Quantum Mechanics II

1) Formal Principles of Quantum Mechanics:
harmonic oscillator, hydrogen atom
→ hypergeometric functions
2) Time-independent perturbation theory:
non-degenerate / degenerate
Brillouin - Wigner
3) Time-dependent perturbation theory:
absorption and emission of radiation
4) Scattering theory:
scattering amplitude, cross-section
5.) Addition of angular momenta:
Clebsch - Gordon coefficients, Landé factors, LS-coupling
6) Relativistic wave equations:
Klein-Gordon-equation, Dirac equation: hydrogen atom

special case

application

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7) Path integral description of quantum mechanics
free particle ⟺ harmonic oscillator

Chapter 1: Overview about Quantum Mechanics

1.1 Classical Mechanics:

particle in 3 D, mass M, potential $V(\vec{x})$

$$A[\vec{x}(\cdot)] = \int_{t_a}^{t_b} dt\, L\left(\vec{x}(t), \dot{\vec{x}}(t)\right), \quad L(x,\dot{x}) = \frac{M}{2}\dot{\vec{x}}^2 - V(\vec{x})$$

"functional"

action is a functional of the path $\vec{x}(t)$

Hamilton principle of Lagrangian mechanics:

$$\frac{\delta A[\vec{x}(\cdot)]}{\delta \vec{x}(t)} = 0 \qquad \text{(functional derivative)}$$

$$\frac{dx}{dx} = 1, \qquad \frac{\partial x_i}{\partial x_j} = \delta_{ij}, \qquad \boxed{\frac{\delta x(t)}{\delta x(t')} = \delta(t-t')} \quad (*)$$

total derivative, partial derivative, functional derivative

This is the basic definition for a functional derivative, all basic rules of differentiation can be extended to functional derivatives

$$\frac{\delta A[x(\cdot)]}{\delta x(t)} = \frac{\delta}{\delta x(t)} \int_{t_a}^{t_b} dt'\, L\left(x(t'), \dot{x}(t')\right)$$

$$= \int_{t_a}^{t_b} dt' \left\{ \frac{\partial L}{\partial x(t')} \frac{\delta x(t')}{\delta x(t)} + \frac{\partial L}{\partial \dot{x}(t')} \frac{\delta \dot{x}(t')}{\delta x(t)} \right\}$$

$$= \frac{\delta}{\delta x(t)} \frac{d}{dt'} x(t') = \frac{d}{dt'} \frac{\delta}{\delta x(t)} x(t')$$

$$= \Big[\frac{\partial L}{\partial \dot{x}(t')} \underbrace{\frac{\delta x(t')}{\delta x(t)}}_{(*)\ = \delta(\cancel{t} - t')} \Big]_{t_a}^{t_b} + \int_{t_a}^{t_b} dt' \left\{ \frac{\partial L}{\partial x(t')} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}(t')} \right\} \underbrace{\frac{\delta x(t')}{\delta x(t)}}_{(*)\ = \delta(t - t')}$$

$= 0 \quad t_a < t < t_b$

$$= \frac{\partial L}{\partial x(t)} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}(t)} = 0$$

Euler-Lagrange equation

$$\underbrace{\frac{\partial L}{\partial \vec{x}(t)}}_{= -\vec{\nabla} V(\vec{x}(t))} - \frac{d}{dt} \underbrace{\frac{\partial L}{\partial \dot{\vec{x}}(t)}}_{\frac{m}{2} 2 \dot{\vec{x}}} = 0 \quad , \quad L = \frac{m}{2} \dot{\vec{x}}^2 - V(\vec{x})$$

$\Rightarrow$ Newton equation: $m \ddot{\vec{x}} = -\frac{\partial V}{\partial \vec{x}}$

Lagrange mechanics $\longrightarrow$ Hamilton mechanics

$$\vec{p} = \frac{\partial L}{\partial \dot{\vec{x}}} = m \dot{\vec{x}} \quad \Rightarrow \quad \dot{\vec{x}} = \frac{\vec{p}}{m}$$

