L1

Particle moving along a line:

$x(t)$, $\dot{x}(t)$, $\ddot{x}(t)$, $V(x)$

position, v, a, potential

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

$$\begin{cases} i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t) \\ \hat{H}\psi(x) = E\psi(x) \end{cases}$$

$$\int_0^{\psi(x,t)} i\hbar\frac{\partial\psi(x,t)}{\psi(x,t)} = \int_0^t E\,dt$$

$i\hbar\ln(\psi(x,t)) = Et + d$

$\ln(\psi(x,t)) = \frac{Et}{i\hbar} = \frac{-iEt}{\hbar}$

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

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

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

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

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

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

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

Hilbert Space

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

$\psi_3(x) = C_1\psi_1(x) + C_2\psi_2(x)$ (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.

$|\psi_3(x)|^2 = |C_1\psi_1(x) + C_2\psi_2(x)|^2 = |C_1|^2|\psi_1(x)|^2 + |C_2|^2|\psi_2(x)|^2 + C_1^*C_2\psi_1^*(x)\psi_2(x) + C_2^*C_1\psi_2^*(x)\psi_1(x)$

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, 干涉项消失)

Operator

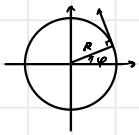
$\hat{p} = -i\hbar\frac{\partial}{\partial x}$

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

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

L 2

Particle moving on a ring:



① $dl = Rd\varphi$

② $d\varphi = \dot{\varphi}dt$

$\frac{dl}{dt} = R\dot{\varphi}$

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

Angular momentum: $L = \underbrace{\vec{r} \times \vec{p}}_{\text{(in x-y plane)}}$ $(L_z = mR^2\dot{\varphi})$

Classical Hamiltonian function: $H = T = \frac{L^2}{2mR^2} = \frac{L^2}{2I}$ (I: momentum of inertia and L_z)

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

$\dot{L} = -\frac{\partial H}{\partial \varphi} = 0$ (H中不显含 φ) → 角动量L守恒

$\varphi(t) = \varphi(t_0) + \frac{\dot{\varphi}}{\frac{L}{mR^2}}(t - t_0)$ ($\dot{\varphi} = \frac{L}{mR^2}$, $dt = t - t_0$)

Eigenvalue problem of the angular momentum operator

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

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

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

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

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

$\ln\psi(\varphi) = -\frac{i\hbar}{L}\varphi + A$

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

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

$C\exp(-\frac{i\hbar}{L}\varphi \cdot \frac{2\pi i\hbar k}{L}) = C\exp(-\frac{i\hbar}{L}\varphi)$

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

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

$\cos(-\frac{2\pi\hbar k}{L}) = 1$, $\sin(-\frac{2\pi\hbar k}{L}) = 0$

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

$L = \hbar k$

$L_k = k\hbar$

Operator

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

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

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

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

TISE

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

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

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

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

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

形式为 $\psi''(x) + \lambda\psi(x) = 0$

$y(x) = \psi(\varphi)$

$\lambda = k^2$ 是一个常数

$Try\ \psi(\varphi) = e^{r\varphi}$

$\psi''(\varphi) + \lambda\psi(\varphi) = r^2e^{r\varphi} + k^2e^{r\varphi} = 0$

$r^2 = k^2 \Rightarrow r = \pm ik$

$\psi(\varphi) = Ae^{ik\varphi} + Be^{-ik\varphi}$

Euler: $e^{ix} = \cos(x) + i\sin(x)$

$\psi(\varphi) = C_1\cos(k\varphi) + D_1\sin(k\varphi)$

$\Downarrow$

$\psi_k(\varphi) = Ce^{ik\varphi}$

Normalized

$\int_0^{2\pi} C^2\exp(\frac{1}{2}ik\varphi)\, d\varphi = 1$

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

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

TDSE

$i\hbar\frac{\partial}{\partial t}\psi(t,\varphi) = \hat{H}\psi(t,\varphi)$ (波函数随时间变化的量 / 总能量(动能+势能))

