

Quantum Mechanics II - Lecture Notes

→ Aim: Going beyond the basics taught in Quantum Mechanics I (T2)

Syllabus

- Recap of QM I basics
- Feynman's path integral approach
- Scattering theory
 - cross section
 - phase shift, partial waves
 - optical theorem, S-matrix, unitarity
- Relativistic quantum mechanics
 - Klein-Gordon equation
 - Dirac equation
- Electro-magnetism in quantum mechanics
- Quantization of the electro-magnetic field
 - atomic transitions
 - time-dependent perturbation theory
- Second quantization, quantum field theory (basics)
- Quantum information

Literature

- Quantum mechanics I lecture notes
- These lecture notes
- F. Schwabl, Quantenmechanik I + II
- Griffiths, Quantum mechanics
- Teilchenphysik-Gruppe Web Site "Stadion"

Chapter 1: Principles of Non-Relativistic Quantum Mechanics (Recap)

1.1. State Vectors, Hilbert Space and Operators

→ At each instant in time t for a physical system there exists a state vector $|\Psi(t)\rangle$, which contains all information on what one can possibly know about the system at this time.

↪ Dirac-Notation (ket vector): $|\Psi\rangle \rightarrow$ vector in an (in general)

\Rightarrow -dimensional complex-valued linear vector space \mathcal{H} (\rightarrow Hilbert space)

Properties: $(\alpha, \beta, \gamma, \dots \in \mathbb{C})$

- $|\psi\rangle, |\varphi\rangle \in \mathcal{H} \Rightarrow \alpha|\psi\rangle + \beta|\varphi\rangle \in \mathcal{H}$
- There exists a null vector $|0\rangle$ with $|0\rangle + |\alpha\rangle = |\alpha\rangle$ for all $|\alpha\rangle \in \mathcal{H}$
- To each state $|\psi\rangle \in \mathcal{H}$ there is an inverse state $|\psi'\rangle$ with $|\psi\rangle + |\psi'\rangle = 0$.
- $|\psi\rangle + |\varphi\rangle = |\varphi\rangle + |\psi\rangle$ (addition commutes)
- $(|\psi\rangle + |\varphi\rangle) + |\chi\rangle = |\psi\rangle + (|\varphi\rangle + |\chi\rangle)$ (associative law for addition)
- $\alpha(\beta|\psi\rangle) = (\alpha \cdot \beta)|\psi\rangle$ (associative law for multiplication)
- $(\alpha + \beta)|\psi\rangle = \alpha|\psi\rangle + \beta|\psi\rangle$ (distributive law for multiplication)
- $\alpha(|\psi\rangle + |\varphi\rangle) = \alpha|\psi\rangle + \alpha|\varphi\rangle$ (distributive law for addition)
- For each state vector $|\psi\rangle$ there is a dual state $\langle\psi|$ that is physically equivalent and with which one can define a scalar product.

→ dual vector property: $|\psi\rangle = \alpha|\psi\rangle + \beta|\psi\rangle \Rightarrow \langle\psi| = \alpha^* \langle\psi| + \beta^* \langle\psi|$

- The scalar product has the properties:

$$\langle\psi|\varphi\rangle = \langle\varphi|\psi\rangle \in \mathbb{C}$$

$$\langle\psi|(\alpha|\varphi\rangle + \beta|\chi\rangle) = \alpha\langle\psi|\varphi\rangle + \beta\langle\psi|\chi\rangle$$

$$\langle\psi|\varphi\rangle = \langle\varphi|\psi\rangle^*$$

$$\langle\psi|\psi\rangle \in \mathbb{R}$$

$$\langle\psi|\psi\rangle \geq 0 \quad (= 0 \text{ if and only if } |\psi\rangle = |0\rangle)$$

$$|\langle\psi|\varphi\rangle|^2 \leq \langle\psi|\psi\rangle \langle\varphi|\varphi\rangle \quad (\text{Schwartz inequality})$$

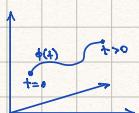
The scalar product is used to define:

→ norm of state ψ : $\|\psi\| = \sqrt{\langle\psi|\psi\rangle}$

→ orthogonality: ψ and φ (both not null vectors) are orthogonal if $\langle\psi|\varphi\rangle = 0$

↪ ψ and φ are then also physically inequivalent

States can be time-dependent and are therefore the basis to describe the dynamics of any system.



