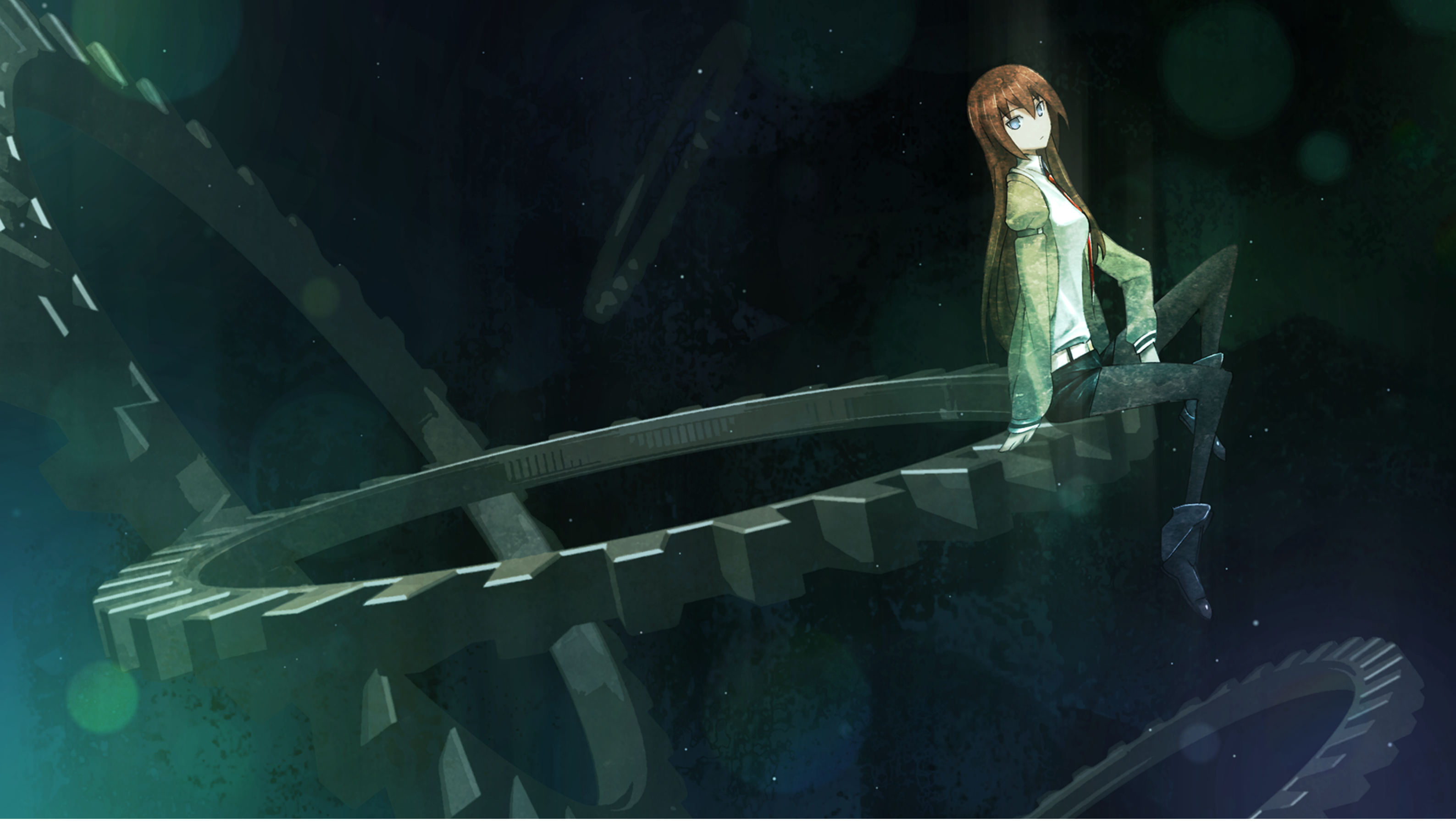

Lecture Notes on Quantum Mechanics

Alpha Version

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Typeset with LaTeX

This note is compiled based on the content of the Quantum Mechanics course taught by Professor Hong Guo from School of Electronics, Peking University.

Contents

1 Review of Preparatory Knowledge

1.1 Classical Mechanics

1. $\boxed{\delta S \equiv 0}$ Principle of Least Action

2. $\boxed{\dfrac{\mathrm{d}}{\mathrm{d}t}\dfrac{\partial \mathscr{L}}{\partial \dot{q}_\alpha} = \dfrac{\partial \mathscr{L}}{\partial q_\alpha} \quad (\alpha = 1, 2, \cdots, D)}$ Euler-Lagrange eqs.

3. $\boxed{\begin{cases} \dot{q}_\alpha = \dfrac{\partial H}{\partial p_\alpha} \\ \dot{p}\alpha = -\dfrac{\partial H}{\partial q_\alpha} \end{cases} \quad (\alpha = 1, 2, \cdots, D)}$ Hamilton's Canonical eqs.

4. $\boxed{\dfrac{\mathrm{d}f}{\mathrm{d}t} = \dfrac{\partial f}{\partial t} + [f, H]_{\mathrm{PB}}[f, H]_{\mathrm{PB}}}$ Poisson Bracket

5. $\boxed{\dfrac{\partial S}{\partial t} + H(q, \dfrac{\partial S}{\partial q}, t) = 0}$ Hamilton-Jacobi eq.

1.2 Newtonian Mechanics

Euclidean Space (Physical Space) $\longrightarrow$ Cartesian (Descartes) Coordinates

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \boldsymbol{F},\ \boldsymbol{p} = m\boldsymbol{v} \text{ (Momentum \& Force)}$$

$$\frac{\mathrm{d}\boldsymbol{L}}{\mathrm{d}t} = \boldsymbol{M},\ \boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p},\ \boldsymbol{M} = \boldsymbol{x} \times \boldsymbol{F} \text{ (Angular Momentum \& Torque)}$$

Mass point $\longrightarrow$ Mass point system $\longrightarrow$ Rigid Body $\longrightarrow$ Inertia $\begin{cases} \text{Mass: } m \\ \text{Inertia of Rotation: } mr^2 \end{cases}$

1.3 Lagrangian Mechanics - Analytical M.

1.3.1 Constraint

$x_1, x_2, \cdots, x_{3N}$ are dependent $\Longrightarrow$ $q_1, q_2, \cdots, q_D$ are independent $\left(\dfrac{\partial q_i}{\partial q_j} = 0,\ i \neq j\right)$

constraint $\begin{cases} \text{holonomic: } f(x; t) \equiv 0 \\ \text{non-holonomic: } f(x, \dot{x}; t) \equiv 0 \end{cases}$

1.3.2 Coordinates and Space

Generalized Coordinates $q_\alpha(t),\ \alpha = 1, 2, \cdots, D \leq 3N$
Configuration Space (Abstract Space): D-dim

1.3.3 Functional

Example of functionals (function of function):

1. Lagrangian:

$$\mathscr{L}(q(t), \dot{q}(t); t)$$

   generalized velocity: $\dot{q} = \dfrac{\mathrm{d}q}{\mathrm{d}t}$

2. Hamiltonian:

$$H(q(t), p(t); t)$$

   canonical position: $q(t)$; canonical momentum: $p_\alpha = \dfrac{\partial \mathscr{L}}{\partial \dot{q}_\alpha}$ (in Phase Space)

3. Action:

$$S[q(t)] = \int_{t_1}^{t_2} \mathscr{L}(q(t), \dot{q}(t); t)\mathrm{d}t$$

Dimensions of these functionals:
$[\mathscr{L}] = [H] = [\text{Energy}]$, $[S] = [\text{Energy}] \cdot [\text{Time}] = [\text{Length}] \cdot [\text{Momentum}] = [\hbar]$
Reduced Planck's Constant: $\hbar = \dfrac{h}{2\pi}$

1.3.4 Difference & Differential & Variation

$$f(x_2) - f(x_1) = \underbrace{\Delta f}_{\text{difference}} \xrightarrow[\Delta x = x_2 - x_1]{\Delta x \to 0} \underbrace{\mathrm{d}f}_{\text{differential}}, \text{ variation: } \delta q(t) = q_2(t) - q_1(t)$$

$$f(q, \dot{q}; t) : \begin{cases} \Delta f = \dfrac{\partial f}{\partial q}\Delta q + \dfrac{\partial f}{\partial \dot{q}}\Delta \dot{q} \\ \mathrm{d}f = \dfrac{\partial f}{\partial q}\mathrm{d}q + \dfrac{\partial f}{\partial \dot{q}}\mathrm{d}\dot{q} \\ \delta f = \dfrac{\partial f}{\partial q}\delta q + \dfrac{\partial f}{\partial \dot{q}}\delta \dot{q} \ (\delta q(t_1) = \delta q_2 = 0; \delta t = 0) \end{cases}$$

1.3.5 Principle of Least Action (Hamilton's Principle)

$$\boxed{\delta S \equiv 0} \Longrightarrow \text{ dynamical equations}$$

1.3.6 Euler-Lagrange Equations

$$\boxed{\frac{\partial \mathscr{L}}{\partial q_\alpha} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{q}_\alpha}\right), \ \alpha = 1, 2, \cdots, D}$$

D 2nd-order ODE

$$
\begin{aligned}
0 \equiv \delta S = \delta \int_{t_1}^{t_2} \mathscr{L}(q,\dot{q};t)\mathrm{d}t &= \int_{t_1}^{t_2} \left(\frac{\partial \mathscr{L}}{\partial q}\delta q + \frac{\partial \mathscr{L}}{\partial \dot{q}}\delta \dot{q} \right) \mathrm{d}t \\
&= \int_{t_1}^{t_2} \left[\frac{\partial \mathscr{L}}{\partial q}\delta q + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{q}}\delta q \right) - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{q}} \right) \delta q \right] \mathrm{d}t \\
&= \int_{t_1}^{t_2} \left[\frac{\partial \mathscr{L}}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{q}} \right) \right] \delta q \mathrm{d}t + \underbrace{\frac{\partial \mathscr{L}}{\partial \dot{q}}\delta q\Big|_{t_1}^{t_2}}_{=0} \Longrightarrow \frac{\partial \mathscr{L}}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{q}} \right) \equiv 0
\end{aligned}
$$

1.4 Hamiltonian Mechanics - Analytical M.

1.4.1 Legendre Transformations

$$
\begin{cases}
p_\alpha = \dfrac{\partial \mathscr{L}}{\partial \dot{q}_\alpha}, \ \alpha = 1, 2, \cdots, D \\
H(q,p;t) = \displaystyle\sum_\alpha p_\alpha \dot{q}_\alpha - \mathscr{L}(q,\dot{q};t)
\end{cases}
$$

$$
\Longrightarrow \frac{\partial H}{\partial \dot{q}_\alpha} = p_\alpha - \frac{\partial \mathscr{L}}{\partial \dot{q}_\alpha} \equiv 0 \Longrightarrow H \text{ is } \dot{q} \text{ - independent, } \mathscr{L} \text{ is } p \text{ - independent}
$$

1.4.2 Hamilton's Canonical Equations of Motion

$$
\boxed{\begin{cases}
\dot{q}_\alpha = \dfrac{\partial H}{\partial p_\alpha} \\
\dot{p}_\alpha = -\dfrac{\partial H}{\partial q_\alpha}
\end{cases} \quad \alpha = 1, 2, \cdots, D}
$$

$2D$ 1st-order ODE

$$
0 \equiv \frac{\partial \mathscr{L}}{\partial p_\alpha} = \dot{q}_\alpha - \frac{\partial H}{\partial p_\alpha} \Longrightarrow \dot{q}_\alpha = \frac{\partial H}{\partial p_\alpha};\ \dot{p}_\alpha = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{q}_\alpha} \right) = \frac{\partial \mathscr{L}}{\partial q_\alpha},\ \frac{\partial H}{\partial q_\alpha} = -\frac{\partial \mathscr{L}}{\partial q_\alpha} \Longrightarrow \dot{p}_\alpha = -\frac{\partial H}{\partial q_\alpha}
$$

$$
\begin{aligned}
\mathrm{d}H &= \frac{\partial H}{\partial t}\mathrm{d}t + \frac{\partial H}{\partial q}\mathrm{d}q + \frac{\partial H}{\partial p}\mathrm{d}p = \mathrm{d}\big(p\dot{q} - \mathscr{L}(q,\dot{q};t)\big) \\
&= (\mathrm{d}p)\dot{q} + p\mathrm{d}\dot{q} - \frac{\partial \mathscr{L}}{\partial t}\mathrm{d}t - \frac{\partial \mathscr{L}}{\partial q}\mathrm{d}q - \frac{\partial \mathscr{L}}{\partial \dot{q}}\mathrm{d}\dot{q} = \dot{q}\mathrm{d}p - \dot{p}\mathrm{d}q - \frac{\partial \mathscr{L}}{\partial t}\mathrm{d}t \\
&\Longrightarrow \dot{q} = \frac{\partial H}{\partial p},\ \dot{p} = -\frac{\partial H}{\partial q}
\end{aligned}
$$

$$
0 \equiv \delta S = \delta \int (p\dot{q} - H(q,p;t))\mathrm{d}t \Longrightarrow \dot{q} = \frac{\partial H}{\partial p},\ \dot{p} = -\frac{\partial H}{\partial q}
$$

1.4.3 Poisson Bracket (Classical Canonical Commutator)

$$\boxed{[A,B]_{\text{PB}} = \sum_\alpha \left(\frac{\partial A}{\partial q_\alpha}\frac{\partial B}{\partial p_\alpha} - \frac{\partial A}{\partial p_\alpha}\frac{\partial B}{\partial q_\alpha}\right)}$$

$\Longrightarrow$ Quantum Canonical Commutator $\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$

$$\forall f(q,p;t),\ \frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \sum_\alpha \left(\frac{\partial f}{\partial q_\alpha}\dot{q}_\alpha + \frac{\partial f}{\partial p_\alpha}\dot{p}_\alpha\right) = \frac{\partial f}{\partial t} + \sum_\alpha \left(\frac{\partial f}{\partial q_\alpha}\frac{\partial H}{\partial p_\alpha} - \frac{\partial f}{\partial p_\alpha}\frac{\partial H}{\partial q_\alpha}\right) = \frac{\partial f}{\partial t} + [f,H]_{\text{PB}}$$

if $f(q,p;t) = q_\alpha \Longrightarrow \dfrac{\mathrm{d}q_\alpha}{\mathrm{d}t} = \dfrac{\partial H}{\partial p_\alpha}$, if $f(q,p;t) = p_\alpha \Longrightarrow \dfrac{\mathrm{d}p_\alpha}{\mathrm{d}t} = -\dfrac{\partial H}{\partial q_\alpha}$

1.4.4 Fundamental Commutation Relations in CM

$$[q_\alpha, p_\beta]_{\text{PB}} = \delta_{\alpha\beta} \longleftrightarrow [\hat{q}_\alpha, \hat{p}_\beta] = \mathrm{i}\hbar\delta_{\alpha\beta}$$
$$[q_\alpha, q_\beta]_{\text{PB}} = [p_\alpha, p_\beta]_{\text{PB}} \equiv 0 \longleftrightarrow [\hat{q}_\alpha, \hat{q}_\beta] = [\hat{p}_\alpha, \hat{p}_\beta] \equiv 0$$

$$[q_\alpha, p_\beta] = \sum_\gamma \left(\frac{\partial q_\alpha}{\partial q_\gamma}\frac{\partial p_\beta}{\partial p_\gamma} - \frac{\partial q_\alpha}{\partial p_\gamma}\frac{\partial p_\beta}{\partial q_\gamma}\right) = \delta_{\alpha\gamma}\delta_{\beta\gamma} - 0 = \delta_{\alpha\beta}$$
$$[q_\alpha, q_\beta] = \sum_\gamma \left(\frac{\partial q_\alpha}{\partial q_\gamma}\frac{\partial q_\beta}{\partial p_\gamma} - \frac{\partial q_\alpha}{\partial p_\gamma}\frac{\partial q_\beta}{\partial q_\gamma}\right) = \delta_{\alpha\gamma}\cdot 0 - 0\cdot\delta_{\beta\gamma} = 0$$