Legendre transformation:

$$\boxed{H(\vec{p}, \vec{x}) = \vec{p} \cdot \dot{\vec{x}} - L} = \vec{p} \cdot \frac{\vec{p}}{m} - \left\{ \frac{m}{2} \left(\frac{\vec{p}}{m} \right)^2 - V(\vec{x}) \right\} = \frac{\vec{p}^2}{2m} + V(\vec{x})$$

action in phase space

$$A = A[\vec{x}(\cdot), \vec{p}(\cdot)] = \int_{t_a}^{t_b} dt\, L = \int_{t_a}^{t_b} dt \left\{ \vec{p}(t) \dot{\vec{x}}(t) - H(\vec{p}(t), \vec{x}(t)) \right\}$$

$$\frac{\delta A}{\delta \vec{x}(t)} = 0 \quad \Rightarrow \ldots \Rightarrow$$

Euler-Lagrange

$$\dot{\vec{p}}(t) = -\frac{\partial H}{\partial \vec{x}(t)} = -\vec{\nabla} V(\vec{x}) \quad \Big\} \text{ Hamilton}$$

$$\frac{\delta \mathcal{A}}{\delta \vec{p}(t)} = 0 \quad \Rightarrow \; --- \Rightarrow \qquad \dot{\vec{x}}(t) = +\frac{\partial H}{\partial \vec{p}(t)} = \frac{\vec{p}(t)}{m}$$ | equations

1.2 Quantization:

classical observables $\longrightarrow$ hermitian operators

$\vec{x} \longrightarrow \hat{\vec{x}}$, $\quad \vec{p} \longrightarrow \hat{\vec{p}}$; $\quad H(\vec{p}, \vec{x}) \longrightarrow \boxed{\hat{H} = H(\hat{\vec{p}}, \hat{\vec{x}})}$

$p\, f(x)\, p\, g(x) \longrightarrow$ operator ordering problem

Heisenberg uncertainty relation enforces:

$$[\hat{x}_j, \hat{x}_k]_- = 0 = [\hat{p}_j, \hat{p}_k]_-, \qquad [\hat{p}_j, \hat{x}_k]_- = \frac{\hbar}{i}\delta_{jk}$$

$$[\hat{A}, \hat{B}]_- = \hat{A}\hat{B} - \hat{B}\hat{A}$$

Dirac notation: generic representation

state: $|\Psi(t)\rangle$ state vector

time evolution: time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}\, |\Psi(t)\rangle$$

coordinate representation: choose a basis $\Rightarrow$ eigenstates of $\hat{\vec{x}}$

$$\hat{\vec{x}}\, |\vec{x}\rangle = \vec{x}\, |\vec{x}\rangle$$

orthonormality: $\langle \vec{x} | \vec{x}' \rangle = \delta(\vec{x} - \vec{x}')$

completeness: $\int d^3x\, |\vec{x}\rangle \langle \vec{x}| = 1$

coordination representation for $\vec{p}$: Jordan rule

$$\langle \vec{x} | \hat{\vec{p}} = \frac{\hbar}{i} \vec{\nabla} \langle \vec{x} |$$

$$|\psi(t)\rangle = \hat{1} \cdot |\psi(t)\rangle = \int d^3x\, |\vec{x}\rangle \underbrace{\langle \vec{x} | \psi(t) \rangle}_{\psi(\vec{x},t)}$$