Note: The ground (vacuum) state of the harmonic oscillator is frequently also written as $|0\rangle$ (for $n=0$), but it is not a null state.

Orthonormal basis (ONB):

A ONB for the Hilbert space \mathcal{H} is a set of state vectors $\{|u\rangle\}$ with

$$\langle u|v \rangle = \begin{cases} \delta(u-v), & u \text{ and } v \text{ continuous} \\ \delta_{uv}, & \text{otherwise} \end{cases}$$

n : counting variable
(countable or continuous)

and the property $\sum_n |u\rangle \langle u| = \mathbb{1}$ (completeness relation)

$$\Rightarrow |\psi\rangle = \sum_n |u\rangle \langle u|\psi\rangle = \sum_n \langle u|\psi\rangle \cdot |u\rangle = \sum_n c_u^* |u\rangle$$

$$|\psi\rangle \approx \begin{pmatrix} c_1^* \\ c_2^* \\ c_3^* \\ \vdots \end{pmatrix}$$

$$\langle \psi|\psi \rangle = \sum_n \langle \psi| |u\rangle \langle u|\psi \rangle = \sum_n \langle u|\psi \rangle^* \langle u|\psi \rangle = \sum_n c_u^{**} c_u^*$$

$$|\psi\rangle \approx (c_1^{**}, c_2^{**}, c_3^{**}, \dots)$$

1.2 Operators

→ Operators are the mathematical instrument to describe

- the dynamics of the system ($\frac{d}{dt}|\psi(t)\rangle = \dots$)
- the outcome of measurements

Linear operator: An operator $A: \mathcal{H} \rightarrow \mathcal{H}$ that assigns each vector $|v\rangle \in \mathcal{H}$ the vector $A|v\rangle \in \mathcal{H}$ is a linear operator, if

$$A(c_1|v_1\rangle + c_2|v_2\rangle) = c_1 A|v_1\rangle + c_2 A|v_2\rangle \quad \forall |v_{1,2}\rangle \in \mathcal{H} \text{ and } c_{1,2} \in \mathbb{C}$$

↪ Let $\{|u\rangle\}$ be ONB:

$$\begin{aligned} A|\psi\rangle &= \sum_n |u\rangle \langle u|A|v\rangle = \sum_n \sum_m |u\rangle \langle u|A|m\rangle \langle m|\psi\rangle \\ &= \sum_n \sum_m \langle u|A|m\rangle \langle m|\psi\rangle \cdot |u\rangle = \sum_n \sum_m a_{nm} c_m^* \cdot |u\rangle \end{aligned}$$

↑ operator matrix elements

$$A \approx \begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots \\ a_{21} & a_{22} & a_{23} & \dots \\ a_{31} & a_{32} & a_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Adjoint operator: The operator A^+ is called the adjoint operator to the linear operator A , if (and only if)

$$\langle \phi|A^+|v\rangle = \langle A\phi|v\rangle \quad \forall \phi, v \in \mathcal{H}$$

$$A^+ \approx "A\text{-dagger"}$$

↪ The following rules apply: $(aA+bB)^+ = a^+A^++b^+B^+$, $A^+ = (A^T)^* = (A^*)^T$ (matrix notation)

$$(AB)^+ = B^+A^+$$

$$(A^+)^+ = A$$

Hermitian (or self-adjoint) operator: A linear operator A is called Hermitian, if also $A^+ = A$

Unitary operator: A linear operator is called unitary if also $UU^+ = U^+U = \mathbb{1}$

Eigenvalues and eigenvectors: A $\psi \in \mathcal{X}$ is called eigenvector to the linear operator A with the eigenvalue a if and only if it has the property $A\psi = a\psi$ for all $a \in \mathbb{C}$

$$A\psi = a\psi \text{ for all } a \in \mathbb{C}$$

↳ If $A|\psi_n\rangle = a_n|\psi_n\rangle$, $A|\psi_m\rangle = a_m|\psi_m\rangle$ and $a_n = a_m$ for $n \neq m$, then the eigenvalue a_n is called degenerate.