1.4.5 Properties of Poisson Bracket

1. $[A,B]_{\text{PB}} = -[B,A]_{\text{PB}}$
2. $[A+B,C]_{\text{PB}} = [A,C]_{\text{PB}} + [B,C]_{\text{PB}}$, $[A,B+C]_{\text{PB}} = [A,B]_{\text{PB}} + [A,C]_{\text{PB}}$
3. $[A,BC]_{\text{PB}} = [A,B]_{\text{PB}}C + B[A,C]_{\text{PB}}$, $[AB,C]_{\text{PB}} = [A,C]_{\text{PB}}B + A[B,C]_{\text{PB}}$
4. $[A,B^n]_{\text{PB}} = n[A,B]_{\text{PB}}B^{n-1}$
5. $[A,f(B)]_{\text{PB}} = [A,B]_{\text{PB}}\dfrac{\partial f}{\partial B}$
6. $[L_i,L_j]_{\text{PB}} = \epsilon_{ijk}L_k$
7. $[L_i,\boldsymbol{L}^2]_{\text{PB}} = 0$
8. $[L_i,x_j]_{\text{PB}} = \epsilon_{ijk}x_k$
9. $[L_i,p_j]_{\text{PB}} = \epsilon_{ijk}p_k$

$$
\begin{aligned}
[L_i, L_j]_{\mathrm{PB}} &= [\epsilon_{iab}x_a p_b, \epsilon_{jcd}x_c p_d]_{\mathrm{PB}} = \epsilon_{iab}\epsilon_{jcd}\left(x_a \underbrace{[p_b, x_c]_{\mathrm{PB}}}_{=-\delta_{bc}} p_d + x_c \underbrace{[x_a, p_d]_{\mathrm{PB}}}_{=\delta_{ad}} p_b\right) \\
&= \epsilon_{iab}\epsilon_{jca}x_c p_b - \epsilon_{iab}\epsilon_{jbd}x_a p_d = (\delta_{bj}\delta_{ic} - \delta_{bc}\delta_{ij})x_c p_b - (\delta_{ij}\delta_{ad} - \delta_{id}\delta_{aj})x_a p_d \\
&= x_i p_j - \delta_{ij}(\boldsymbol{x}\cdot\boldsymbol{p}) + \delta_{ij}(\boldsymbol{x}\cdot\boldsymbol{p}) - x_j p_i = x_i p_j - x_j p_i = \epsilon_{ijk}L_k
\end{aligned}
$$

1.4.6 Hamilton-Jacobi Equation

$$
\boxed{\frac{\partial S}{\partial t} + H(q, \frac{\partial H}{\partial q}; t) = 0}
$$

$$
\begin{aligned}
\delta S &= \int_{t_0}^{t} \mathscr{L}(q, \dot{q}; t)\mathrm{d}t = \int_{t_0}^{t}\left[\frac{\partial \mathscr{L}}{\partial q}\delta q + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{q}}\delta q\right) - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{q}}\right)\delta q\right] \\
&= \int_{t_0}^{t} \underbrace{\left(\frac{\partial \mathscr{L}}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{q}}\right)}_{=0 \text{ (physical path)}}\delta q \mathrm{d}t + \frac{\partial \mathscr{L}}{\partial \dot{q}}\delta q(t) - \underbrace{\frac{\partial \mathscr{L}}{\partial \dot{q}}\delta q(t_0)}_{=0 \text{ (fixed)}} = \frac{\partial \mathscr{L}}{\partial \dot{q}}\delta q = p\delta q
\end{aligned}
$$

$$
\begin{cases}
\delta S = p\delta q \\
\delta S[q(t), t] = \dfrac{\partial S}{\partial q}\delta q
\end{cases}
\Longrightarrow p = \frac{\partial S}{\partial q},
\begin{cases}
\dfrac{\mathrm{d}S}{\mathrm{d}t} = \dfrac{\partial S}{\partial t} + \dfrac{\partial S}{\partial q}\dot{q} \\
\dfrac{\mathrm{d}S}{\mathrm{d}t} = \mathscr{L} = p\dot{q} - H
\end{cases}
\Longrightarrow \frac{\partial S}{\partial t} + H = 0
$$

1.4.7 Phase Space (Dynamics)

phase point $(q, p) \longrightarrow$ state

$$
\int \rho(q, p; t)\mathrm{d}^D q\,\mathrm{d}^D p = 1
$$

ρ: probability

$$
\boxed{\frac{\partial \rho}{\partial t} = [H, \rho]_{\mathrm{PB}}} \text{ Liouville Theorem}
$$

$$
0 = \frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{\partial \rho}{\partial t} + [\rho, H]_{\mathrm{PB}} \xrightarrow{QM} \frac{\partial \hat{\rho}}{\partial t} = \frac{1}{\mathrm{i}\hbar}\left[\hat{H}, \hat{\rho}\right]
$$

1.4.8 Regular Lagrangian

$$
\left|\frac{\partial^2 \mathscr{L}}{\partial q_i \partial q_j}\right| \neq 0 \Longrightarrow
\begin{cases}
\mathscr{L} = T - V \\
H = T + V
\end{cases}
$$

2 Classical Electrodynamics

2.1 Vector Analysis

$$\boldsymbol{v} = v_1\boldsymbol{e}_1 + v_2\boldsymbol{e}_2 + v_3\boldsymbol{e}_3 = \sum_i v_i\boldsymbol{e}_i = v_i\boldsymbol{e}_i \text{ (Einstein convention)},\ i = 1,2,3$$

2.1.1 Generalized Stokes' Theorem

$$\boxed{\int_\Omega \mathrm{d}\omega = \int_{\partial\Omega} \omega}$$

1. Newton-Leibniz formula

$$\int_a^b \mathrm{d}f = f(b) - f(a)$$

2. Green's theorem

$$\oint f\,\mathrm{d}x + g\,\mathrm{d}y = \iint \left(\frac{\partial g}{\partial x} - \frac{\partial f}{\partial y}\right)\mathrm{d}x\,\mathrm{d}y$$

3. Stokes' theorem

$$\oint \boldsymbol{F}\cdot\mathrm{d}\boldsymbol{l} = \iint (\nabla\times\boldsymbol{F})\cdot\mathrm{d}\boldsymbol{S}$$

$$\Longrightarrow \oint \psi\,\mathrm{d}\boldsymbol{l} = \iint \mathrm{d}\boldsymbol{S}\times\nabla\psi$$

4. Gauss-Ostrogradsky's theorem

$$\oiint \boldsymbol{F}\cdot\mathrm{d}\boldsymbol{S} = \iiint (\nabla\cdot\boldsymbol{F})\,\mathrm{d}V$$

$$\Longrightarrow \begin{cases} \oiint \psi\,\mathrm{d}\boldsymbol{S} = \iiint (\nabla\psi)\,\mathrm{d}V \\ \oiint \mathrm{d}\boldsymbol{S}\nabla\boldsymbol{A} = \iiint (\nabla\times\boldsymbol{A})\,\mathrm{d}V \end{cases}$$

2.1.2 Helmholtz's theorem

For all continuous differentiable $\boldsymbol{F}$,

$$\boxed{\boldsymbol{F} = \boldsymbol{F}_\perp + \boldsymbol{F}_\parallel}$$

1. transverse component

$$\nabla\cdot\boldsymbol{F}_\perp = 0 \quad \& \quad \boldsymbol{F}_\perp = \nabla\times\boldsymbol{A}$$

2. longitudinal component

$$\nabla\times\boldsymbol{F}_\parallel = 0 \quad \& \quad \boldsymbol{F}_\parallel = -\nabla\phi$$

For magnetic field $\boldsymbol{B}$

$$\nabla \cdot \boldsymbol{B} \equiv 0$$

For electric field $\boldsymbol{E}$

$$\begin{cases} \nabla \times \boldsymbol{E} = 0 & \text{for static electric field} \\ \nabla \times \boldsymbol{E} \neq 0 & \text{for AC electric field} \end{cases}$$

2.2 Experimental Laws and Maxwell's Equations

2.2.1 Coulomb's Law

$$\boldsymbol{E}(\boldsymbol{x}) = \int \frac{\rho(\boldsymbol{x}')(\boldsymbol{x} - \boldsymbol{x}')}{|\boldsymbol{x} - \boldsymbol{x}'|^3} \, \mathrm{d}V' = -\nabla\phi, \quad \phi = \int \frac{\rho(\boldsymbol{x}')}{|\boldsymbol{x} - \boldsymbol{x}'|} \, \mathrm{d}V'$$

$$\Longrightarrow \boxed{\nabla \cdot \boldsymbol{E} = 4\pi\rho(\boldsymbol{x})} \quad \text{Gauss' Law}$$

2.2.2 Biot-Savart's Law

$$\boldsymbol{B} = \int \frac{\boldsymbol{j}(\boldsymbol{x}') \times (\boldsymbol{x} - \boldsymbol{x}')}{|\boldsymbol{x} - \boldsymbol{x}'|^3} \, \mathrm{d}V' = \nabla \times \boldsymbol{A}(\boldsymbol{x})$$

3 Fundamental Postulates (Axioms)

3.1 SOME IS

1. State
2. Observable (Operation)
3. Measurement
4. Evolution
5. Identical Particals and Symmetrization

3.1.1 State

system $\longleftrightarrow$ state vector
ket: $|\psi\rangle$
bra: $\langle\psi|$

$$(|\psi\rangle)^\dagger = \langle\psi|$$
$$[(|\psi\rangle)^\dagger]^\dagger = (\langle\psi|)^\dagger = |\psi\rangle$$

$\dagger$: adjoint or Hermitian conjugate

3.1.2 Observable

Physical Quantity $\longleftrightarrow$ Observable $\longleftrightarrow$ Operation $\hat{A}$ (Linear & Hermitian)

3.1.3 Measurement

1. Measurement + Outcomes
$$\underset{\text{Eigenvalue equation}}{\hat{A}\left|\psi\right\rangle = A_n\left|\psi_n\right\rangle} \tag{1}$$
$\hat{A}$: operation (q-number); A_n: eigenvalue (c-number); ψ_n: eigenstate.

2. Probability of Measurement Outcomes
$$\left|\psi\right\rangle = \sum_n c_n\left|\psi_n\right\rangle,\ c_n = \left\langle\psi_n|\psi\right\rangle \tag{2}$$
$$P(A_n) = \left|c_n\right|^2 = \left|\left\langle\psi_n|\psi\right\rangle\right|^2 \tag{3}$$

3. Expectation Value of the Observable A
$$\left\langle\hat{A}\right\rangle = \left\langle\psi\right|\hat{A}\left|\psi\right\rangle = \sum_n P(A_n)A_n = \sum_n \left|\left\langle\psi_n|\psi\right\rangle\right|^2 A_n \tag{4}$$

4. State Collapse
$$\left|\psi\right\rangle \xrightarrow{\hat{A}\text{-measurement}} \left|\psi_n\right\rangle \tag{5}$$

3.1.4 Evolution (Dynamics)

3.1.5 Schrödinger Picture

state: change; observable: no change

$$\begin{cases} \boxed{\mathrm{i}\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle} \text{ Schrödinger Equation} \\ \left|\psi(t=0)\right\rangle = \left|\psi_0\right\rangle \end{cases}$$

where $\hat{H} = \hat{T} + \hat{V} = \dfrac{\hat{\boldsymbol{p}}^2}{2m} + \hat{V}(\hat{\boldsymbol{x}})$

representation: coordinate system
$\boldsymbol{x}$-representation (position):

$$\hat{\boldsymbol{x}}\left|\boldsymbol{x}\right\rangle = \boldsymbol{x}\left|\boldsymbol{x}\right\rangle,\ \left|\psi\right\rangle \longrightarrow \left\langle\boldsymbol{x}|\psi\right\rangle = \psi(\boldsymbol{x}) \to \text{wave-function}$$

$$\Longrightarrow \boxed{\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{x},t) + \hat{V}(\boldsymbol{x},t)\psi(\boldsymbol{x},t)}$$

$\boldsymbol{p}$-representation (momentum): $\hat{\boldsymbol{p}}\left|\boldsymbol{p}\right\rangle = \boldsymbol{p}\left|\boldsymbol{p}\right\rangle$

3.1.6 Heisenberg Picture

state: no change; observable: change

$$\boxed{\frac{\mathrm{d}\hat{F}}{\mathrm{d}t} = \frac{\partial\hat{F}}{\partial t} + \frac{1}{\mathrm{i}\hbar}\left[\hat{F},\hat{H}\right]} \text{ Heisenberg Equation}$$

3.2 Identical Particles and Symmetrization

3.2.1 Identical Particles

$$\begin{cases} \text{boson: } s = 0, 1, 2, \cdots \ \text{Bose-Einstein Statistics} \\ \text{fermion: } s = \dfrac{1}{2}, \dfrac{3}{2}, \cdots \ \text{Fermi-Dirac Statistics} \end{cases} \xrightarrow[\text{reduce}]{\text{classical}} \text{Maxwell-Boltzmann Statistics}$$

3.2.2 Symmetrization

$$\begin{cases} \text{Boson: symmetric} \\ \text{Femion: anti-symmetric} \end{cases}$$

3.3 State Vector

3.3.1 Euclidean Space $\mathbb{R}^3$

$$\boldsymbol{v} = v_1\boldsymbol{e}_1 + v_2\boldsymbol{e}_2 + v_3\boldsymbol{e}_3$$

$$\boldsymbol{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \ \boldsymbol{e}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \ \boldsymbol{e}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\boldsymbol{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}, \ \boldsymbol{v}^T = \begin{pmatrix} v_1 & v_2 & v_3 \end{pmatrix}$$

1. vector addition: $\boldsymbol{v}_1 + \boldsymbol{v}_2 = \boldsymbol{v}_2 + \boldsymbol{v}_1$
2. scalar multiplication: $\begin{cases} a(\boldsymbol{v}_1 + \boldsymbol{v}_2) = a\boldsymbol{v}_1 + a\boldsymbol{v}_2 \\ (a+b)\boldsymbol{v} = a\boldsymbol{v} + b\boldsymbol{v} \end{cases} \quad \forall a, b \in \mathbb{R}$
3. inner product (dot product): $\boldsymbol{v}_1^T\boldsymbol{v}_2 = \boldsymbol{v}_1 \cdot \boldsymbol{v}_2 = \boldsymbol{v}_2 \cdot \boldsymbol{v}_1 = \boldsymbol{v}_2^T\boldsymbol{v}_1$
4. dyadic: $\boldsymbol{v}_1\boldsymbol{v}_2 \neq \boldsymbol{v}_2\boldsymbol{v}_1$
5. basis: $\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \longrightarrow$ orthonormal $\boldsymbol{e}_i\boldsymbol{e}_i = \boldsymbol{I} = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$
6. $\boldsymbol{v}_1 \cdot \boldsymbol{v}_2 = r \in \mathbb{R}$
   $\boldsymbol{v} \cdot \boldsymbol{v} = r \in \mathbb{R}, r \geq 0$ (equality iff $\boldsymbol{v} = \boldsymbol{0}$)

3.3.2 State Vector Space $\mathbb{H}$ (Hilbert Space)

$$|\psi\rangle = \begin{pmatrix} \vdots \\ \vdots \\ \vdots \end{pmatrix}, \ \langle\psi| = \begin{pmatrix} \cdots & \cdots & \cdots \end{pmatrix}$$