Variable Separation 分离变量

① $\psi(t,\varphi) = T(t)\phi(\varphi)$

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

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

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

① ②

① $i\hbar\frac{\partial T(t)}{\partial t} = T(t)E$ (Time 时间)

$\int_0^{T(t)}\frac{i\hbar}{T(t)}\frac{\partial T(t)}{\partial t} = \int_0^t E\,\partial t$

$i\hbar\ln T(t) = Et$

$T(t) = \exp(-\frac{iEt}{\hbar})$

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

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

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

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

Same

Features of the eigenvalue spectrum, degeneracy

简并性

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

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

Non-degeneracy: E_0

Doubly degeneracy: $E_{-k} = E_k = \frac{\hbar^2k^2}{2mR^2}$ (两项相同能量)

$\int_0^{2\pi}\psi_{-k}^*(\varphi)\psi_k^*(\varphi)d\varphi = 0$ → orthonormal

$\begin{cases}\psi_k(\varphi) = \frac{1}{\sqrt{2\pi}}\exp(+ik\varphi)\\ \psi_k(\varphi) = \frac{1}{\sqrt{2\pi}}\exp(-ik\varphi)\end{cases} \Rightarrow \begin{cases}\psi_{k,1}(\varphi) = \frac{1}{\sqrt{\pi}}\cos(k\varphi)\\ \psi_{k,2}(\varphi) = \frac{1}{\sqrt{\pi}}\sin(k\varphi)\end{cases}$

Standing wave 驻波

Physical meaning of the obtained eigensolutions

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

$\hat{L}$ = Angular momentum operator

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

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

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

$\frac{1}{\sqrt{\pi}}\cos(k\varphi)\, e^{-\frac{i}{\hbar}E_k t}$, $\frac{1}{\sqrt{\pi}}\sin(k\varphi)\, e^{-\frac{i}{\hbar}E_k t}$ (时间演化因子)

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

Experimental relevance (spectroscopy)

$E_{k\,initial} - E_{k\,final} = \frac{2\pi\hbar c}{\lambda}$ ↳ 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: $\int_0^{2\pi} d\varphi\, |\psi(\varphi)|^2 = \sum_{k=-\infty}^{k=\infty} |C_n|^2 = 1$

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

$\psi(t_0,\varphi) = \sum_{k=-\infty}^{k=\infty} C_k \psi_k(\varphi)$

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

L 3

Quantum measurement: Particle on a ring as an example

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

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

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

$p(\varphi_1 \le \varphi \le \varphi_2) = \int_0^{2\pi} |\psi(\varphi)|^2 d\varphi = \sum_{k \in \mathbb{Z}} |C_k|^2 = \sum_{k \in \mathbb{Z}} |\phi(L_k)|^2 = 1$ (Normalization)

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

Particle moving along a line

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

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

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

$\hat{\frac{L}{R}} = -i\hbar \frac{\partial}{\partial R\varphi} = -i\hbar \frac{\partial}{\partial x} = \hat{p} \rightarrow$ momentum operator $\hat{p}$ $\qquad$ For $R \to \infty$, $d\rho = \frac{\hbar}{R}$

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

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

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

Normalization: $\int_{-\infty}^{+\infty} |\phi(p_k)|^2 \underbrace{dp_k}_{\downarrow \frac{\hbar}{R}} = 1$

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

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

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

$$\Phi(p_k) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-R\pi}^{+R\pi} \mathrm{d}x\ \psi(x)\, e^{-\frac{i}{\hbar} p_k x} \quad . \tag{20}$$

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

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \Phi(p)\, e^{+\frac{i}{\hbar} px}\, \mathrm{d}p \quad ; \tag{21}$$

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(x)\, e^{-\frac{i}{\hbar} px}\, \mathrm{d}x \quad . \tag{22}$$