↳ The set of eigenvalues of a linear operator A is called the spectrum of A .

↳ Eigenvalues of Hermitian operators are real.

Proof: $\langle \psi | A \psi \rangle = a \langle \psi | \psi \rangle = \langle A^\dagger \psi | \psi \rangle = \langle A \psi | \psi \rangle = \langle \psi | A^\dagger \psi \rangle = a^* \langle \psi | \psi \rangle \Rightarrow a = a^* \Rightarrow a \in \mathbb{R}$ \square

↳ The eigenvectors of a Hermitian operator to two different eigenvalues $a_1 \neq a_2$ are orthogonal.

Proof: $A|\psi_1\rangle = a_1|\psi_1\rangle \Rightarrow \langle \psi_1 | A \psi_2 \rangle = \langle A \psi_1 | \psi_2 \rangle = a_1 \langle \psi_1 | \psi_2 \rangle = a_2 \langle \psi_1 | \psi_2 \rangle \Rightarrow (a_1 - a_2) \langle \psi_1 | \psi_2 \rangle = 0 \Rightarrow \langle \psi_1 | \psi_2 \rangle = 0$ \square

Spectral Theorem: For each Hermitian operator A there is a ONB to \mathcal{X} made of eigenvectors $\{|\psi_n\rangle\}$ to A , i.e. $A|\psi_n\rangle = a_n|\psi_n\rangle$ for some $a_n \in \mathbb{C}$.

↳ Spectral representation: $A = \sum_n a_n |\psi_n\rangle \langle \psi_n|$

↳ A, B Hermitian and $[A, B] = AB - BA = 0$:

There exists an ONB $\{|\psi_n\rangle\}$ made of eigenvectors to both A and B , i.e. $A|\psi_n\rangle = a_n|\psi_n\rangle$, $B|\psi_n\rangle = b_n|\psi_n\rangle$

1.3. Observables

Correspondence Principle:

Each observable quantity ("observable") in quantum mechanics is represented by a Hermitian operator.

The set of eigenvalues (spectrum) of the Hermitian operator associated to an observable in quantum mechanics is the set of measurable values of the observable.

↳ Observable A : ONB $\{|\psi_n\rangle\}$ of eigenvectors: $A|\psi_n\rangle = a_n|\psi_n\rangle$

System in normalized state $|\psi\rangle$: $|\psi\rangle = \sum_n c_n |\psi_n\rangle$, $c_n = \langle \psi_n | \psi \rangle$

→ Probability to measure value a_n : $P(a_n) = \sum_{\psi_n} |c_n|^2 = \sum_{\psi_n} |\langle \psi_n | \psi \rangle|^2$
(in each measurement)

Sum over set of states ψ_n which have eigenvalue a_n
(can be more than one state if a_n is degenerate.)

→ Average of many repeated measurements on identical system in the state $|4\rangle$:

$$\sum_n a_n |c_n|^2 = \sum_n a_n \langle \phi_n | 4 \rangle \langle 4 | \phi_n \rangle = \langle 4 | \sum_n a_n | \phi_n \rangle \langle \phi_n | 4 \rangle = \langle 4 | A | 4 \rangle =: \langle A \rangle_4$$

$$\text{Variance of these measurements: } (\Delta A)^2 = \langle (A - \langle A \rangle_4)^2 \rangle_4 = \langle A^2 \rangle_4 - \langle A \rangle_4^2$$

$$\text{Standard deviation: } \Delta A = (\langle A^2 \rangle_4 - \langle A \rangle_4^2)^{1/2}$$

→ **Collapse of the State:** If the measurement does not minimally, so that the system is not destroyed during the measurement, the system is after measurement of value a_m in the (still unnormalized) state

$$|4\rangle_{am} = \sum_m c_m |\phi_m\rangle = \sum_m |\phi_m\rangle \langle \phi_m | 4 \rangle$$