1. vector addition: $|\psi_1\rangle + |\psi_2\rangle = |\psi_2\rangle + |\psi_1\rangle$
2. scalar multiplication: $\begin{cases} c(|\psi_1\rangle + |\psi_2\rangle) = c\,|\psi_1\rangle + c\,|\psi_2\rangle \\ (c + c')\,|\psi\rangle = c\,|\psi\rangle + c'\,|\psi\rangle \end{cases} \quad \forall c \in \mathbb{C}$
3. inner product: $\langle\psi_1|\psi_2\rangle = (\langle\psi_2|\psi_1\rangle)^*$
4. outer product: $|\psi\rangle\langle\phi| \neq |\phi\rangle\langle\psi|$
$$(|\psi\rangle\langle\phi|)^\dagger = (\langle\phi|)^\dagger(|\psi\rangle)^\dagger = |\phi\rangle\langle\psi|$$
5. basis: for Hermitian operation $\begin{cases} \hat{A}\,|\psi_n\rangle = A_n\,|\psi_n\rangle \ \text{discrete} \\ \hat{A}\,|a\rangle = a\,|a\rangle \ \text{continuous} \end{cases}$
$$\text{discrete:} \begin{cases} \langle\psi_n|\psi_m\rangle = \delta_{nm} = \begin{cases} 1, \ n = m \\ 0, \ n \neq m \end{cases} \\ \displaystyle\sum_n |\psi_n\rangle\langle\psi_n| = \hat{I} \end{cases}$$
$$\text{continuous:} \begin{cases} \langle a|a'\rangle = \delta(a - a') = \begin{cases} \infty, \ a = a' \\ 0, \ a \neq a' \end{cases} \\ \displaystyle\int |a\rangle\langle a| \ \mathrm{d}a = \hat{I} \end{cases}$$
6. $\langle\psi_1|\psi_2\rangle = c \in \mathbb{C}$
$(\langle\psi_1|\psi_2\rangle)^* = \langle\psi_2|\psi_1\rangle$
$\langle\psi|\psi\rangle = \||\psi\rangle\|^2 = r \in \mathbb{R}, r \geq 0$ (equality iff $|\psi\rangle = \mathbf{0}$)

3.4 Operator

$$\hat{A}\,|\phi\rangle = |\psi\rangle, \ \hat{A}^{-1}\,|\psi\rangle = |\phi\rangle$$

3.4.1 Linear Operator

$$\forall\,|\psi_1\rangle, |\psi_2\rangle \in \mathbb{H}, a, b \in \mathbb{C}, \ \hat{A}(a\,|\psi_1\rangle + b\,|\psi_2\rangle) = a\hat{A}\,|\psi_1\rangle + b\hat{A}\,|\psi_2\rangle$$

then, $\hat{A}$ is a linear operator

$$\hat{A}(a\,|\psi_1\rangle + b\,|\psi_2\rangle) = a^*\hat{A}\,|\psi_1\rangle + b^*\hat{A}\,|\psi_2\rangle$$

then, $\hat{A}$ is an anti-linear operation

3.4.2 Two Kinds of Linear Operators

$$\begin{cases} \text{Hermitian operator: } \hat{A}^\dagger = \hat{A} \\ \text{Unitary operator: } \hat{U}^\dagger = \hat{U}^{-1} \end{cases}$$

3.4.3 Rules

$$\forall \left|\psi\right\rangle, \text{ if } \hat{A}\left|\psi\right\rangle = \hat{B}\left|\psi\right\rangle \Longleftrightarrow \hat{A} = \hat{B}$$

1. $\hat{A} + \hat{B} = \hat{B} + \hat{A}$
   def: $\forall \left|\psi\right\rangle, \ \hat{A}\left|\psi\right\rangle + \hat{B}\left|\psi\right\rangle = (\hat{A} + \hat{B})\left|\psi\right\rangle$
2. $(\hat{A} + \hat{B}) + \hat{C} = \hat{A} + (\hat{B} + \hat{C})$
3. $\hat{A}\hat{B} \neq \hat{B}\hat{A}$
   def commutator: $\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} \longleftrightarrow [A, B]_{\mathrm{PB}} \longleftrightarrow \dfrac{1}{\mathrm{i}\hbar}\left[\hat{A}, \hat{B}\right]$
4. adjoint (Hermitian conjugate): $(\hat{A}\left|\phi\right\rangle)^\dagger = \left\langle\phi\right|\hat{A}^\dagger \Longleftrightarrow \left\langle\phi\right|\hat{A}^\dagger\left|\psi\right\rangle = (\left\langle\psi\right|\hat{A}\left|\phi\right\rangle)^*$
   $\Longrightarrow$ Hermitian operation: $\hat{A}^\dagger = \hat{A}$ (Hermitian matrix) $\Longrightarrow A_{ij} = A_{ji}^*$

3.4.4 Properties

1. Identity: $\forall \left|\psi\right\rangle, \exists \hat{I}, \hat{I}\left|\psi\right\rangle = \left|\psi\right\rangle$
2. Inverse: $\hat{A}\left|\psi\right\rangle = \left|\phi\right\rangle \Longrightarrow \left|\psi\right\rangle = \hat{A}^{-1}\left|\phi\right\rangle$, $\hat{A}\hat{A}^{-1} = \hat{A}^{-1}\hat{A} = \hat{I}$
   $(\hat{A}_1\hat{A}_2\cdots\hat{A}_n)^{-1} = \hat{A}_n^{-1}\cdots\hat{A}_2^{-1}\hat{A}_1^{-1}$
3. $(\hat{A}_1\hat{A}_2\cdots\hat{A}_n)^\dagger = \hat{A}_n^\dagger\cdots\hat{A}_2^\dagger\hat{A}_1^\dagger$

4 Overview of QM

ROSE P... M

4.1 Roles: State Vector & Operator

4.1.1 Operator

$$\begin{cases} \text{Observable} \\ \text{Transformation} \end{cases} \quad \begin{cases} \text{Hermitian: } \hat{A}^\dagger = \hat{A} \\ \text{Unitary: } \hat{A}^\dagger = \hat{A}^{-1} \end{cases}$$

4.1.2 State

$$\begin{cases} \text{ket } \left|\psi\right\rangle \text{ (vector): } (\left|\psi\right\rangle)^\dagger = \left\langle\psi\right| \\ \text{bra } \left\langle\psi\right| \text{ (dual vector): } (\left\langle\psi\right|)^\dagger = \left|\psi\right\rangle \end{cases}$$

4.1.3 Eigenspectrum

$$\begin{cases}\text{discrete (bound state)}\\ \text{continuous (unbound state)}\end{cases}$$

4.2 Properties

Wave Particle Duality

4.3 Problems

4.3.1 Eigenvalue Problem

$$\hat{A}\left|\psi\right\rangle = \lambda\left|\psi\right\rangle \begin{cases} \hat{A}\left|u_n\right\rangle = A_n\left|u_n\right\rangle \begin{cases}\left\langle u_n|u_m\right\rangle = \delta_{nm}\\ \displaystyle\sum_n \left|u_n\right\rangle\left\langle u_n\right| = \hat{I}\end{cases}\\ \hat{A}\left|a\right\rangle = a\left|a\right\rangle \begin{cases}\left\langle a|a'\right\rangle = \delta(a-a')\\ \displaystyle\int \mathrm{d}a\left|a\right\rangle\left\langle a\right| = \hat{I}\end{cases}\end{cases}$$

4.3.2 Evolution Problem

$$\begin{cases} \mathrm{i}\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle \text{ Schrödinger eq.}\\ \dfrac{\mathrm{d}\hat{F}}{\mathrm{d}t} = \dfrac{\partial\hat{F}}{\partial t} + \dfrac{1}{\mathrm{i}\hbar}\left[\hat{F},\hat{H}\right] \text{ Heisenberg eq.}\end{cases}$$

4.4 Picture

4.4.1 Schrödinger Picture

$$\frac{\mathrm{d}\hat{F}}{\mathrm{d}t} = \frac{\partial\hat{F}}{\partial t} \equiv 0$$

4.4.2 Heisenberg Picture

$$\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle \equiv 0$$

4.5 Particles

$$\begin{cases}\text{Boson: s=integer} \longrightarrow \text{Bose-Einstein Statistics}\\ \text{Femion: s=half-integer} \longrightarrow \text{Fermi-Dirac Statistics}\end{cases} \xrightarrow{\hbar\to 0} \text{Maxwell-Boltzmann Statistics}$$

4.6 Perturbation Theories

$$\begin{cases} \text{Non-degenerate} \\ \text{Degenerate} \end{cases}$$

4.7 Angular Momentum and Magnetic Moment

$$\begin{cases} \text{Orbital Angular Momentum} \\ \text{Spin Angular Momentum} \end{cases} \Longleftrightarrow \begin{cases} \text{Orbital Magnetic Moment} \\ \text{Intrinsic Magnetic Moment} \end{cases}$$

4.8 Mechanics

$$\begin{cases} \text{Wave Mechanics: wavefunction} \longleftrightarrow \text{state vector} \\ \text{Matrix Mechanics: matrix forms of } \begin{cases} \text{state vector} \\ \text{operator: } n \times n \text{ matrix} \end{cases} \end{cases}$$

4.9 Theorem of Hermitian Operator

$$\hat{A}^{\dagger} = \hat{A}, \quad \hat{A} |\psi_n\rangle = A_n |\psi_n\rangle \text{ (non-degenerate, discrete)}$$

1. eigenvalue $A_n \in \mathbb{R}$
2. eigenstate $\longrightarrow$ orthonarmal and complete basis

$$\langle\psi_n| \hat{A}^{\dagger} |\psi_n\rangle = (\langle\psi_n| \hat{A} |\psi_n\rangle)^* = A_n^* \langle\psi_n|\psi_n\rangle = \langle\psi_n| \hat{A} |\psi_n\rangle = A_n \langle\psi_n|\psi_n\rangle$$
$$\Longrightarrow A_n^* = A_n \Longrightarrow A_n \in \mathbb{R}$$

$$\begin{cases} \hat{A} |\psi_n\rangle = A_n |\psi_n\rangle \\ \hat{A} |\psi_m\rangle = A_m |\psi_m\rangle \end{cases} \Longrightarrow \langle\psi_n| \hat{A}^{\dagger} |\psi_m\rangle = (\langle\psi_m| \hat{A} |\psi_n\rangle)^* = A_n^* (\langle\psi_m|\psi_n\rangle)^* = A_n^* \langle\psi_n|\psi_m\rangle$$

$$\langle\psi_n| \hat{A} |\psi_m\rangle = A_m \langle\psi_n|\psi_m\rangle \Longrightarrow (A_n - A_m) \langle\psi_n|\psi_m\rangle = 0$$
$$n \neq m \Longrightarrow A_n \neq A_m \Longrightarrow \langle\psi_n|\psi_m\rangle = 0 \Longrightarrow |\psi_n\rangle \perp |\psi_m\rangle$$

Remark: Degenerate,

$$\hat{A} \left|\psi_n^i\right\rangle = A_n \left|\psi_n^i\right\rangle \quad (i = 1, 2, \cdots, \underset{\text{degeneracy}}{g_n}) \Longrightarrow \left|\psi_n^i\right\rangle \neq c \left|\psi_n^j\right\rangle \text{ (linear independent)}$$

$$\left|\psi_n^i\right\rangle \xrightarrow{\text{Gram-Schmidt Orthogonalization}} \left|\phi_n^i\right\rangle \begin{cases} \langle\phi_n^i|\phi_m^j\rangle = \delta_{nm}\delta_{ij} \\ \sum_{n,i} \left|\phi_n^i\right\rangle \left\langle\phi_n^i\right| = \hat{1} \end{cases}$$

5 Wave Mechanics & Matrix Mechanics

5.1 Wave Mechanics: wavefunction

$$\text{wavefunction}\begin{cases}\text{matter wave (Schrödinger)}\\ \text{probabilistic wave (Born): } |\Psi(\boldsymbol{x},t)|^2 \sim \text{probability density}\end{cases}$$

wavefunction is the projection of state vector in $\underset{\text{basis}}{\text{representation}}$

$$|\psi\rangle = \hat{1}\,|\psi\rangle = \begin{cases}\left(\sum_n |u_n\rangle\langle u_n|\right)|\psi\rangle = \sum_n c_n\,|u_n\rangle\,, \quad c_n = \langle u_n|\psi\rangle & \text{discrete}\\ \left(\int \mathrm{d}a\ |a\rangle\langle a|\right)|\psi\rangle = \int \mathrm{d}a\,\psi(a)\,|a\rangle\,, \quad \psi(a) = \langle a|\psi\rangle & \text{continuous}\end{cases}$$

c_n is the wavefunction in $\{|u_n\rangle\}$-representation, $\psi(a)$ is the wavefunction in $\{|a\rangle\}$-representation.

$$|\psi\rangle = \sum_n c_n\,|\psi_n\rangle\,, \quad c_n = \langle\psi_n|\psi\rangle\,, \hat{A}\,|\psi\rangle = A_n\,|\psi_n\rangle$$

$$\text{continuous}\begin{cases}\boldsymbol{x}\text{-representation: } \hat{\boldsymbol{x}}\,|\boldsymbol{x}\rangle = \boldsymbol{x}\,|\boldsymbol{x}\rangle \begin{cases}\langle\boldsymbol{x}|\boldsymbol{x}'\rangle = \delta(\boldsymbol{x}-\boldsymbol{x}')\\ \int \mathrm{d}^3x\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}| = \hat{1}\end{cases}\\ \boldsymbol{p}\text{-representation: } \hat{\boldsymbol{p}}\,|\boldsymbol{p}\rangle = \boldsymbol{p}\,|\boldsymbol{p}\rangle \begin{cases}\langle\boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}')\\ \int \mathrm{d}^3x\ |\boldsymbol{p}\rangle\langle\boldsymbol{p}| = \hat{1}\end{cases}\end{cases}$$

