partial}{\partial x} = \hat{p} \rightarrow \text{momentum operator } \hat{p}$$

$$\text{For } R \rightarrow \infty, \quad \delta p = \frac{\hbar}{R}$$

$$\text{Normalization: } \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1, \quad |\psi(x)|^2 dx = |\psi(\varphi)|^2 d\varphi = |\psi(\varphi)|^2 \frac{dx}{R}$$

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \int_0^{2\pi} |\psi(\varphi)|^2 \frac{dx}{R} = 1$$

$$\psi(R) = \psi(\varphi) \cdot \frac{1}{\sqrt{R}}$$

$$\text{Normalization: } \int_{-\infty}^{+\infty} |\phi(p_k)|^2 dp_k = 1$$

$$\int_{-\infty}^{+\infty} |\phi(L_k)|^2 \cdot \frac{\hbar}{R} dL_k = 1$$

$$\sqrt{\frac{R}{\hbar}} \phi(L_k) = \phi(p_k)$$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \sum_{k=-\infty}^{+\infty} \phi(p_k) e^{+\frac{i}{\hbar} p_k x} (\delta p) \quad ; \quad (19)$$

$$\phi(p_k) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-R\pi}^{+R\pi} dx \psi(x) e^{-\frac{i}{\hbar} p_k x} \quad . \quad (20)$$

After pushing $R \rightarrow \infty$, we may regard the momentum as a continuous variable, and write even more insightfully

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \phi(p) e^{+\frac{i}{\hbar} px} dp \quad ; \quad (21)$$

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(x) e^{-\frac{i}{\hbar} px} dx \quad . \quad (22)$$

Formulas

$$|\psi(\varphi)|^2 d\varphi = |\psi(x)|^2 dx \quad (23)$$

and

$$|\phi(L_k)|^2 = |\phi(p)|^2 \delta p \quad (24)$$

reveal that $|\psi(x)|^2$ is the appropriate probability density for position x (as expected), whereas $|\phi(p)|^2$ is the appropriate probability density for momentum p (as we see right now, given the previously established interpretation of $|\phi(L_k)|^2$).

What do you need to know for the exam?

The Fourier transform formulas (21)-(22)

converting the wavefunction $\psi(x)$ of our particle moving along a straight line

into the equivalent **momentum representation wavefunction** $\phi(p)$.

Physical meaning of $\phi(p)$: Quantity $|\phi(p)|^2$ is the probability density of momentum.

Calculation of the mean $\bar{p}$ and uncertainty (Δp) of the momentum,

following completely analogous methods as we used before for calculations of $\bar{x}$ and (Δx) .

Mutual equivalence between the x -representation $\psi(x)$ and the p -representation $\phi(p)$.²

$$\bar{p} = \int_{-\infty}^{+\infty} p |\phi(p)|^2 dp$$

$$\Delta p = \sqrt{\bar{p}^2 - \bar{p}^2}$$

$$\bar{p}^2 = \int_{-\infty}^{+\infty} p^2 |\phi(p)|^2 dp$$



TDSE for a free particle moving along a straight line

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

$$i\hbar \frac{\partial}{\partial t} \psi(t, x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(t, x)$$

$$\psi(t, x) = \psi(0, x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \phi(p) e^{+\frac{i}{\hbar} px} dp$$

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(0, x) e^{-\frac{i}{\hbar} px} dx$$

$$\psi(t, x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \phi(p) e^{-\frac{i}{\hbar} \left(\frac{p^2}{2m}\right) t} e^{+\frac{i}{\hbar} px} dp$$

时间演化因子

$e^{+\frac{i}{\hbar} p x}$ is an eigenfunction of both $\hat{p}$ and $\hat{H}$. (but not square integrable function $\int_{-\infty}^{+\infty} e^{+\frac{i}{\hbar} p x} dx$)

The Heisenberg uncertainty principle

$\psi(x) \rightarrow$ mean $\bar{x}$ and uncertainty (Δx)

$\phi(p) \rightarrow$ mean $\bar{p}$ and uncertainty (Δp)

$(\Delta x)(\Delta p) \geq \frac{\hbar}{2} \Rightarrow$ Quantum particle have no trajectory.

Quantum harmonic oscillator:

Ladder operator: $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega} \hat{p} \right)$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega} \hat{p} \right)$$

L 4

Ket / bra vector, closure, Scalar production (Dirac)

$$\overset{\text{bra}}{\langle \psi_1 |} \overset{\text{ket}}{\psi_2 \rangle} = \int_{-\infty}^{\infty} \psi_1^*(x) \psi_2(x) dx$$

$$\langle \psi_1 | \psi_2 \rangle = \langle \psi_2 | \psi_1 \rangle^*$$

$$\langle \phi_i | \phi_j \rangle = \delta_{ij}$$

1. Describe, in your own words, what is Quantum Mechanics (QM),

what kind of objects does QM deal with ?