Complete Set of physical observables

⇒ Sufficiently large set of commuting Hermitian operators $\{A_1, A_2, \dots, A_n\}$ ($[A_i, A_j] = 0$) such that each eigenvector of their common (and unique) ONB can be unambiguously identified by the eigenvalues wr. to these operators.

$$A_i |\phi_m\rangle = a_i^m |\phi_m\rangle \Rightarrow |\phi_m\rangle \approx |a_1^m, a_2^m, \dots, a_n^m\rangle$$

The set $\{a_1^m, a_2^m, \dots, a_n^m\}$ are called the quantum numbers of state $|\phi_m\rangle$.

spin-less particle:

⇒ Complete set: $\{\vec{x}\}$, $[\vec{x}_i, \vec{x}_j] = 0$, $\vec{x}| \vec{x} \rangle = \vec{x} | \vec{x} \rangle$, $\int d^3x | \vec{x} \rangle \vec{x} | \vec{x} \rangle = 1$, $\langle \vec{x} | \vec{y} \rangle = \delta^{(3)}(\vec{x} - \vec{y})$

$$|\psi\rangle = \int d^3x \underbrace{| \vec{x} \rangle}_{\psi(\vec{x})} \langle \vec{x} | \psi \rangle = \int d^3x \psi(\vec{x}) | \vec{x} \rangle \quad \psi(\vec{x}): \text{contig. space wave function}$$

→ Interpretation of $\psi(\vec{x})$: $\frac{1}{(2\pi\hbar)^{3/2}} |\psi(\vec{x})|^2 d^3x \triangleq \text{probability that particle is found at } \vec{x} \text{ within volume element } d^3x \text{ in a location measurement}$

Complete set: $\{\vec{p}\}$, $[\vec{p}_i, \vec{p}_j] = 0$, $\vec{p} | \vec{p} \rangle = \vec{p} | \vec{p} \rangle$, $\int d^3p | \vec{p} \rangle \vec{p} | \vec{p} \rangle = 1$, $\langle \vec{p} | \vec{q} \rangle = \delta^{(3)}(\vec{p} - \vec{q})$

$$| \psi \rangle = \int d^3p \underbrace{| \vec{p} \rangle}_{\tilde{\psi}(\vec{p})} \langle \vec{p} | \psi \rangle = \int d^3p \tilde{\psi}(\vec{p}) | \vec{p} \rangle \quad \tilde{\psi}(\vec{p}): \text{mom space wave function}$$

$$\langle \vec{x} | \vec{p} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p} \cdot \vec{x}/\hbar},$$

$$\langle \vec{x} | \vec{P} | \vec{q} \rangle = \int d^3p \vec{p} \langle \vec{x} | \vec{p} \rangle \langle \vec{p} | \vec{q} \rangle = i\hbar \frac{\partial}{\partial \vec{x}} \langle \vec{x} | \vec{q} \rangle = i\hbar \frac{\partial}{\partial \vec{x}} \delta^{(3)}(\vec{x} - \vec{q}) = -i\hbar \frac{\partial}{\partial \vec{x}} \delta^{(3)}(\vec{p} - \vec{q})$$

$$\langle \vec{p} | \vec{X} | \vec{q} \rangle = \int d^3x \vec{x} \langle \vec{p} | \vec{x} \rangle \langle \vec{x} | \vec{q} \rangle = -i\hbar \frac{\partial}{\partial \vec{q}} \langle \vec{p} | \vec{q} \rangle = -i\hbar \frac{\partial}{\partial \vec{q}} \delta^{(3)}(\vec{p} - \vec{q}) = i\hbar \frac{\partial}{\partial \vec{q}} \delta^{(3)}(\vec{p} - \vec{q})$$

particle with spin- $\frac{1}{2}$:

Compl. set: $\{\vec{x}, \vec{n} \vec{S}\}$, $[x_i, \vec{n} \vec{S}] = 0$, $\vec{S}^2 = \frac{1}{2} \vec{\sigma}^2$, $|\vec{n}|^2 = 1$, \vec{n} : quantization axis
 Pauli matrices
 direct prod.