Energy-representation, Fork-state representation (occupation number representation)

$$\begin{aligned}|\psi\rangle &= \left(\int \mathrm{d}^3x\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\right)|\psi\rangle = \int \mathrm{d}^3x\,\psi(\boldsymbol{x})\,|\boldsymbol{x}\rangle\\ &= \left(\int \mathrm{d}^3p\ |\boldsymbol{p}\rangle\langle\boldsymbol{p}|\right)|\psi\rangle = \int \mathrm{d}^3p\,\tilde{\psi}(\boldsymbol{p})\,|\boldsymbol{p}\rangle\end{aligned}$$

$$\psi(\boldsymbol{x}) = \langle\boldsymbol{x}|\psi\rangle \quad \tilde{\psi}(\boldsymbol{p}) = \langle\boldsymbol{p}|\psi\rangle$$

$$\begin{aligned}\tilde{\psi}(\boldsymbol{p}) &= \langle\boldsymbol{p}|\psi\rangle = \langle\boldsymbol{p}|\,\hat{1}\,|\psi\rangle = \langle\boldsymbol{p}|\left(\int \mathrm{d}^3x\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\right)|\psi\rangle = \int \mathrm{d}^3x\ \langle\boldsymbol{p}|\boldsymbol{x}\rangle\,\psi(\boldsymbol{x})\\ &= \int \mathrm{d}^3x\,\psi(\boldsymbol{x})\psi_{\boldsymbol{p}}^*(\boldsymbol{x}) \quad \text{where } \psi_{\boldsymbol{p}}(\boldsymbol{x}) = \langle\boldsymbol{x}|\boldsymbol{p}\rangle = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}\\ &\Longrightarrow \text{in } \boldsymbol{x}\text{-representation, } \hat{\boldsymbol{x}} = \boldsymbol{x},\ \hat{\boldsymbol{p}} = -\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{x}}\end{aligned}$$

$$\Longrightarrow \begin{cases} \mathrm{i}\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\,|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle \\ \hat{H} = \dfrac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{x}}) \end{cases} \xrightarrow{\int \mathrm{d}^3x\,|\boldsymbol{x}\rangle\langle\boldsymbol{x}|=\hat{I}} \mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{x},t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\boldsymbol{x},t) + V(\boldsymbol{x})\Psi(\boldsymbol{x},t)$$

$$\text{where } \begin{cases} \Psi(\boldsymbol{x},t) = \langle\boldsymbol{x}|\psi(t)\rangle \\ \hat{\boldsymbol{x}} = \boldsymbol{x}, \quad \hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla \end{cases}$$

$$\text{in } \boldsymbol{p}\text{-representation, } \hat{x} = +\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{p}},\ \hat{\boldsymbol{p}} = \boldsymbol{p}$$

$$\text{Schrödinger eq. } \xrightarrow{\int \mathrm{d}^3p\,|\boldsymbol{p}\rangle\langle\boldsymbol{p}|=\hat{I}} \mathrm{i}\hbar\frac{\partial}{\partial t}\tilde{\psi}(\boldsymbol{p},t) = \frac{\boldsymbol{p}^2}{2m}\tilde{\psi}(\boldsymbol{p},t) + V\left(\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{p}}\right)\tilde{\psi}(\boldsymbol{p},t)$$

$$\text{where } \begin{cases} \tilde{\psi}(\boldsymbol{p}) = \langle\boldsymbol{p}|\psi(t)\rangle \\ \hat{\boldsymbol{p}} = \boldsymbol{p}, \quad \hat{\boldsymbol{x}} = +\mathrm{i}\hbar\dfrac{\partial}{\partial\boldsymbol{p}} \end{cases}$$

5.2 Matrix Mechanics: State Vector

$$|\psi\rangle = \hat{1}\,|\psi\rangle = \sum_n c_n\,|u_n\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \\ \vdots \end{pmatrix} = \begin{pmatrix} c_1 & c_2 & \cdots & c_n & \cdots \end{pmatrix}^{\mathrm{T}}$$

$$\hat{A} = \boldsymbol{I}\hat{A}\boldsymbol{I} = \left(\sum_n |u_n\rangle\langle u_n|\right)\hat{A}\left(\sum_m |u_m\rangle\langle u_m|\right) = \sum_{n,m}\underbrace{\langle u_n|\,\hat{A}\,|u_m\rangle}_{=A_{nm}}(|u_n\rangle\langle u_m|) = \begin{pmatrix} & A_{nm} & \end{pmatrix}$$

5.3 Matrix Mechanics: Hermitian Conjugate

if the operator $\hat{A}$ can be written as a matrix,

$$\langle\psi|\,\hat{A}^\dagger\,|\phi\rangle = \left(\langle\phi|\,\hat{A}\,|\psi\rangle\right)^* \Longrightarrow \hat{A}^\dagger = \left(\hat{A}^{\mathrm{T}}\right)^*$$

Pf. Let $\begin{cases} |\psi\rangle = \sum_n c_n |u_n\rangle \\ |\phi\rangle = \sum_n d_n |u_n\rangle \end{cases}$,

$$\langle\psi| \hat{A}^\dagger |\phi\rangle = \left(\sum_n c_n^* \langle u_n|\right) \hat{A}^\dagger \left(\sum_m d_m |u_m\rangle\right) = \sum_{n,m} c_n^* d_m \langle u_n| \hat{A}^\dagger |u_m\rangle = \sum_{n,m} c_n^* d_m \left(\hat{A}^\dagger\right)_{nm}$$

$$\begin{aligned}\Big(\langle\phi| \hat{A} |\psi\rangle\Big)^* &= \left[\left(\sum_n d_n^* \langle u_n|\right) \hat{A} \left(\sum_m c_m |u_m\rangle\right)\right]^* = \left(\sum_{n,m} d_n^* c_m \langle u_n| \hat{A} |u_m\rangle\right)^* \\ &= \sum_{n,m} d_n c_m^* A_{nm}^* = \sum_{n,m} d_m c_n^* A_{mn}^* = \sum_{n,m} c_n^* d_m A_{mn}^* \Longrightarrow \left(\hat{A}^\dagger\right)_{nm} = \left(\hat{A}\right)_{mn}^* = \left(\hat{A}^{\mathrm{T}}\right)_{nm}^*\end{aligned}$$

6 Commutation

6.0.1 Definition

$$\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{6}$$

6.0.2 Compare

$$\begin{cases} \text{q-number}: & \hat{A}\hat{B} \neq \hat{B}\hat{A} \quad \text{(QM)} \\ \text{c-number}: & AB = BA \quad \text{(CM)} \end{cases}$$

$$\underbrace{[A, B]_{\mathrm{PB}} = \sum_\alpha \left(\frac{\partial A}{\partial q_\alpha}\frac{\partial B}{\partial p_\alpha} - \frac{\partial A}{\partial p_\alpha}\frac{\partial B}{\partial q_\alpha}\right)}_{\text{Classical Canonical Commutator}} \tag{7}$$

6.0.3 Relation

$$\boxed{[A, B]_{\mathrm{PB}} \longleftrightarrow \frac{1}{\mathrm{i}\hbar}\left[\hat{A}, \hat{B}\right]} \tag{8}$$

7 Properties of Commutations

$\left[\hat{A}, \hat{B}\right] \neq 0 \Longrightarrow$ Uncertainty Relation

$$\Delta\hat{A} \cdot \Delta\hat{B} \geq \frac{\left|\left\langle\left[\hat{A}, \hat{B}\right]\right\rangle\right|}{2} \tag{9}$$

$\left[\hat{A}, \hat{B}\right] = 0 \Longrightarrow \underset{\text{Simultaneous}}{\text{Common}}$ Eigenstates

1. **Linearity**
$$\left[a\hat{A}, b\hat{B}+c\hat{C}\right] = ab\left[\hat{A},\hat{B}\right] + ac\left[\hat{A},\hat{C}\right] \tag{10}$$

2. **Leibniz rule**
$$\begin{cases}\left[\hat{A},\hat{B}\hat{C}\right] = \left[\hat{A},\hat{B}\right]\hat{C} + \hat{B}\left[\hat{A},\hat{C}\right] \\ \left[\hat{A}\hat{B},\hat{C}\right] = \left[\hat{A},\hat{C}\right]\hat{B} + \hat{A}\left[\hat{B},\hat{C}\right]\end{cases} \tag{11}$$

3. **Power related**
$$\left[\hat{A},\hat{B}^n\right] = n\left[\hat{A},\hat{B}\right]\hat{B}^{n-1} \tag{12}$$

   provided that $\left[\hat{B},\left[\hat{A},\hat{B}\right]\right] = 0$

   Pf. $\left[\hat{A},\hat{B}\right] = 1\left[\hat{A},\hat{B}\right]\hat{B}^{1-1}$ $(n=1)$. Suppose $\left[\hat{A},\hat{B}^k\right] = k\left[\hat{A},\hat{B}\right]\hat{B}^{k-1}$, then when $n=k+1$, one has $\left[\hat{A},\hat{B}^{k+1}\right] = \left[\hat{A},\hat{B}^k\right]\hat{B} + \hat{B}^k\left[\hat{A},\hat{B}\right] = (k+1)\left[\hat{A},\hat{B}\right]\hat{B}^k$
   $\Longrightarrow \left[\hat{A},\hat{B}^n\right] = n\left[\hat{A},\hat{B}\right]\hat{B}^{n-1}$

4.
$$\left[\hat{A}, f(\hat{B})\right] = \left[\hat{A},\hat{B}\right]\frac{\partial f}{\partial \hat{B}} \tag{13}$$

   provided that $\left[\hat{B},\left[\hat{A},\hat{B}\right]\right] = 0$

   Pf. $\left[\hat{A}, f(\hat{B})\right] = \left[\hat{A}, \sum_n \frac{f^{(n)}(0)}{n!}\hat{B}^n\right] = \sum_n \frac{f^{(n)}(0)}{n!}\left[\hat{A},\hat{B}^n\right] = \sum_n \frac{f^{(n)}(0)}{(n-1)!}\hat{B}^{n-1}\left[\hat{A},\hat{B}\right]$
   $= \sum_n \frac{f^{(n)}(0)}{n!}\left[\hat{A},\hat{B}\right]\hat{B}^n = \left[\hat{A},\hat{B}\right]\frac{\partial f}{\partial \hat{B}}$

5. **Jacobi identity** $\longrightarrow$ Lie Algebra

$$[A,[B,C]_{\text{PB}}]_{\text{PB}} + [B,[C,A]_{\text{PB}}]_{\text{PB}} + [C,[A,B]_{\text{PB}}]_{\text{PB}} \quad \text{(CM)} \tag{14}$$

$$\boldsymbol{A}\times(\boldsymbol{B}\times\boldsymbol{C}) + \boldsymbol{B}\times(\boldsymbol{C}\times\boldsymbol{A}) + \boldsymbol{C}\times(\boldsymbol{A}\times\boldsymbol{B}) = 0 \quad \text{(VA)} \tag{15}$$

$$\boldsymbol{F}_{\mu\nu,\lambda} + \boldsymbol{F}_{\nu\lambda,\mu} + \boldsymbol{F}_{\lambda\mu,\nu} = 0 \quad \text{(CED)} \tag{16}$$

$$\left[\hat{A},\left[\hat{B},\hat{C}\right]\right] + \left[\hat{B},\left[\hat{C},\hat{A}\right]\right] + \left[\hat{C},\left[\hat{A},\hat{B}\right]\right] = 0 \quad \text{(QM)} \tag{17}$$

8 Fundamental Commutation Relations

$$\text{CM}\begin{cases}[x_i,p_j]_{\text{PB}} = \delta_{ij} \\ [x_i,x_j]_{\text{PB}} = [p_i,p_j]_{\text{PB}} = 0\end{cases} \longleftrightarrow \boxed{\text{QM}\begin{cases}[\hat{x}_i,\hat{p}_j] = \mathrm{i}\hbar\delta_{ij} \\ [\hat{x}_i,\hat{x}_j] = [\hat{p}_i,\hat{p}_j] = 0\end{cases}} \tag{18}$$

Pf. in $\boldsymbol{x}$-representation, $\hat{\boldsymbol{x}} = \boldsymbol{x}$, $\hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla \Longrightarrow \hat{x} = x$, $\hat{p}_x = -\mathrm{i}\hbar\dfrac{\partial}{\partial x}$. $\forall\psi(x)$,

$$
\begin{aligned}
[\hat{x}, \hat{p}_x]\psi(x) &= (\hat{x}\hat{p}_x - \hat{p}_x\hat{x})\,\psi(x) = -\mathrm{i}\hbar\left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right)\psi(x) = -\mathrm{i}\hbar\left[x\frac{\partial\psi}{\partial x} - \frac{\partial}{\partial x}(x\psi)\right] \\
&= \mathrm{i}\hbar\psi(x) \Longrightarrow [\hat{x}, \hat{p}_x] = \mathrm{i}\hbar.
\end{aligned}
$$

Similarly, $[\hat{y}, \hat{p}_y] = [\hat{z}, \hat{p}_z] = \mathrm{i}\hbar$. $[\hat{x}_i, \hat{p}_j] = 0, (i \neq j)$.

9 Commutation Relations of Orbital Angular Momentum

$$
\hat{\boldsymbol{L}} = \hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}} \Longleftrightarrow \hat{L}_i = \varepsilon_{ijk}\hat{x}_j\hat{p}_k \tag{19}
$$

$$
\Longrightarrow \boxed{\left[\hat{L}_i, \hat{L}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{L}_k \Longleftrightarrow \hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} = \mathrm{i}\hbar\hat{\boldsymbol{L}}} \tag{20}
$$

$$
\Longrightarrow \left[\hat{L}_i, \hat{\boldsymbol{L}}^2\right] = 0 \Longrightarrow \left[\hat{L}_z, \hat{\boldsymbol{L}}^2\right] = 0,\ z\text{: quantum axis} \tag{21}
$$

$$
\begin{cases}
\left[\hat{L}_i, \hat{x}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{x}_k \Longleftrightarrow \hat{\boldsymbol{L}} \times \hat{\boldsymbol{x}} + \hat{\boldsymbol{x}} \times \hat{\boldsymbol{L}} = 2\mathrm{i}\hbar\hat{\boldsymbol{x}} \\
\left[\hat{L}_i, \hat{p}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{p}_k \Longleftrightarrow \hat{\boldsymbol{L}} \times \hat{\boldsymbol{p}} + \hat{\boldsymbol{p}} \times \hat{\boldsymbol{L}} = 2\mathrm{i}\hbar\hat{\boldsymbol{p}}
\end{cases} \tag{22}
$$

$$
\forall \text{ vector } \hat{\boldsymbol{v}},\ \left[\hat{L}_i, \hat{v}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{v}_k \Longleftrightarrow \hat{\boldsymbol{L}} \times \hat{\boldsymbol{v}} + \hat{\boldsymbol{v}} \times \hat{\boldsymbol{L}} = 2\mathrm{i}\hbar\hat{\boldsymbol{v}} \tag{23}
$$

$$
\text{for } V(\boldsymbol{x}) = V(r),\ \left[\hat{L}_i, V(r)\right] = 0 \tag{24}
$$

$$
\text{for } \hat{T} = \frac{\hat{\boldsymbol{p}}^2}{2m},\ \left[\hat{L}_i, \hat{T}\right] = 0 \tag{25}
$$

$$
\text{for } \hat{H} = \hat{T} + V(r),\ \left[\hat{L}_i, \hat{H}\right] = \left[\hat{\boldsymbol{L}}^2, \hat{H}\right] = 0 \tag{26}
$$

Pf. $(\hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}})_i = \varepsilon_{ijk}\hat{L}_j\hat{L}_k = \frac{1}{2}\varepsilon_{ijk}\hat{L}_j\hat{L}_k - \frac{1}{2}\varepsilon_{ijk}\hat{L}_k\hat{L}_j = \frac{1}{2}\varepsilon_{ijk}\left[\hat{L}_j, \hat{L}_k\right]$

$$
= \frac{1}{2}\varepsilon_{ijk}(\mathrm{i}\hbar)\varepsilon_{jkl}\hat{L}_l = \mathrm{i}\hbar\delta_{il}\hat{L}_l = \mathrm{i}\hbar\hat{L}_i \Longrightarrow \hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} = \mathrm{i}\hbar\hat{\boldsymbol{L}}
$$

$$
\begin{aligned}
\left[\hat{L}_i, \hat{L}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{L}_k \Longrightarrow \left[\hat{L}_i, \hat{\boldsymbol{L}}^2\right] &= \left[\hat{L}_i, \hat{L}_j\hat{L}_j\right] = \left[\hat{L}_i, \hat{L}_j\right]\hat{L}_j + \hat{L}_j\left[\hat{L}_i, \hat{L}_j\right] \\
&= \mathrm{i}\hbar\varepsilon_{ijk}(\hat{L}_k\hat{L}_j + \hat{L}_j\hat{L}_k) = 0
\end{aligned}
$$

$$
\left[\hat{L}_i, \hat{x}_j\right] = [\varepsilon_{iab}\hat{x}_a\hat{p}_b, \hat{x}_j]
$$

$$
\left[\hat{L}_i, V(r)\right] = \left[\hat{L}_i, \hat{x}_j\right]\frac{\partial V}{\partial x_j} = \mathrm{i}\hbar\varepsilon_{ijk}\hat{x}_k\frac{\mathrm{d}V}{\mathrm{d}r}\frac{\hat{x}_j}{r} = \left(\frac{\mathrm{i}\hbar}{r}\frac{\mathrm{d}V}{\mathrm{d}r}\right)\varepsilon_{ijk}\hat{x}_k\hat{x}_j = 0
$$

$$
\left[\hat{L}_i, \hat{\boldsymbol{p}}^2\right] = \left[\hat{L}_i, \hat{p}_j\hat{p}_j\right] = \left[\hat{L}_i, \hat{p}_j\right]\hat{p}_j + \hat{p}_j\left[\hat{L}_i, \hat{p}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}(\hat{p}_k\hat{p}_j + \hat{p}_j\hat{p}_k) = 0
$$