At which length scales does the quantum mechanical description become important ?

Why is QM important for Chemistry and Engineering ?

How does QM differ from Classical Mechanics ? (give at least 4 differences)

QC : Discipline of physics dealing with microworld.

Object of microworld : elementary particles (electrons, photon, ...), atoms, molecules

Length scale : $< 1 \mu\text{m}$ (10^{-6} m) example: nanostructure, molecules, atoms

Why important : Understanding the property of matter { atoms, molecules, materials } from first principles

Time dependent Schrödinger eq.

QM gives foundation of electronic

structure theory of atoms and molecules

spectroscopy

theory of reaction mechanisms, rate constants

QM enables to predict new phenomena

Difference : can not imagine how does a Quantum particle look like.

wavefunction, operators

uncertainty principle $(\Delta x)(\Delta p) \geq \frac{\hbar}{2}$

quantization (energy levels, angular momentum)

play dice (stochastic nature of QM, probability)

quantum entanglement
纠缠

wave - particle duality
波粒二象性

2. Consider a particle moving in 1D along $x \in (-\infty, +\infty)$. The particle has no spin. Describe, in your own words, how do you perform the passage from Classical Mechanics into Quantum Mechanics. Write down the corresponding procedure mathematically, and build up in this manner the time dependent Schrödinger equation (TDSE). Explain, in your own words, what is the TDSE good for. Write down the corresponding time independent Schrödinger equation (TISE), and explain what are the associated eigenvalues of $\hat{H}$ good for. Explain how can solutions of the TISE be used to solve TDSE.

Classical mechanics $\Rightarrow$ Hamiltonian $H = \overset{\text{kinetic}}{\frac{p^2}{2m}} + \overset{\text{potential}}{V(x)}$

Passage to QM: $p \rightarrow \hat{p} = -i\hbar \frac{\partial}{\partial x}$ $\hat{p}\psi(x) = -i\hbar \frac{\partial \psi(x)}{\partial x}$

$x \rightarrow \hat{x} = x$ $\hat{x}\psi(x) = x\psi(x)$

$H \rightarrow \hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$

TDSE: $i\hbar \frac{\partial}{\partial t} \psi(x, t) = \hat{H} \psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x) \psi(x, t)$

What is TDSE good for: suppose at $t = t_0$, $\psi(x, t_0) = \psi_0(x)$

TDSE enables us solving $\psi(x, t)$ ($t \neq t_0$)

$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \hat{H} \psi(x, t)$; $\psi(x, t_0) = \psi_0(x)$

TISE: $\hat{H} \psi_m(x) = E_m \psi_m(x)$ m : labels different solutions

Eigenvalues good for: measurements of energy of our particles gives one of the E_m 's.

one can't get a measurement outcome which is not one of the E_m 's.

TISE $\rightarrow$ TDSE: We expand

$$\begin{aligned} \phi_0(x) &= \sum_m C_m \psi_m(x) \\ C_m &= \langle \psi_m | \phi_0 \rangle = \int_{-\infty}^{\infty} \psi_m^*(x) \phi_0(x) dx \\ \psi(t, x) &= \psi_0(x) \cdot \exp\left(-\frac{i}{\hbar} E_m (t - t_0)\right) = \sum_m C_m \psi_m(x) \cdot \exp\left(-\frac{i}{\hbar} E_m (t - t_0)\right) \end{aligned}$$

3. Consider a particle of mass m moving on a circle (radius R). The particle has no spin.
 Write down the corresponding Hamiltonian $\hat{H}$ and the angular momentum operator $\hat{L}$.
 Solve the eigenvalue problems of $\hat{L}$ and $\hat{H}$ (eigenvalues and unit normalized eigenfunctions),
 and represent the obtained eigenvalue spectra graphically.
 Write down the orthonormality relations for the eigenfunctions.
 Write down the time dependent Schrödinger equation (TDSE) for our particle on the ring,
 and explain how can the just constructed eigenfunctions be used
 to propagate a given ($t = 0$) initial state in time.

$$\hat{H} = -\frac{\hbar^2}{2mR^2} \frac{\partial^2}{\partial \varphi^2}$$

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

$$\hat{H} \psi(\varphi) = E \psi(\varphi)$$

$$\hat{L} \psi(\varphi) = L \psi(\varphi)$$

$-\hbar^2 \left(\frac{\partial^2}{\partial \varphi^2} \right) \psi(\varphi) = E \psi(\varphi) \Rightarrow \psi(\varphi) = A e^{ik\varphi}$