$$|\vec{x}, \pm\rangle = |\vec{x}\rangle \otimes |\pm\rangle, \quad \vec{x}|\vec{x}, \pm\rangle = \vec{x}|\vec{x}, \pm\rangle, \quad \vec{n} \vec{S}|\vec{x}, \pm\rangle = \pm \frac{1}{2} |\vec{x}, \pm\rangle$$

$$|\psi\rangle = \sum_{s=\pm} \left(a_{\vec{x}}^s |\vec{x}, s\rangle + a_{\vec{x}, -}^s |\vec{x}, -s\rangle \right) = \left(a_{\vec{x}}^s \begin{pmatrix} 1 & 0 \\ 0 & e^{i\vec{x} \cdot \vec{s}} \end{pmatrix} \right) |\vec{x}\rangle$$

↳ Observables suitable as quantum numbers:

\vec{x} (location), \vec{p} (momentum), \vec{L} (angular momentum), $\vec{S}^2, \vec{n} \vec{S}$ (spin)

but also: electric charge Q , weak isospin I , color charge, ...

Canonical Commutation Relations: $[x_i, p_j] = i\delta_{ij}\hat{t}$, $[x_i, x_j] = [p_i, p_j] = 0$

1.4. Temporal Dynamics

Schrödinger Picture (S)

- mostly used for time-independent, stationary problems
bound states, exactly solvable problems
- standard picture for construction of observable operators
using the correspondence principle

Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H|\psi(t)\rangle$$

H: Hamilton operator (e.g. sum of terms)

Determined from the total energy and the
correspondence principle

$$\begin{array}{c} E = T + V + \dots \\ \downarrow \\ i\hbar \frac{\partial}{\partial t} \quad \underbrace{\qquad}_{H = H(\vec{p}, \vec{x}, \dots)} \end{array}$$

Observables: time-independent
States: time-dependent

special case: H time-independent $\rightarrow |\psi(t)\rangle_s = \exp(-i \frac{H(t-t_0)}{\hbar} t) |\psi(t_0)\rangle_s = U(t, t_0) |\psi(t_0)\rangle_s$

↳ There is a DNS of energy eigenstates for H.

Unitary time evolution operator $U(t, t_0)$

Separation ansatz: $\psi_s(\vec{x}, t) = f(t) \psi_s(\vec{x})$

$$\hookrightarrow i\hbar \frac{\partial}{\partial t} f(t) \psi_s(\vec{x}) = H f(t) \psi_s(\vec{x})$$

eigenfunction to some
energy eigenvalue E

$$\Leftrightarrow \underbrace{i\hbar \frac{1}{f(t)} \frac{\partial}{\partial t} f(t)}_{\text{indep. of } \vec{x}} = \underbrace{\frac{1}{f(\vec{x})} H f(\vec{x})}_{\text{indep. of } t} = E = \text{const}$$

$$\hookrightarrow f(t) = e^{-i \frac{Et}{\hbar}}, \quad H f(\vec{x}) = E f(\vec{x})$$

$$\hookrightarrow |\psi(\vec{x}, t)|^2 = |\psi(\vec{x})|^2 \text{ stationary}$$

time-independent Schrödinger equation

see Stern-Gerlach experiment
Clip 5.3. QM1-lecture

Heisenberg Picture (H)

- very useful to calculate time-evolution of quantum effects in "almost" classical problems
- Does not involve determination of eigenfunctions to H.

$$\text{Observable: } A_H(t) = U^\dagger(t) A_S U(t) \quad U(t) = \exp(-i \frac{Ht}{\hbar}) \quad (\text{reference time } t_0 = 0)$$

↓
Observable operator in the Schrödinger picture

↳ Heisenberg equation: $\dot{A}_H(t) = i \frac{\hbar}{\hbar} [H, A_H] + \frac{\partial}{\partial t} A_H$ if A_S time-dependent

$$\frac{d}{dt} A_H(t) = \frac{i}{\hbar} [H, A_H] + \frac{\partial}{\partial t} A_H$$

$$H_H = H_S \quad (\text{always!})$$

Observables: time-dependent
States: time-independent

$$\text{States: } |\psi(t)\rangle_h = U^\dagger(t) |\psi(t)\rangle_s = |\psi(t_0)\rangle_s$$