10 Eigenvalue Problem

11 Observables

1. Position (canonical)

$$\hat{\boldsymbol{x}} = \begin{cases} \boldsymbol{x} & \boldsymbol{x}\text{-representation} \\ +\mathrm{i}\hbar\dfrac{\partial}{\partial \boldsymbol{p}} & \boldsymbol{p}\text{-representation} \end{cases} \tag{27}$$

2. Momentum (canonical)

$$\hat{\boldsymbol{p}} = \begin{cases} -\mathrm{i}\hbar\dfrac{\partial}{\partial \boldsymbol{x}} & \boldsymbol{x}\text{-representation} \\ \boldsymbol{p} & \boldsymbol{p}\text{-representation} \end{cases} \tag{28}$$

Fundamental Commutation Relation $\begin{cases} [\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar\delta_{ij} \\ [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0 \end{cases}$

3. Orbital Angular Momentum

$$\hat{\boldsymbol{L}} = \hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}} \text{ or } \hat{L}_i = \varepsilon_{ijk}\hat{x}_j\hat{p}_k$$

Commutation Relations $\left[\hat{L}_i, \hat{L}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{L}_k \Longrightarrow \left[\hat{L}_i, \hat{\boldsymbol{L}}^2\right]$

Remark $\hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} \neq 0$, but $\hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}} = -\hat{\boldsymbol{p}} \times \hat{\boldsymbol{x}}$

4. Intrinsic Angular Momentum (No classical correspondence) - SPIN

$$\left[\hat{S}_i, \hat{S}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{S}_k \Longleftrightarrow \hat{\boldsymbol{S}} \times \hat{\boldsymbol{S}} = \mathrm{i}\hbar\hat{\boldsymbol{S}}$$
$$\left[\hat{L}_i, \hat{S}_j\right] = 0$$

5. Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{\boldsymbol{p}}^2}{2m} + \hat{V}(\boldsymbol{x}) \quad \begin{cases} \hat{T}: & \hat{\boldsymbol{p}}\text{-dependent only} \\ \hat{V}: & \hat{\boldsymbol{x}}\text{-dependent only} \end{cases}$$

6. Energy

$$\begin{cases} \hat{E} = \mathrm{i}\hbar\dfrac{\partial}{\partial t} & \text{wavefuncitons} \\ \hat{E} = \mathrm{i}\hbar\dfrac{\mathrm{d}}{\mathrm{d}t} & \text{state vector} \end{cases}$$

Remark In non-relativistic QM, time t is NOT observable.

12 Eigenvalue & Eigenstates

1. Position

$$\underbrace{\hat{\boldsymbol{x}}\,|\boldsymbol{x}'\rangle = \boldsymbol{x}'\,|\boldsymbol{x}'\rangle}_{\text{eigenvalue eq.}}$$

$$\begin{cases} \langle \boldsymbol{x}'|\boldsymbol{x}''\rangle = \delta(\boldsymbol{x}' - \boldsymbol{x}'') & \text{(ON)} \\ \displaystyle\int \mathrm{d}^3x\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}| = \hat{1} & \text{(RI)} \end{cases}$$

$$\langle \boldsymbol{x}|\,\hat{\boldsymbol{x}}\,|\boldsymbol{x}'\rangle = \boldsymbol{x}'\delta(\boldsymbol{x} - \boldsymbol{x}')$$

In $\hat{\boldsymbol{x}}$-representation, wavefunction of $|\boldsymbol{x}\rangle$ is $\langle \boldsymbol{x}'|\boldsymbol{x}\rangle = \delta(\boldsymbol{x} - \boldsymbol{x}')$, and eigenvalue eq. is

$$\hat{\boldsymbol{x}}\,\delta(\boldsymbol{x} - \boldsymbol{x}') = \boldsymbol{x}'\delta(\boldsymbol{x} - \boldsymbol{x}')$$

2. Momentum

$$\hat{\boldsymbol{p}}\,|\boldsymbol{p}'\rangle = \boldsymbol{p}'\,|\boldsymbol{p}'\rangle$$

$$\begin{cases} \langle \boldsymbol{p}'|\boldsymbol{p}''\rangle = \delta(\boldsymbol{p}' - \boldsymbol{p}'') & \text{(ON)} \\ \displaystyle\int |\boldsymbol{p}\rangle\langle\boldsymbol{p}|\ \mathrm{d}\boldsymbol{p} = \boldsymbol{I} & \text{(RI)} \end{cases}$$

In $\hat{\boldsymbol{p}}$-representation, wavefunction of $|\boldsymbol{p}\rangle$ is $\langle \boldsymbol{p}'|\boldsymbol{p}\rangle = \delta(\boldsymbol{p} - \boldsymbol{p}')$, and eigenvalue eq. is

$$\hat{\boldsymbol{p}}\,\delta(\boldsymbol{p} - \boldsymbol{p}') = \boldsymbol{p}'\delta(\boldsymbol{p} - \boldsymbol{p}')$$

Remark eigenspectrum: set of eigenvalues of observable

3. Relation

$$\psi(\boldsymbol{x}) = \psi_{\boldsymbol{p}}(\boldsymbol{x})\tilde{\psi}(\boldsymbol{p}), \quad \psi_{\boldsymbol{p}}(\boldsymbol{x}) = \langle \boldsymbol{x}|\boldsymbol{p}\rangle$$

$$|\psi\rangle = \hat{I}\,|\psi\rangle = \begin{cases} \displaystyle\int \mathrm{d}\boldsymbol{x}\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\psi\rangle = \int \mathrm{d}\boldsymbol{x}\ |\boldsymbol{x}\rangle\,\psi(\boldsymbol{x}) \\ \displaystyle\int \mathrm{d}\boldsymbol{p}\ |\boldsymbol{p}\rangle\langle\boldsymbol{p}|\psi\rangle = \int \mathrm{d}\boldsymbol{p}\ |\boldsymbol{p}\rangle\,\tilde{\psi}(\boldsymbol{p}) \end{cases} = \begin{cases} \psi(\boldsymbol{x}) & \hat{\boldsymbol{x}}\text{-representation} \\ \tilde{\psi}(\boldsymbol{p}) & \hat{\boldsymbol{p}}\text{-representation} \end{cases}$$

$$\begin{aligned} |\psi\rangle &= \int \mathrm{d}\boldsymbol{p}\ |\boldsymbol{p}\rangle\,\tilde{\psi}(\boldsymbol{p}) = \int \mathrm{d}\boldsymbol{x}\ |\boldsymbol{x}\rangle\Big(\langle\boldsymbol{x}|\boldsymbol{p}\rangle\,\tilde{\psi}(\boldsymbol{p})\Big) = \int \mathrm{d}\boldsymbol{x}\ |\boldsymbol{x}\rangle\,\psi(\boldsymbol{x}) \\ &\Longrightarrow \psi(\boldsymbol{x}) = \langle\boldsymbol{x}|\boldsymbol{p}\rangle\,\tilde{\psi}(\boldsymbol{p}) = \psi_{\boldsymbol{p}}(\boldsymbol{x})\tilde{\psi}(\boldsymbol{p}) \end{aligned}$$

$$\begin{aligned} \hat{\boldsymbol{p}}\,|\boldsymbol{p}\rangle = \boldsymbol{p}\,|\boldsymbol{p}\rangle &\Longrightarrow \int \mathrm{d}\boldsymbol{x}\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\,\hat{\boldsymbol{p}}\,|\boldsymbol{p}\rangle = \boldsymbol{p}\int \mathrm{d}\boldsymbol{x}\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\boldsymbol{p}\rangle \quad (\hat{\boldsymbol{p}} = -\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{x}}) \\ &\Longrightarrow -\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{x}}\psi_{\boldsymbol{p}}(\boldsymbol{x}) = \boldsymbol{p}\psi_{\boldsymbol{p}}(\boldsymbol{x}) \end{aligned}$$

$$-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\psi_p(x) = p\psi_p(x) \Longrightarrow \psi_p(x) = N\exp\left(\frac{\mathrm{i}}{\hbar}px\right) \Longrightarrow \psi_{\boldsymbol{p}}(\boldsymbol{x}) = N\exp\left(\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}\right)$$

13 Spin and Pauli Matrices

13.1 Stern-Gerlach Experiment

13.1.1 Meanings

1. Quantization of Spatial Orientation of Angular Momentum
2. Intrinsic Angular Momentum (Spin)
3. S-G experiment $\longrightarrow$ Rabi oscillation $\longrightarrow$ Ramsey (atom clock, Hydrogen maser) $\longrightarrow$ Quantum measurement

13.1.2 Analysis

1. (Silver) neutral atom beam $\Longrightarrow$ no Lorentz force
2. Magnetic field is inhomogeneous

$$\boldsymbol{F} = -\nabla W_{\mathrm{m}} = \boldsymbol{\mu} \cdot \nabla \boldsymbol{B} \tag{29}$$

$$W_{\mathrm{m}} = -\boldsymbol{\mu} \cdot \boldsymbol{B} \tag{30}$$

   $\boldsymbol{\mu}$: magnetic dipole moment

3. Deflection: two values $\begin{cases} \text{up} & 50\% \\ \text{dowm} & 50\% \end{cases}$

4. furnace: low-temperature $\longrightarrow$ $\boldsymbol{v}$ is small $\longrightarrow$ $\boldsymbol{p}$ is small $\longrightarrow$ $\boldsymbol{L}$ is small $\xrightarrow{\boldsymbol{\mu}_L \propto \boldsymbol{L}}$ $\boldsymbol{\mu}_L$ is small $\Longrightarrow$ Intrinsic freedom?

13.1.3 History

1921-1922 Stern, Gerlach - S-G experiment
1924 Pauli - Two-valuedness not described classically $\longrightarrow$ Pauli exclusion principle
1925 Kronig - Self-rotation of electron (unpublished)
1925 Uhlenbeck, Gordsmit - Self-rotation
1927 Pauli - Pauli matrices, Pauli equation (wavefunction is a spinor with 2-component)
1928 Dirac - Relativistic QM, Dirac equation (4-component spinor)

13.1.4 Cascaded S-G Experiment

$$\text{Ag} \xrightarrow{\uparrow \boldsymbol{B}} \mu_z \to \begin{cases} +\mu_{\mathrm{B}} \text{ up } 50\% \\ -\mu_{\mathrm{B}} \text{ down } 50\% \end{cases} \quad \mu_{\mathrm{B}} = \frac{e\hbar}{2mc} \quad \text{(Bohr magneton)}$$

$$\text{Ag} \longrightarrow \mu_x \to \begin{cases} |\mu_{x,+}\rangle \to \mu_z \to \begin{cases} +\mu_{\mathrm{B}} & 50\% \\ -\mu_{\mathrm{B}} & 50\% \end{cases} \\ |\mu_{x,-}\rangle \to | \end{cases}$$

14 Spin Angular Momentum

14.0.1 Significance

1. Spin is an Intrinsic Angular Momentum
2. Spin is a signiture to distinguish two families
   (a) $\begin{cases} s = 0, 1, 2, \cdots \text{ (integer)} & \text{Bosons} \\ s = \frac{1}{2}, \frac{3}{2}, \cdots \text{ (half-integer)} & \text{Fermion} \end{cases}$
   (b) Boson $\begin{cases} \text{Statistics: Bose-Einstein statistics} \\ \text{Permutation: } \underbrace{\psi_{\mathrm{S}}(\cdots, x_i, \cdots, x_j, \cdots) = \psi_{\mathrm{S}}(\cdots, x_j, \cdots, x_i, \cdots)}_{\text{unchanged}} \end{cases}$
   (c) Fermion $\begin{cases} \text{Statistics: Fermi-Dirac statistics} \\ \text{Permutation: } \underbrace{\psi_{\mathrm{A}}(\cdots, x_i, \cdots, x_j, \cdots) = -\psi_{\mathrm{A}}(\cdots, x_j, \cdots, x_i, \cdots)}_{\text{opposite sign}} \end{cases}$
   (d) Quantum Statistics $\begin{cases} \text{Bose-Einstein} \\ \text{Fermi-Dirac} \end{cases} \xrightarrow{\hbar\to 0}$ Maxwell-Boltzmann statistics

$$\left[\hat{S}_i, \hat{S}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{S}_k \Longleftrightarrow \hat{\boldsymbol{S}} \times \hat{\boldsymbol{S}} = \mathrm{i}\hbar\hat{\boldsymbol{S}} \tag{31}$$

$$\Longrightarrow \left[\hat{\boldsymbol{S}}^2, \hat{S}_i\right] = 0 \Longrightarrow \begin{cases} \hat{\boldsymbol{S}}^2 \left|s, m_s\right\rangle = \hbar^2 s(s+1)\left|s, m_s\right\rangle \\ \hat{S}_z \left|s, m_s\right\rangle = \hbar m_s \left|s, m_s\right\rangle \end{cases} \quad \text{common eigenstates: } \left|s, m_s\right\rangle$$

$$\text{Dirac eq.} \longleftrightarrow s = \frac{1}{2} \quad \text{(electron \& positron, proton, neutron, } \cdots) \tag{32}$$

$$\left|s = \frac{1}{2}, m_s = +\frac{1}{2}\right\rangle = |+\rangle = |\uparrow\rangle = |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{33}$$

$$\left|s = \frac{1}{2}, m_s = -\frac{1}{2}\right\rangle = |-\rangle = |\downarrow\rangle = |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{34}$$

$$\begin{cases} |0\rangle\langle 0| + |1\rangle\langle 1| = \boldsymbol{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ \langle 0|0\rangle = \langle 1|1\rangle = 1; \ \langle 1|0\rangle = \langle 0|1\rangle = 0 \end{cases}$$

$$\Longrightarrow \text{In } \hat{S}_z\text{-representation} \begin{cases} \hat{S}_z |0\rangle = +\frac{\hbar}{2}|0\rangle \\ \hat{S}_z |1\rangle = -\frac{\hbar}{2}|0\rangle \end{cases} \Longrightarrow \hat{\boldsymbol{S}} = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}} \Longrightarrow \begin{cases} \hat{\boldsymbol{\sigma}}_z |0\rangle = |0\rangle \\ \hat{\boldsymbol{\sigma}}_z |1\rangle = -|1\rangle \end{cases}$$

$$\Longrightarrow \hat{\boldsymbol{\sigma}}_z = |0\rangle\langle 0| - |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\hat{\boldsymbol{S}}^2 = \frac{3}{4}\hbar^2\boldsymbol{I} \Longrightarrow \hat{\boldsymbol{\sigma}}^2 = 3\boldsymbol{I} \Longrightarrow [\hat{\boldsymbol{\sigma}}_i, \hat{\boldsymbol{\sigma}}_j] = 2\mathrm{i}\varepsilon_{ijk}\hat{\boldsymbol{\sigma}}_k$$

15 Algebraic Method to Eigenvalue Problem of Angular Momentum

16 Review

Fundamental Commutations

$$[\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar\delta_{ij} \quad [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0 \tag{35}$$