$-i\hbar \frac{\partial}{\partial \varphi} \psi(\varphi) = L \psi(\varphi)$

$\int_0^{2\pi} \frac{\partial \psi(\varphi)}{\psi(\varphi)} = \int_0^{2\pi} L \frac{\partial \varphi}{-i\hbar}$

$\ln \psi(\varphi) = \frac{iL\varphi}{\hbar} + k$

$\psi(\varphi) = A e^{\frac{iL\varphi}{\hbar}} \quad (k = \frac{L}{\hbar})$

$\psi_k(\varphi) = \frac{1}{\sqrt{2\pi}} e^{ik\varphi}$

Normalization:

$$\int_0^{2\pi} \psi_k^*(\varphi) \psi_k(\varphi) d\varphi = 1$$

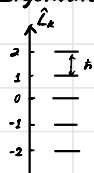
$$A^2 \int_0^{2\pi} (e^{ik\varphi})^* e^{ik\varphi} d\varphi = 1$$

$$\downarrow$$

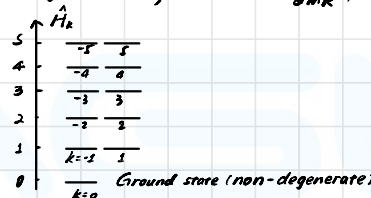
$$A = \frac{1}{\sqrt{2\pi}}$$

$$\psi_k(\varphi) = \frac{1}{\sqrt{2\pi}} e^{ik\varphi}$$

Eigenvalue of $\hat{L}$ ($L_k = k\hbar$)



Eigenvalue of $\hat{H}$ ($E_k = \frac{\hbar^2 k^2}{2mR^2}$)



Orthonormality relations

$$\langle \psi_k | \psi_{k'} \rangle = \int_{-\infty}^{\infty} \psi_k^*(\varphi) \psi_{k'}(\varphi) d\varphi = \delta_{kk'} \begin{cases} k=k', 1 \\ k \neq k', 0 \end{cases}$$

TDSE: $i\hbar \frac{\partial}{\partial t} \psi(\varphi, t) = \hat{H} \psi(\varphi, t)$

Expand $\phi(\varphi)$ in the orthonormal basis set $\phi(\varphi) = \sum_{n=-\infty}^{\infty} C_n \psi_n(\varphi)$; $C_n = \langle \psi_n | \phi \rangle = \int_0^{2\pi} \psi_n^*(\varphi) \phi(\varphi) d\varphi$

Propagate in the time: $\phi(\varphi, t) = \sum_{n=-\infty}^{\infty} C_n \psi_n(\varphi) \cdot e^{-\frac{i}{\hbar} E_n t}$

4. Consider a particle moving along $x \in (-\infty, +\infty)$, without spin.

Let the quantum state of this particle be described by wavefunction $\psi(x)$.

Explain what it means when we say that $\psi(x)$ must be square integrable.

Describe how do we normalize a given square integrable wavefunction $\psi(x)$ (which is given to you without normalization).

Suppose now that $\psi(x)$ is unit normalized. What is the meaning of $|\psi(x)|^2$?

How do we determine the probability of finding our particle between $x = -7$ and $x = +3$?

Explain how do we get from $\psi(x)$ an information about the momentum probability density.

Write down the definitions of the mean momentum $\bar{p}$ and the standard deviation (Δp) .

What it means if $\psi(x)$ must be square integrable: $\int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty$

Normalization: $\phi(x) = C\psi(x)$

$$\int_{-\infty}^{\infty} |\phi(x)|^2 dx = C^2 \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

$$C^2 = \frac{1}{\int_{-\infty}^{\infty} |\psi(x)|^2 dx} \Rightarrow \phi(x) = \frac{1}{\sqrt{\int_{-\infty}^{\infty} |\psi(x)|^2 dx}} \psi(x)$$

Meaning of $|\psi(x)|^2$ ($\psi(x)$ is normalized): Probability density around x .

Probability between $x = -7$ and $x = 3$: $\int_{-7}^3 |\psi(x)|^2 dx = P(-7 \leq x \leq 3)$

How to get from $\psi(x)$ an information about the momentum probability density?

Fourier transform into p -presentation: $\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-\frac{i}{\hbar} p x} dx$ Exom

$|\psi(p)|^2 =$ momentum probability density

$$\bar{p} = \int_{-\infty}^{\infty} p |\psi(p)|^2 dp$$

$$\bar{p}^2 = \int_{-\infty}^{\infty} p^2 |\psi(p)|^2 dp$$

$$(\Delta p)^2 = \bar{p}^2 - (\bar{p})^2$$