Formulas

$$\left| \psi(\varphi) \right|^2 \mathrm{d}\varphi = \left| \psi(x) \right|^2 \mathrm{d}x \tag{23}$$

and

$$\left| \phi(L_k) \right|^2 = \left| \Phi(p) \right|^2 \delta p \tag{24}$$

reveal that $|\psi(x)|^2$ is the appropriate probability density for position x (as expected), whereas $|\boldsymbol{\Phi(p)}|^2$ ***is the appropriate probability density for momentum*** $\boldsymbol{p}$ (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]

$$\bar{p} = \int_{-\infty}^{\infty} p\,|\phi(p)|^2\,dp$$
$$\Delta p = \sqrt{\overline{p^2} - \bar{p}^2}$$
$$\overline{p^2} = \int_{-\infty}^{\infty} p^2\,|\phi(p)|\,dp$$

TDSE for a free particle moving along a straight line

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

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

$\psi_1(x) =$

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

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

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

$\frac{p^2}{2m} \to E_p$ (时间演化因子)

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

The Heisenberg uncertainty principle

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

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

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

Quantum harmonic oscillator:

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

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

L4

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

$$\langle \psi_1 | \psi_2 \rangle = \int_{-\infty}^{\infty} \psi_1^*(x)\, \psi_2(x)\, dx$$

(bra: $\langle \psi_1 |$, ket: $| \psi_2 \rangle$)

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

$$\langle \phi_l | \phi_{l'} \rangle = \delta_{ll'}$$

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 μm (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 phenomenia

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.

kinetic potential

Classical mechanisms $\Rightarrow$ Hamiltonian $H = \frac{p^2}{2m} + V(x)$

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

$x \to \hat{x} = x$ $\quad \hat{x}\psi(x) = x\psi(x)$

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

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

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: $\hat{H}\psi_m(x) = E_m\psi_m(x)$ $\quad m$: 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 $\longrightarrow$ TDSE: We expand

$$\phi_0(x) = \sum_m C_m\psi_m(x)$$

$$C_m = \langle \psi_m | \phi_0 \rangle = \int_{-\infty}^{\infty} \psi_m^*(x)\,\phi_0(x)\,dx$$

$$\psi(t,x) = \psi_0(x)\cdot \exp\left(-\tfrac{i}{\hbar}E_m(t-t_0)\right) = \sum_m C_m\psi_m(x)\cdot\exp\left(-\tfrac{i}{\hbar}E_m(t-t_0)\right)$$

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.

$\hat{H} = -\frac{\hbar^2}{2mR^2}\frac{\partial^2}{\partial\varphi^2}$ $\quad \hat{H}\psi(\varphi) = E\psi(\varphi)$

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

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

$-k^2 \left(\hat{L}^2 = \frac{\hbar^2 k^2}{2mR^2}\right)$ (eigenvalue)

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

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

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

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

$\psi(\varphi) = Ae^{\frac{iL\varphi}{\hbar}} \quad \left(k = \frac{L}{\hbar}\right)$

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

Normalization:

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

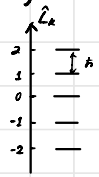
$A^2 \int_0^{2\pi} (e^{ik\varphi})^2 d\varphi = 1$

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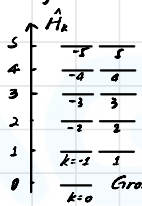
$A = \frac{1}{\sqrt{2\pi}}$

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

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



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



Ground state (non-degenerate)

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

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

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

Propagate in the time: $\quad \phi(\varphi, t) = \sum_{-\infty}^{\infty} C_m \psi_m(\varphi) \cdot e^{-\frac{i}{\hbar}E_m t}$

4. Consider a particle moving along $x \in (-\infty, +\infty)$, without spin.
Let the quantum state if this particle be described by wavefunction $\psi(x)$.
Explain what it means when we say that $\psi(x)$ must be 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 $x = 3$: $\int_{-7}^{3} |\psi(x)|^2 dx = p(-7 \le x \le 3)$

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

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

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

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

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

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