16.1 Orbital Angular Momentum

16.1.1 Definition of Orbital AM

$$\hat{\boldsymbol{L}} = \hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}} \quad \text{or} \quad \hat{L}_i = \varepsilon_{ijk}\hat{x}_j\hat{p}_k \tag{36}$$

16.1.2 Commutation Relations of Orbital AM

$$\left[\hat{L}_i, \hat{L}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{L}_k \Longleftrightarrow \hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} = \mathrm{i}\hbar\hat{\boldsymbol{L}} \tag{37}$$

$$\left[\hat{L}^2, \hat{L}_i\right] = 0 \Longrightarrow \text{Common Eigenstates} \tag{38}$$

16.1.3 Eigenvalue Equation

$$\begin{cases} \hat{\boldsymbol{L}}^2 |l, m_l\rangle = \hbar^2 l(l+1) |l, m_l\rangle \\ \hat{L}_z |l, m_l\rangle = \hbar m_l |l, m_l\rangle \end{cases} \quad m_l = \underbrace{-l, -l+1, \cdots, l-1, l}_{2l+1} \tag{39}$$

16.2 Intrinsic Angular Momentum (Spin)

Generalize to Intrinsic AM (Spin):

$$\left[\hat{S}_i, \hat{S}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{S}_k \Longleftrightarrow \hat{\boldsymbol{S}} \times \hat{\boldsymbol{S}} = \mathrm{i}\hbar\hat{\boldsymbol{S}} \tag{40}$$

$$\left[\hat{S}^2, \hat{S}_i\right] = 0 \Longrightarrow \text{Common Eigenstates} \tag{41}$$

16.2.1 Eigenvalue Equation

$$\begin{cases} \hat{\boldsymbol{S}}^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle \\ \hat{S}_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle \end{cases} \quad m_s = \underbrace{-s, -s+1, \cdots, s-1, s}_{2s+1} \tag{42}$$

$$s = \frac{1}{2} \Longrightarrow |s, m_s\rangle = \begin{cases} |+\rangle = |0\rangle = \begin{pmatrix} 1 & 0 \end{pmatrix}^{\mathrm{T}} \\ |-\rangle = |1\rangle = \begin{pmatrix} 0 & 1 \end{pmatrix}^{\mathrm{T}} \end{cases} \tag{43}$$

16.3 Pauli Matrix

$$\hat{\boldsymbol{S}} = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}} \tag{44}$$

$$\begin{cases} \hat{\boldsymbol{S}}^2 = \dfrac{3}{4}\hbar\hat{1}_2 \Longrightarrow \hat{\boldsymbol{\sigma}}^2 = 3\hat{1}_2 \\ \hat{S}_z^2 = \dfrac{1}{4}\hbar\hat{1}_2 \Longrightarrow \hat{\sigma}_z^2 = \hat{1}_2 \end{cases} \tag{45}$$

$$\text{Cascaded SGE} \Longrightarrow \begin{cases} |\mu_x, +\rangle = c_1\,|0\rangle + c_2\,|1\rangle \\ |c_1|^2 = |c_2|^2 = \dfrac{1}{2} \end{cases} \Longrightarrow \hat{\sigma_x}^2 = \hat{\sigma_y}^2 = \hat{1}_2$$

$$\hat{\sigma}_i = \hat{1}_2 \tag{46}$$

$$\{\hat{\sigma}_1, \hat{\sigma}_j\} = 2\delta_{ij}\hat{1}_2 \tag{47}$$

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 2\mathrm{i}\varepsilon_{ijk}\hat{\sigma}_k \tag{48}$$

$$\hat{\sigma}_i\hat{\sigma}_j = \delta_{ij}\hat{1}_2 + \mathrm{i}\varepsilon_{ijk}\hat{\sigma}_k \tag{49}$$

$$\mathrm{tr}(\hat{\sigma}_i) = 0 \quad \mathrm{tr}(\hat{\sigma}_i\hat{\sigma}_j) = 2\delta_{ij} \tag{50}$$

$$\hat{S}_\pm = \hat{S}_x \pm \mathrm{i}\hat{S}_y = \frac{\hbar}{2}(\hat{\sigma}_x \pm \mathrm{i}\hat{\sigma}_y) = \hbar\hat{\sigma}_\pm \tag{51}$$

$$\begin{cases} \hat{\sigma}_x = \hat{\sigma}_+ + \hat{\sigma}_- \\ \hat{\sigma}_y = -\mathrm{i}(\hat{\sigma}_+ - \hat{\sigma}_-) \end{cases} \tag{52}$$

16.3.1 Ladder / Raising & Lowering / Transition Operator

$$\hat{\sigma}_+ = |0\rangle\langle 1| \quad \& \quad \hat{\sigma}_- = |1\rangle\langle 0| \tag{53}$$

16.3.2 Pauli Matrices ($S_z(\sigma_z)$-representation)

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \quad \hat{\sigma}_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{54}$$

17 Arbitrary Angular Momentum

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}} \tag{55}$$

$$\left[\hat{J}_i, \hat{J}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{J}_k \tag{56}$$

OAM & Spin are in DIFFERENT State Vector Spaces:

$$\left[\hat{L}_i, \hat{S}_j\right] \equiv 0 \tag{57}$$

$$\left[\hat{J}_i, \hat{J}_j\right] = \left[\hat{L}_i + \hat{S}_i, \hat{L}_j + \hat{S}_j\right] = \left[\hat{L}_i, \hat{L}_j\right] + \left[\hat{S}_i, \hat{S}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}(\hat{L}_k + \hat{S}_k) = \mathrm{i}\hbar\varepsilon_{ijk}\hat{J}_k$$

17.1 Ladder Operator

17.1.1 Definition of Ladder Operators

$$\hat{J}_{\pm} = \hat{J}_x \pm \mathrm{i}\hat{J}_y \tag{58}$$

$$\left[\hat{J}_i, \hat{\boldsymbol{J}}^2\right] = 0 \Longrightarrow \begin{cases} \hat{\boldsymbol{J}}^2 \left|j, m_j\right\rangle = \hbar j(j+1) \left|j, m_j\right\rangle \\ \hat{J}_z \left|j, m_j\right\rangle = \hbar m_j \left|j, m_j\right\rangle \end{cases} \quad j \geq 0,\ m_j = \underbrace{-j, -j+1, \cdots, j-1, j}_{(2j+1)\text{-fold (degeneracy)}} \tag{59}$$

$$\begin{cases} j\text{: azimuthal quantum number} \\ m_j\text{: magnetic quantum number} \end{cases}$$

17.1.2 Effect of Ladder Operators on Common Eigenstates

$$\hat{J}_{\pm} \left|j, m_j\right\rangle = \hbar\sqrt{j(j+1) - m_j(m_j \pm 1)} \left|j, m_j \pm 1\right\rangle \tag{60}$$

17.1.3 Restriction

$$\hat{J}_{+} \left|j, j\right\rangle = \hat{J}_{-} \left|j, -j\right\rangle = 0 \tag{61}$$

17.1.4 Commutations

1. $\left[\hat{J}_i, \hat{J}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{J}_k$

2. $\left[\hat{\boldsymbol{J}}^2, \hat{J}_i\right] = 0$

3. $\left[\hat{\boldsymbol{J}}^2, \hat{J}_{\pm}\right] = 0$

4. $\left[\hat{J}_z, \hat{J}_{\pm}\right] = \pm\hbar\hat{J}_{\pm}$

$$\left[\hat{J}_z, \hat{J}_{\pm}\right] = \left[\hat{J}_z, \hat{J}_x \pm \mathrm{i}\hat{J}_y\right] = \left[\hat{J}_z, \hat{J}_x\right] \pm \mathrm{i}\left[\hat{J}_z, \hat{J}_y\right] = \mathrm{i}\hbar\hat{J}_y \pm \mathrm{i}(-\mathrm{i}\hbar)\hat{J}_x = \pm\hbar\hat{J}_{\pm}$$

5. $\hat{J}_{+}\hat{J}_{-} = \hat{\boldsymbol{J}}^2 - \hat{J}_z^2 + \hbar\hat{J}_z$

$$\hat{J}_{+}\hat{J}_{-} = (\hat{J}_x + \mathrm{i}\hat{J}_y)(\hat{J}_x - \mathrm{i}\hat{J}_y) = \hat{J}_x^2 + \hat{J}_y^2 - \mathrm{i}\left[\hat{J}_x, \hat{J}_y\right] = \hat{\boldsymbol{J}}^2 - \hat{J}_z^2 + \hbar\hat{J}_z$$

6. $(\hat{J}_{\pm})^{\dagger} = \hat{J}_{\mp}$

$\hat{J}_{\pm}$ are NOT Hermitian Operators, but $\hat{J}_{+}$ & $\hat{J}_{-}$ are mutually Hermitian Conjugates.

17.2 Eigenvalue Equation of Angular Momentum Operator

$$\begin{cases} \hat{\boldsymbol{J}}^2 \left|\lambda, m\right\rangle = \hbar^2 \lambda \left|\lambda, m\right\rangle \\ \hat{J}_z \left|\lambda, m\right\rangle = \hbar m \left|\lambda, m\right\rangle \end{cases} \tag{62}$$

$$\left[\hat{\boldsymbol{J}}^2, \hat{J}_\pm\right] = 0 \Longrightarrow \hat{J}_\pm \hat{\boldsymbol{J}}^2 \left|\lambda, m\right\rangle = \hat{\boldsymbol{J}}^2 \hat{J}_\pm \left|\lambda, m\right\rangle \Longrightarrow \lambda\hbar^2(\hat{J}_\pm \left|\lambda, m\right\rangle) = \hat{\boldsymbol{J}}^2(\hat{J}_\pm \left|\lambda, m\right\rangle) \tag{63}$$

$$\begin{aligned} \left[\hat{J}_\pm, \hat{J}_z\right] &= \pm\hbar\hat{J}_\pm \Longrightarrow \hat{J}_z\hat{J}_\pm = \hat{J}_\pm\hat{J}_z \pm \hbar\hat{J}_\pm \\ \Longrightarrow \hat{J}_z\left(\hat{J}_\pm \left|\lambda, m\right\rangle\right) &= (\hat{J}_\pm\hat{J}_z \pm \hbar\hat{J}_\pm)\left|\lambda, m\right\rangle = m\hbar\hat{J}_\pm \left|\lambda, m\right\rangle \pm \hbar\hat{J}_\pm \left|\lambda, m\right\rangle \\ &= (m \pm 1)\hbar\left(\hat{J}_\pm \left|\lambda, m\right\rangle\right) \end{aligned} \tag{64}$$

$\Longrightarrow \hat{J}_\pm \left|\lambda, m\right\rangle$ is an eigenstate of $\hat{J}_z$, with eigenvalue of $(m \pm 1)\hbar$.

$$\Longrightarrow \hat{J}_\pm \left|\lambda, m\right\rangle = C_\pm \left|\lambda, m \pm 1\right\rangle \tag{65}$$

$$\Longrightarrow \hat{J}_\pm^n \left|\lambda, m\right\rangle = D_\pm \left|\lambda, m \pm n\right\rangle \tag{66}$$

$$\begin{cases} \left\langle \hat{\boldsymbol{J}}^2 \right\rangle = \left\langle\lambda, m\right| \hat{\boldsymbol{J}}^2 \left|\lambda, m\right\rangle = \lambda\hbar^2 \\ \left\langle \hat{J}_z^2 \right\rangle = \left\langle\lambda, m\right| \hat{J}_z^2 \left|\lambda, m\right\rangle = m^2\hbar^2 \end{cases} \tag{67}$$

$$\left\langle \hat{\boldsymbol{J}}^2 \right\rangle \geq \left\langle \hat{J}_z \right\rangle \Longrightarrow \lambda \geq m^2 \geq 0 \tag{68}$$

$\exists m_0$ (minimal), $\exists N$ (integer), $m_0 + N$ is the maximal

$$\hat{J}_- \left|\lambda, m_0\right\rangle = 0 \quad \hat{J}_+ \left|\lambda, m_0 + N\right\rangle = 0 \tag{69}$$

$$0 = \hat{J}_+\hat{J}_- \left|\lambda, m_0\right\rangle = (\hat{\boldsymbol{J}}^2 - \hat{J}_z^2 + \hbar\hat{J}_z)\left|\lambda, m_0\right\rangle = \hbar^2(\lambda - m_0^2 + m_0) \tag{70}$$

$$0 = \hat{J}_-\hat{J}_+ \left|\lambda, m_0 + N\right\rangle = (\hat{\boldsymbol{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z)\left|\lambda, m_0 + N\right\rangle = \hbar^2[\lambda - (m_0 + N)^2 - (m_0 + N)] \tag{71}$$

$$\begin{cases} \lambda - m_0^2 + m_0 = 0 \\ \lambda - (m_0 + N)^2 - (m_0 + N) = 0 \end{cases} \Longrightarrow \begin{cases} m_0 = -\dfrac{N}{2} \\ m_0 + N = \dfrac{N}{2} \\ \lambda = -\dfrac{N}{2}\left(\dfrac{N}{2} + 1\right) \end{cases} \tag{72}$$

let $j = \dfrac{N}{2}$, $\lambda = j(j + 1)$, $m_j = \underbrace{-j, -j + 1, \cdots, j - 1, j}_{2j+1}$

$$\Longrightarrow \boxed{\begin{cases} \hat{\boldsymbol{J}}^2 \left|j, m_j\right\rangle = j(j + 1)\hbar^2 \left|j, m_j\right\rangle \\ \hat{J}_z \left|j, m_j\right\rangle = m_j\hbar \left|j, m_j\right\rangle \end{cases}} \tag{73}$$

$$\hat{J}_\pm \left|j, m_j\right\rangle = C_\pm \left|j, m_j \pm 1\right\rangle \tag{74}$$

$$\langle j, m_j | j', m_{j'} \rangle = \delta_{jj'}\delta_{m_j m_{j'}} \quad (\hat{J}_\pm)^\dagger = \hat{J}_\mp \tag{75}$$

$$\Longrightarrow 1 = \langle j, m_j \pm 1 | j, m_j \pm 1 \rangle = \langle j, m_j | \hat{J}_\mp \hat{J}_\pm | j, m_j \rangle = |C_\pm|^2 \langle j, m_j | j, m_j \rangle \tag{76}$$

$$\hat{J}_\mp \hat{J}_\pm = (\hat{J}_x \mp \mathrm{i}\hat{J}_y)(\hat{J}_x \pm \mathrm{i}\hat{J}_y) = \hat{J}_x^2 + \hat{J}_y^2 \pm \mathrm{i}\left[\hat{J}_x, \hat{J}_y\right] = \hat{\boldsymbol{J}}^2 - \hat{J}_z^2 \mp \hbar\hat{J}_z \tag{77}$$

$$\begin{aligned}\Longrightarrow \langle j, m_j | \hat{J}_\mp \hat{J}_\pm | j, m_j \rangle &= \langle j, m_j | (\hat{\boldsymbol{J}}^2 - \hat{J}_z^2 \mp \hbar\hat{J}_z) | j, m_j \rangle \\ &= \hbar^2[j(j+1) - m_j^2 \mp m_j] \langle j, m_j | j, m_j \rangle = |C_\pm|^2 \langle j, m_j | j, m_j \rangle \\ \Longrightarrow |C_\pm|^2 &= [j(j+1) - m_j(m_j \pm 1)]\hbar^2\end{aligned} \tag{78}$$

for simplicity, let $C_\pm \in \mathbb{R}$

$$\Longrightarrow C_\pm = \hbar\sqrt{j(j+1) - m_j(m_j \pm 1)} \tag{79}$$

$$\Longrightarrow \boxed{\hat{J}_\pm |j, m_j\rangle = \hbar\sqrt{j(j+1) - m_j(m_j \pm 1)}\, |j, m_j \pm 1\rangle} \tag{80}$$