$\psi(\vec{x},t)$ wave function

$| \langle \vec{x} | \cdot$

$$i\hbar \frac{\partial}{\partial t} \underbrace{\langle \vec{x} | \psi(t) \rangle}_{=\psi(\vec{x},t)} = \langle \vec{x} | \left\{ \frac{\hat{\vec{p}}^2}{2m} + V(\hat{\vec{x}}) \right\} | \psi(t) \rangle$$

$$= \hat{H} \psi(\vec{x},t)$$

$$\Rightarrow \hat{H} = -\frac{\hbar^2}{2m} \underbrace{\Delta}_{=\vec{\nabla}^2} + V(\vec{x})$$

time-independent potential

stationarity: $\psi(\vec{x},t) = e^{-\frac{i}{\hbar}Et} \psi_E(\vec{x})$, $|\psi(\vec{x},t)|^2 = |\psi(\vec{x})|^2$ independent of time

time-independent Schrödinger equation: $\hat{H} \psi_E(\vec{x}) = \underbrace{E}_{} \psi_E(\vec{x})$ ⇐ energy eigenfunction

energy eigenvalue

- solvable as a partial differential equation of second order for any energy E
- boundary conditions in addition yield the quantization of the energy (usually: dirichlet boundary condition)

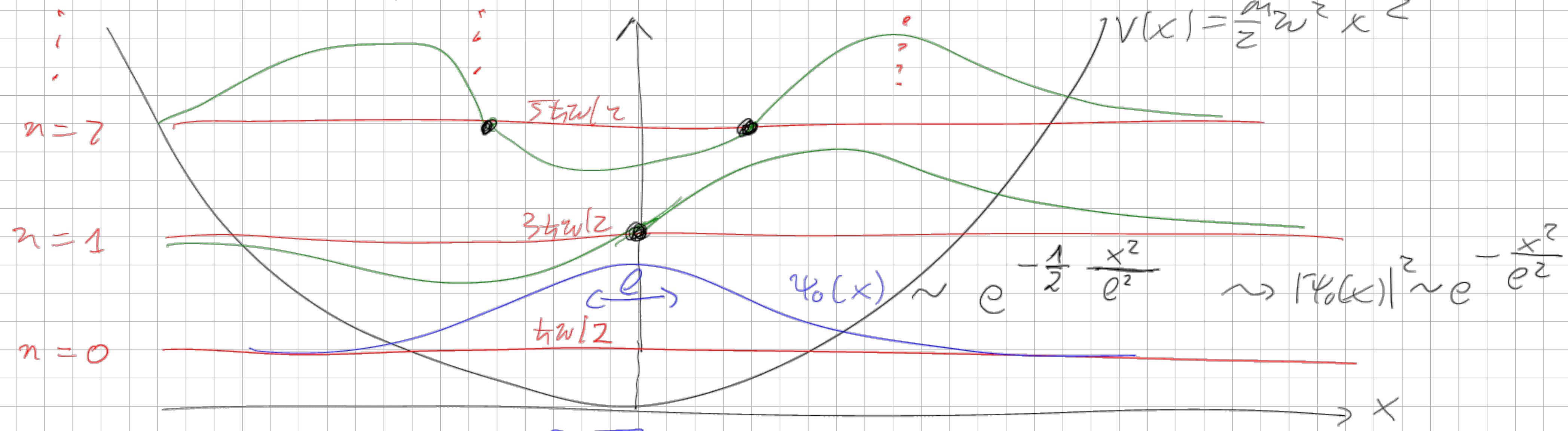
1.3 Harmonic oscillator: (example for 1D)

many applications: lattice vibrations, quantum optics, QFT

$$\left\{ -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + \frac{M}{2}\omega^2 x^2 \right\} \Psi_E(x) = E\,\Psi_E(x)$$

ω ↑ frequency

Dirichlet boundary condition: $\lim_{x\to\pm\infty} \Psi_E(x) = 0$



oscillator length: $\ell = \sqrt{\frac{\hbar}{M\omega}}$ energy eigenvalues: $E_n = \hbar\omega(n+\frac{1}{2});\ n \in \mathbb{N}_0$

^{87}Rb, $M = 87u$, $u = 1.66\,10^{-27}\,kg$, $\omega = 2\pi\cdot 100\,Hz$ $\Rightarrow$ $\ell = 1.16\,\mu m$

$\Psi_n(-x) = (-1)^n\,\Psi_n(x)$;

node rule: $\Psi_n(x)$ has n nodes