18 Commutation Relations between Angular Momentum Operators and Hamiltonian

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(r) + \xi(r)\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} \tag{81}$$

$V(r)$: central potential, $\xi(r)\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}$: $\hat{\boldsymbol{L}}$-$\hat{\boldsymbol{S}}$ coupling $\longleftrightarrow$ fine structure

$$\left[\hat{L}_i, \hat{p}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{p}_k \Longrightarrow \left[\hat{L}_i, \hat{\boldsymbol{p}}^2\right] = \left[\hat{L}_i, \hat{p}_j\right]\hat{p}_j + \hat{p}_j\left[\hat{L}_i, \hat{p}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}(\hat{p}_k\hat{p}_j + \hat{p}_j\hat{p}_k) = 0 \tag{82}$$

$$\left[\hat{S}_i, \hat{\boldsymbol{p}}^2\right] = 0 \Longrightarrow \left[\hat{J}_i, \hat{\boldsymbol{p}}^2\right] = 0 \tag{83}$$

$$\left[\hat{L}_i, V(r)\right] = 0 \quad \& \quad \left[\hat{S}_i, V(r)\right] = 0 \Longrightarrow \quad \left[\hat{J}_i, V(r)\right] = 0 \tag{84}$$

$$\left[\hat{L}_i, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}\right] = \left[\hat{L}_i, \hat{L}_j\hat{S}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{L}_k\hat{S}_j \neq 0 \tag{85}$$

$$\left[\hat{\boldsymbol{L}}^2, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}\right] = \left[\hat{L}_i\hat{L}_i, \hat{L}_j\hat{S}_j\right] = \left[\hat{L}_i, \hat{L}_j\right]\hat{L}_i\hat{S}_j + \hat{L}_i\left[\hat{L}_i, \hat{L}_j\right]\hat{S}_j = \mathrm{i}\hbar\varepsilon_{ijk}(\hat{L}_k\hat{L}_i + \hat{L}_i\hat{L}_k) = 0 \tag{86}$$

similarly, $\left[\hat{S}_i, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}\right] \neq 0$, but $\left[\hat{\boldsymbol{S}}^2, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}\right] = 0$. futher, $\left[\hat{J}_i, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}\right] = 0$, $\left[\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}\right] = 0$.

$$\hat{\boldsymbol{L}}^2, \hat{\boldsymbol{S}}^2, \hat{\boldsymbol{J}}^2, \hat{J}_i \text{ commutes with } \hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(r) + \xi(r)\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}$$

19 Addition of Angular Momenta

assume $\hat{\boldsymbol{J}}_1$, $\hat{\boldsymbol{J}}_2$, $\hat{\boldsymbol{J}} = \hat{\boldsymbol{J}}_1 + \hat{\boldsymbol{J}}_2$, and Commutation Relations:

$$\left[\hat{J}_{\alpha i}, \hat{J}_{\beta j}\right] = \mathrm{i}\hbar\delta_{\alpha\beta}\varepsilon_{ijk}\hat{J}_{\alpha k} \quad (\alpha, \beta = 1, 2) \tag{87}$$

$$\left[\hat{\boldsymbol{J}}_{\alpha}^2, \hat{J}_{\alpha i}\right] \quad (\alpha = 1, 2) \tag{88}$$

Eigenvalue Equations:

$$\begin{cases} \hat{\boldsymbol{J}}_1^2 \left|j_1, m_1\right\rangle = j_1(j_1+1)\hbar^2 \left|j_1, m_1\right\rangle \\ \hat{J}_{1z} \left|j_1, m_1\right\rangle = m_1\hbar \left|j_1, m_1\right\rangle \end{cases} \tag{89}$$

$$\begin{cases} \hat{\boldsymbol{J}}_2^2 \left|j_2, m_2\right\rangle = j_2(j_2+1)\hbar^2 \left|j_2, m_2\right\rangle \\ \hat{J}_{2z} \left|j_2, m_2\right\rangle = m_2\hbar \left|j_2, m_2\right\rangle \end{cases} \tag{90}$$

$$\left[\hat{J}_i, \hat{J}_j\right] = \mathrm{i}\hbar\varepsilon_{ijk}\hat{J}_k \tag{91}$$

20 Uncertainty Principle

20.1 Heisenberg Uncertainty Principle

$\forall \left|\psi\right\rangle$,

$$\underbrace{\Delta\hat{x}^2 \cdot \Delta\hat{p}^2}_{\text{variance}} \geq \frac{\hbar^2}{4} \quad \text{or} \quad \underbrace{\Delta\hat{x} \cdot \Delta\hat{p}}_{\text{root-mean-square}} \geq \frac{\hbar}{2} \tag{92}$$

20.2 Generalized Uncertainty Principle

$\forall \left|\psi\right\rangle$, if $\left[\hat{A}, \hat{B}\right] \neq 0$, then

$$\Delta\hat{A}^2 \cdot \Delta\hat{B}^2 \geq \frac{\left|\left\langle\left[\hat{A}, \hat{B}\right]\right\rangle\right|^2}{4} \quad \text{or} \quad \Delta\hat{A} \cdot \Delta\hat{B} \geq \frac{\left|\left\langle\left[\hat{A}, \hat{B}\right]\right\rangle\right|}{2} \tag{93}$$

Variance:

$$\Delta\hat{A}^2 = \left\langle(\hat{A} - \left\langle\hat{A}\right\rangle)^2\right\rangle = \left\langle\hat{A}^2\right\rangle - \left\langle\hat{A}\right\rangle^2 \tag{94}$$

root-mean-square:

$$\Delta\hat{A} = \sqrt{\Delta\hat{A}^2} = \sqrt{\left\langle\hat{A}^2\right\rangle - \left\langle\hat{A}\right\rangle^2} \tag{95}$$

20.2.1 Essential Mathematical Tools

1. If $\hat{F}^\dagger = \hat{F}$ (Hermitian), then eigenvalue of $\hat{F}$ is REAL
2. If $\hat{F}^\dagger = -\hat{F}$ (skew-Hermitian), then $\hat{F}$ is IMAGINARY
3. Cauchy-Schwarz Inequality
   (a) $\left(\sum_n a_n^2\right)\left(\sum_n b_n^2\right) \geq \left(\sum_n a_n b_n\right)^2$, equality iff $a_n = kb_n$
   (b) $|\boldsymbol{u}|^2|\boldsymbol{v}|^2 \geq |\boldsymbol{u}\cdot\boldsymbol{v}|^2$, equality iff $\boldsymbol{u} = k\boldsymbol{v}$
   (c) $\boxed{\langle\psi|\psi\rangle\langle\phi|\phi\rangle \geq |\langle\psi|\phi\rangle|^2, \text{ equality iff } |\psi\rangle = \lambda|\phi\rangle}$

20.2.2 Define Deviation Operator

$$\hat{\sigma}_A = \hat{A} - \left\langle\hat{A}\right\rangle \quad \& \quad \hat{\sigma}_B = \hat{B} - \left\langle\hat{B}\right\rangle \tag{96}$$

$$\Longrightarrow \begin{cases} \Delta\hat{A}^2 = \langle\hat{\sigma}_A^2\rangle \\ \Delta\hat{B}^2 = \langle\hat{\sigma}_B^2\rangle \end{cases} \tag{97}$$

20.2.3 Properties of $\hat{\sigma}_A, \hat{\sigma}_B$

1. $\hat{\sigma}_A^\dagger = \hat{\sigma}_A$, $\hat{\sigma}_B^\dagger = \hat{\sigma}_B$ (Hermitian)
2. $\hat{\sigma}_A^\dagger\hat{\sigma}_A = \hat{\sigma}_A^2$, $\hat{\sigma}_B^\dagger\hat{\sigma}_B = \hat{\sigma}_B^2$
3. $[\hat{\sigma}_A, \hat{\sigma}_B] = \left[\hat{A}, \hat{B}\right]$
4. $\hat{\sigma}_A\hat{\sigma}_B = \frac{1}{2}[\hat{\sigma}_A, \hat{\sigma}_B] + \frac{1}{2}\{\hat{\sigma}_A, \hat{\sigma}_B\}$
5. $[\hat{\sigma}_A, \hat{\sigma}_B]^\dagger = -[\hat{\sigma}_A, \hat{\sigma}_B]$ (skew-Hermitian)
6. $\{\hat{\sigma}_A, \hat{\sigma}_B\}^\dagger = \{\hat{\sigma}_A, \hat{\sigma}_B\}$ (Hermitian)
7. $\Delta\hat{A}^2 = \langle\hat{\sigma}_A^2\rangle$, $\Delta\hat{B}^2 = \langle\hat{\sigma}_B^2\rangle$

20.2.4 Proof of GUP

$$\text{def: } \hat{\sigma}_A|\psi\rangle = |\psi_A\rangle \quad \& \quad \hat{\sigma}_B|\psi\rangle = |\psi_B\rangle$$

$$\left\langle\hat{\sigma}_A^2\right\rangle = \langle\psi|\hat{\sigma}_A\hat{\sigma}_A|\psi\rangle = \langle\psi|\hat{\sigma}_A^\dagger\hat{\sigma}_A|\psi\rangle = \langle\psi_A|\psi_A\rangle \quad \& \quad \left\langle\hat{\sigma}_B^2\right\rangle = \langle\psi_B|\psi_B\rangle$$

$$\Longrightarrow \left\langle\hat{\sigma}_A^2\right\rangle\left\langle\hat{\sigma}_B^2\right\rangle = \langle\psi_A|\psi_A\rangle\langle\psi_B|\psi_B\rangle \geq |\langle\psi_A|\psi_B\rangle|^2 = |\langle\psi|\hat{\sigma}_A\hat{\sigma}_B|\psi\rangle|^2 = |\langle\hat{\sigma}_A\hat{\sigma}_B\rangle|^2$$

$$\langle\hat{\sigma}_A\hat{\sigma}_B\rangle = \frac{1}{2}\langle[\hat{\sigma}_A, \hat{\sigma}_B]\rangle + \frac{1}{2}\langle\{\hat{\sigma}_A, \hat{\sigma}_B\}\rangle$$

$$\Longrightarrow |\langle\hat{\sigma}_A\hat{\sigma}_B\rangle|^2 \geq \frac{1}{4}|\langle[\hat{\sigma}_A, \hat{\sigma}_B]\rangle|^2 = \frac{1}{4}\left|\left\langle\left[\hat{A}, \hat{B}\right]\right\rangle\right|^2 \quad \Longrightarrow \text{GUP}$$

20.3 Energy-Time Uncertainty Relation

$$\Delta E \cdot \Delta T \geq \frac{\hbar}{2} \tag{98}$$

20.3.1 Ehrenfest Theorem

$$\left[\hat{A}, \hat{H}\right] \neq 0,\ \frac{\partial \hat{A}}{\partial t} = 0,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{A} \right\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle \left[\hat{A}, \hat{H}\right] \right\rangle \tag{99}$$

20.3.2 Proof

$$\Longrightarrow \Delta \hat{A} \cdot \Delta \hat{H} \geq \frac{1}{2}\left|\left\langle \left[\hat{A}, \hat{H}\right] \right\rangle\right| = \frac{\hbar}{2}\left|\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{A} \right\rangle\right| \quad \Longrightarrow \Delta \hat{H} \frac{\Delta \hat{A}}{\left|\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{A} \right\rangle\right|} = \frac{\hbar}{2}$$

define $\Delta \hat{H} = \Delta E$, $\Delta T = \dfrac{\Delta \hat{A}}{\left|\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{A} \right\rangle\right|}$

$$\Longrightarrow \Delta E \cdot \Delta T \geq \frac{\hbar}{2}$$

20.4 Minimum Uncertainty State

$\dfrac{\hbar}{2}$: quantum limit (Heisenberg limit) $\Longrightarrow$ Minimum Uncertainty State

$$\exists \left|\psi\right\rangle_{\min},\ \Delta \hat{A} \cdot \Delta \hat{B} = \frac{1}{2}\left|\left\langle \left[\hat{A}, \hat{B}\right] \right\rangle\right|$$

$\left|\psi\right\rangle_{\min}$: Minimum Uncertainty State

20.4.1 MUS of $\hat{x}$ & $\hat{p}$

$$\begin{cases} \hat{\sigma}_x = \hat{x} - \langle \hat{x} \rangle \\ \hat{\sigma}_p = \hat{p} - \langle \hat{p} \rangle \end{cases},\ \text{let } |\phi\rangle = (\hat{\sigma}_x - \mathrm{i}\lambda\hat{\sigma}_p)\,|\psi\rangle \text{ (testing state)}$$

$$\begin{aligned}
\langle \phi|\phi \rangle &= \langle \psi|\,(\hat{\sigma}_x + \mathrm{i}\lambda\hat{\sigma}_p)(\hat{\sigma}_x - \mathrm{i}\lambda\hat{\sigma}_p)\,|\psi\rangle = \langle \psi|\,(\hat{\sigma}_x^2 - \mathrm{i}\lambda\hat{\sigma}_x\hat{\sigma}_p + \mathrm{i}\lambda\hat{\sigma}_p\hat{\sigma}_x + \lambda^2\hat{\sigma}_p^2)\,|\psi\rangle \\
&= \langle \psi|\,\hat{\sigma}_x^2\,|\psi\rangle - \mathrm{i}\lambda\,\langle \psi|\,[\hat{\sigma}_x, \hat{\sigma}_p]\,|\psi\rangle + \lambda^2\,\langle \psi|\,\hat{\sigma}_p^2\,|\psi\rangle = \left\langle \hat{\sigma}_x^2 \right\rangle + \lambda\hbar + \lambda^2\left\langle \hat{\sigma}_p^2 \right\rangle \\
|\psi\rangle = 0 &\Longrightarrow \langle \phi|\phi \rangle = 0 \Longrightarrow \left\langle \hat{\sigma}_p^2 \right\rangle \lambda^2 + \hbar\lambda + \left\langle \hat{\sigma}_x^2 \right\rangle = 0 \\
\Delta &= \hbar^2 - 4\left\langle \hat{\sigma}_x^2 \right\rangle\left\langle \hat{\sigma}_p^2 \right\rangle \lambda^2 \leq 0 \Longrightarrow \left\langle \hat{\sigma}_x^2 \right\rangle\left\langle \hat{\sigma}_p^2 \right\rangle \lambda^2 \geq \frac{\hbar^2}{4} \\
&\Longrightarrow \Delta\hat{x}^2 \cdot \Delta\hat{p}^2 \geq \frac{\hbar^2}{4} \quad \text{or} \quad \Delta\hat{x} \cdot \Delta\hat{p} \geq \frac{\hbar}{2}
\end{aligned} \tag{100}$$

$$\Delta = 0 \Longrightarrow \begin{cases} \lambda = -\dfrac{2}{\hbar}\Delta\hat{x}^2 \\ \left|\phi\right\rangle = \left(\hat{\sigma}_x + \dfrac{2\mathrm{i}}{\hbar}\Delta\hat{x}^2\hat{\sigma}_p\right)\left|\psi\right\rangle = 0 \end{cases} \tag{101}$$

$$\left\langle x\right|\left(\hat{x} - \langle\hat{x}\rangle\right) - \mathrm{i}\lambda\left(-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x} - \langle\hat{p}\rangle\right)\left|\psi\right\rangle = (x - \langle\hat{x}\rangle)\psi(x) - \lambda\hbar\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) + \mathrm{i}\lambda\left\langle\hat{p}\right\rangle\psi(x)$$

21 Quantum Dynamics

21.1 Schrödinger Equation

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle \tag{102}$$

where $\hat{H} = \dfrac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{x}})$

21.1.1 Remark

1. Pure State
2. Closed System $\Longrightarrow \langle\psi(t)|\psi(t)\rangle = 1$
3. Non-Relativistic QM
4. Initial Value Problem (IVP): $\left|\psi(t = t_0)\right\rangle = \left|\psi(t_0)\right\rangle$
5. Schrödinger Picture: $\dfrac{\mathrm{d}\hat{A}}{\mathrm{d}t} \equiv 0$

21.1.2 Representation of Position

In $\boldsymbol{x}$-representation: $\hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla$, $\langle\boldsymbol{x}|\psi(t)\rangle = \psi(\boldsymbol{x})$

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle \Longrightarrow \mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x}, t) = \left(-\frac{\hat{p}}{2m} + V(\hat{x})\right)\psi(\boldsymbol{x}, t) \tag{103}$$

1. In general, $\dfrac{\partial\hat{A}}{\partial t} \equiv 0$ & $\dfrac{\partial\hat{H}}{\partial t} \equiv 0$. Unless there is external influence.
2. $\langle\psi(t)|\psi(t)\rangle = 1 \longleftrightarrow \int \mathrm{d}^3x\left|\psi(\boldsymbol{x}, t)\right|^2 = 1$
3. $\psi(\boldsymbol{x}, t = t_0) = \psi(\boldsymbol{x}, t_0)$

21.2 Time Evolution Operator

$$\left|\psi(t)\right\rangle = \hat{U}(t, t_0)\left|\psi(t_0)\right\rangle \tag{104}$$

$$\text{Schrödinger eq.} \Longrightarrow \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left[\hat{U}(t, t_0)\left|\psi(t_0)\right\rangle\right] = \hat{H}\left[\hat{U}(t, t_0)\left|\psi(t_0)\right\rangle\right] \tag{105}$$

$$\Longrightarrow \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t, t_0) = \hat{H}\hat{U}(t, t_0) \tag{106}$$

21.2.1 TEO for Conservative System

If the system is conservative, that is $\dfrac{\partial \hat{H}}{\partial t} \equiv 0$.

$$\Longrightarrow \frac{\mathrm{d}\hat{U}}{\hat{U}} = -\frac{\mathrm{i}}{\hbar}\hat{H}\,\mathrm{d}t \Longrightarrow \boxed{\hat{U}(t,t_0) = \mathrm{e}^{-\mathrm{i}\hat{H}(t-t_0)/\hbar}}$$

If $\dfrac{\partial \hat{H}}{\partial t} \neq 0$, then

$$\begin{aligned}\hat{U}(t,t_0) &= \hat{1} - \frac{\mathrm{i}}{\hbar}\int \mathrm{d}t'\,\hat{U}(t',t_0) \\ &= \hat{1} - \frac{\mathrm{i}}{\hbar}\cdots\text{(Dyson Series)}\end{aligned} \tag{107}$$

21.2.2 Properties of $\hat{U}(t,t_0)$

1. $\hat{U}^\dagger(t,t_0) = \hat{U}^{-1}(t,t_0 = \hat{U}(t_0,t))$ or $\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0) = \hat{1}$
2. $\hat{U}(t,t_1)\hat{U}(t_1,t_0) = \hat{U}(t,t_0) \xrightarrow{\text{expand}} \hat{U}(t,t_n)\hat{U}(t_n,t_{n-1})\cdots\hat{U}(t_2,t_1)\hat{U}(t_1,t_0) = \hat{U}(t,t_0)$
3. $\hat{U}(t,t_0) = \hat{U}(t-t_0) = \hat{U}(\tau)$ ($\tau \xlongequal{\text{def}} t-t_0$)

21.3 Continuity Equation

$$\begin{cases}\mathrm{i}\hbar\dfrac{\partial}{\partial t}\psi(\boldsymbol{x},t) = -\dfrac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t) \\ -\mathrm{i}\hbar\dfrac{\partial}{\partial t}\psi^*(\boldsymbol{x},t) = -\dfrac{\hbar^2}{2m}\nabla^2\psi^*(\boldsymbol{x},t) + V(\boldsymbol{x})\psi^*(\boldsymbol{x},t)\end{cases}$$

$$\Longrightarrow \begin{cases}\psi^*(\boldsymbol{x},t)\dfrac{\partial}{\partial t}\psi(\boldsymbol{x},t) = -\dfrac{\hbar}{2m\mathrm{i}}\psi^*(\boldsymbol{x},t)\nabla^2\psi(\boldsymbol{x},t) + \dfrac{1}{\mathrm{i}\hbar}\psi^*(\boldsymbol{x},t)V(\boldsymbol{x})\psi(\boldsymbol{x},t) \\ \psi(\boldsymbol{x},t)\dfrac{\partial}{\partial t}\psi^*(\boldsymbol{x},t) = \dfrac{\hbar}{2m\mathrm{i}}\psi(\boldsymbol{x},t)\nabla^2\psi^*(\boldsymbol{x},t) - \dfrac{1}{\mathrm{i}\hbar}\psi(\boldsymbol{x},t)V(\boldsymbol{x})\psi(\boldsymbol{x},t)\end{cases}$$

$$\Longrightarrow \psi^*\frac{\partial}{\partial t}\psi + \psi\frac{\partial}{\partial t}\psi^* = \frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\hbar}{2m\mathrm{i}}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right) = -\frac{\hbar}{2m\mathrm{i}}\nabla\cdot(\psi^*\nabla\psi - \psi\nabla\psi^*)$$

$$\Longrightarrow \frac{\partial}{\partial t}(\psi^*\psi) + \nabla\cdot\left[\frac{\hbar}{2m\mathrm{i}}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)\right] = 0$$

Let:

1. Probability Density
$$\rho(\boldsymbol{x},t) = \psi^*(\boldsymbol{x},t)\psi(\boldsymbol{x},t) = |\psi(\boldsymbol{x},t)|^2 \tag{108}$$
2. Probability Current Density
$$\boldsymbol{j} = \frac{\hbar}{2m\mathrm{i}}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) \tag{109}$$
$$\Longrightarrow \boxed{\frac{\partial\rho}{\partial t} + \nabla\cdot\boldsymbol{j} = 0} \tag{110}$$

21.4 Ehrenfest Theorem

$$\begin{cases} \mathrm{i}\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle & \Longrightarrow \dfrac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = \dfrac{\hat{H}}{\mathrm{i}\hbar}\left|\psi(t)\right\rangle \\ -\mathrm{i}\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\left\langle\psi(t)\right| = \left\langle\psi(t)\right|\hat{H} & \Longrightarrow \dfrac{\mathrm{d}}{\mathrm{d}t}\left\langle\psi(t)\right| = -\dfrac{1}{\mathrm{i}\hbar}\left\langle\psi(t)\right|\hat{H} \end{cases}$$

Consider an observable $\hat{O}$, with its expectation value $\left\langle\hat{O}\right\rangle = \left\langle\psi(t)\right|\hat{O}\left|\psi(t)\right\rangle$

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\left\langle\hat{O}\right\rangle(t) &= \left(\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\psi(t)\right|\right)\hat{O}\left|\psi(t)\right\rangle + \left\langle\psi(t)\right|\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}\left|\psi(t)\right\rangle + \left\langle\psi(t)\right|\hat{O}\left(\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle\right) \\ &= -\frac{1}{\mathrm{i}\hbar}\left\langle\psi(t)\right|\hat{H}\hat{O}\left|\psi(t)\right\rangle + \left\langle\psi(t)\right|\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}\left|\psi(t)\right\rangle + \frac{1}{\mathrm{i}\hbar}\left\langle\psi(t)\right|\hat{O}\hat{H}\left|\psi(t)\right\rangle \end{aligned}$$

$$\Longrightarrow \boxed{\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\hat{O}\right\rangle(t) = \left\langle\frac{\partial\hat{O}}{\partial t}\right\rangle + \frac{1}{\mathrm{i}\hbar}\left\langle\left[\hat{O},\hat{H}\right]\right\rangle} \tag{111}$$

21.4.1 Conserved Quantity (Constant of Motion)

If $\dfrac{\partial\hat{Q}}{\partial t} \equiv 0$ & $\left[\hat{O},\hat{H}\right]$, $\hat{O}$ is a conserved quantity. $\hat{O}$ & $\hat{H}$ have common eigenstates.

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}O = \dfrac{\partial O}{\partial t} + [O,H]_{\mathrm{PB}} & \text{CM} \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\hat{O}_{\mathrm{H}} = \left(\dfrac{\partial\hat{O}_{\mathrm{S}}}{\partial t}\right)_{\mathrm{H}} + \dfrac{1}{\mathrm{i}\hbar}\left[\hat{O}_{\mathrm{H}},\hat{H}\right] & \text{QM} \end{cases}$$

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

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\left\langle\hat{x}\right\rangle = \dfrac{1}{\mathrm{i}\hbar}\left\langle\left[\hat{x},\hat{H}\right]\right\rangle = \dfrac{1}{\mathrm{i}\hbar}\left\langle\left[\hat{x},\dfrac{\hat{p}^2}{2m}\right]\right\rangle = \dfrac{\left\langle\hat{p}\right\rangle}{m} \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\left\langle\hat{p}\right\rangle = \dfrac{1}{\mathrm{i}\hbar}\left\langle[\hat{p},V(x)]\right\rangle = -\left\langle V'(\hat{x})\right\rangle \end{cases} \Longrightarrow \frac{\mathrm{d}^2\left\langle\hat{x}\right\rangle}{\mathrm{d}t^2} = \frac{1}{m}\frac{\mathrm{d}\left\langle\hat{p}\right\rangle}{\mathrm{d}t}$$

$$\Longrightarrow m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\left\langle\hat{x}\right\rangle = -\left\langle V'(\hat{x})\right\rangle$$

21.5 Transformation between Schrödinger Picture & Heisenberg Picture

1. Schrödinger Picture

$$\begin{cases} \mathrm{i}\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle_{\mathrm{S}} = \hat{H}_{\mathrm{S}}\left|\psi(t)\right\rangle_{\mathrm{S}} \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\hat{A}_{\mathrm{S}}(t) \equiv 0 \end{cases} \tag{112}$$

2. Heisenberg Picture

$$\begin{cases} \dfrac{\mathrm{d}\hat{F}_{\mathrm{H}}}{\mathrm{d}t} = \left(\dfrac{\partial \hat{F}_{\mathrm{S}}}{\partial t}\right)_{\mathrm{H}} + \dfrac{1}{\mathrm{i}\hbar}\left[\hat{F}_{\mathrm{H}}, \hat{H}\right] \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle_{\mathrm{H}} \equiv 0 \end{cases} \tag{113}$$

21.5.1 from Schrödinger Picture to Heisenberg Picture

Time Evolution Operator

$$\begin{cases} \left|\psi(t)\right\rangle_{\mathrm{S}} = \hat{U}(t)\left|\psi(t)\right\rangle_{\mathrm{H}} \\ \hat{U}(t) = \mathrm{e}^{\mathrm{i}\hat{H}t/\hbar} \end{cases} \tag{114}$$

Invariant Quantities

1. Inner Product (Conservation of Probability)

$$_{\mathrm{S}}\langle\psi(t)|\psi(t)\rangle_{\mathrm{S}} = {_{\mathrm{S}}\langle\psi(t)|}\hat{U}^\dagger(t)\hat{U}(t)\left|\psi(t)\right\rangle_{\mathrm{H}} = {_{\mathrm{H}}\langle\psi(t)|\psi(t)\rangle_{\mathrm{H}}} \tag{115}$$

2. Expectation Value

$$_{\mathrm{S}}\langle\psi(t)|\hat{F}_{\mathrm{S}}\left|\psi(t)\right\rangle_{\mathrm{S}} = {_{\mathrm{H}}\langle\psi(t)|}\hat{U}^\dagger\hat{F}_{\mathrm{S}}\hat{U}\left|\psi(t)\right\rangle_{\mathrm{H}} = {_{\mathrm{H}}\langle\psi(t)|}\,\hat{F}_{\mathrm{H}}\left|\psi(t)\right\rangle_{\mathrm{H}} \tag{116}$$

$$\Longrightarrow \boxed{\hat{F}_{\mathrm{H}} = \hat{U}^\dagger\hat{F}_{\mathrm{S}}\hat{U}} \tag{117}$$

$$\begin{cases} \dfrac{\mathrm{d}\hat{U}}{\mathrm{d}t} = -\dfrac{\mathrm{i}}{\hbar}\hat{H}\hat{U} \quad (\hat{H}\hat{U} = \hat{U}\hat{H}) \\ \dfrac{\mathrm{d}\hat{U}^\dagger}{\mathrm{d}t} = \dfrac{\mathrm{i}}{\hbar}\hat{U}^\dagger\hat{H} \quad (\hat{H}\hat{U}^\dagger = \hat{U}^\dagger\hat{H}) \end{cases} \tag{118}$$

$$\begin{aligned} \frac{\mathrm{d}\hat{F}_{\mathrm{H}}}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{U}^\dagger\hat{F}_{\mathrm{S}}\hat{U}\right) = \frac{\mathrm{d}\hat{U}^\dagger}{\mathrm{d}t}\hat{F}_{\mathrm{S}}\hat{U} + \hat{U}^\dagger\left(\frac{\partial \hat{F}_{\mathrm{S}}}{\partial t}\right)\hat{U} + \hat{U}^\dagger\hat{F}_{\mathrm{S}}\frac{\mathrm{d}\hat{U}}{\mathrm{d}t} \\ &= \left(\frac{\partial \hat{F}_{\mathrm{S}}}{\partial t}\right)_{\mathrm{H}} + \frac{1}{\mathrm{i}\hbar}\left(\hat{U}^\dagger\hat{F}_{\mathrm{S}}\hat{H}\hat{U} - \hat{U}^\dagger\hat{H}\hat{F}_{\mathrm{S}}\hat{U}\right) \\ &= \left(\frac{\partial \hat{F}_{\mathrm{S}}}{\partial t}\right)_{\mathrm{H}} + \frac{1}{\mathrm{i}\hbar}\left[\left(\hat{U}^\dagger\hat{F}_{\mathrm{S}}\hat{U}\right)\left(\hat{U}^\dagger\hat{H}\hat{U}\right) - \left(\hat{U}^\dagger\hat{H}\hat{U}\right)\left(\hat{U}^\dagger\hat{F}_{\mathrm{S}}\hat{U}\right)\right] \\ &= \left(\frac{\partial \hat{F}_{\mathrm{S}}}{\partial t}\right)_{\mathrm{H}} + \frac{1}{\mathrm{i}\hbar}\left[\hat{F}_{\mathrm{H}}, \hat{H}_{\mathrm{H}}\right] \quad \left(\hat{H}_{\mathrm{H}} = \hat{U}^\dagger\hat{H}_{\mathrm{S}}\hat{U} = \hat{H}_{\mathrm{S}}\right) \end{aligned} \tag{119}$$

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle_{\mathrm{H}} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{U}^\dagger\left|\psi(t)\right\rangle_{\mathrm{S}}\right) = \frac{\mathrm{d}\hat{U}^\dagger}{\mathrm{d}t}\left|\psi(t)\right\rangle_{\mathrm{S}} + \hat{U}^\dagger\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle_{\mathrm{S}} \\ &= \frac{\mathrm{i}}{\hbar}\hat{U}^\dagger\hat{H}\left|\psi(t)\right\rangle_{\mathrm{S}} + \hat{U}^\dagger\left(\frac{1}{\mathrm{i}\hbar}\hat{H}_{\mathrm{S}}\left|\psi(t)\right\rangle_{\mathrm{S}}\right) = 0 \end{aligned} \tag{120}$$

21.5.2 from Heisenberg Picture to Schrödinger Picture