Interaction Picture (I) (Dirac representation)

$$H = H_0 + \delta H(t)$$

↑
exactely solvable
Hamiltonian

↑
time-dependent
perturbation: $\delta H \ll H_0$

→ For time-dependent problems where the time-dependence cannot be solved exactly, but leads to "small" effects (suitable for perturbative treatment)

$$\hookrightarrow |\psi(t)\rangle_I = e^{i \frac{H_0 t}{\hbar}} |\psi(t)\rangle_s \quad \leftarrow \text{state contains only "non-trivial" time dependence from } \delta H$$

$$A_I(t) = e^{i \frac{H_0 t}{\hbar}} A_S(t) e^{-i \frac{H_0 t}{\hbar}} \quad \leftarrow \text{operator contains "trivial" time-dependence from } H_0$$

$$\hookrightarrow i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_I = e^{i \frac{H_0 t}{\hbar}} (-H_0 + \delta H) |\psi(t)\rangle_s = \delta H |\psi(t)\rangle_I \quad ([H_0, \delta H] = 0)$$

$$\frac{d}{dt} A_I(t) = \frac{i}{\hbar} [H_0, A_I(t)] + \frac{\partial}{\partial t} A_I(t)$$

→ Later in lecture for describing time-dependent processes that are fast / slow.

1.5. Units

The fundamental constants of nature

$$\hbar = \frac{h}{2\pi} = 6.582 \cdot 10^{-16} \text{ eV}\cdot\text{s} \quad (\text{reduced Planck constant})$$

$$c = 2.998 \cdot 10^8 \frac{\text{m}}{\text{s}} \quad (\text{speed of light}) \rightarrow \text{in vacuum}$$

$$k = 8.617 \cdot 10^{-5} \frac{\text{eV}}{\text{K}} \quad (\text{Boltzmann constant}),$$

intrinsically connect the quantities distance, time, energy, momentum, mass, temperature.

$1 \text{ eV} = \text{kinetic energy of a particle with one electric elementary charge } e \text{ (e.g. proton } p^+, \text{ electron } e^- \dots) \text{ acquires / loses when going through a potential difference of } 1 \text{ V (volt).}$

Classical mechanics: energy (E) and time (t), momentum (p) and distance (x)

↳ are unrelated quantities, can be measured using independent conventions

Quantum mechanics: quantum fluctuations and dynamics determined by products energy \times time ($E \cdot t$), momentum \times distance ($p \cdot x$) in units of \hbar
 ↳ e.g. wave function of free particle with mass μ and momentum \vec{p} :

$$\psi(x, t) = e^{\frac{-iEt}{\hbar}} e^{\frac{i\vec{p}\vec{x}}{\hbar}}, \quad E = \frac{p^2}{2\mu} \xrightarrow{t=1} \psi(x, t) = c e^{\frac{-iEt}{\hbar}} e^{\frac{i\vec{p}\vec{x}}{\hbar}}$$

↳ We can adopt units such that $[E] = [t]^{-1}$, $[p] = [x]^{-1} \rightarrow \boxed{\hbar = 1}$

Non-relativistic physics: time (t) and distance (x), energy (E) and momentum (p)

↳ are unrelated quantities, can be measured using independent conventions

Relativistic physics: Speed of light c (in vacuum) universal, independent of reference frame
 ↳ We can quantify time & positions through the distance light travels.
 Mass is just another form of energy : $E = mc^2$

↳ We can adopt units such that $[t] = [x]^{-1}$, $[E] = [m] \rightarrow \boxed{c = 1}$

$$\text{Recall: } [E_{\text{kin}}] = \left[\frac{p^2}{m} \right] \Rightarrow [E] = [p]$$

↳ "Natural units": $\hbar = c = 1$

→ All quantities can be measured
 e.g. in units (eV) some power → simplifies notation

Note 1: One can always recover (unambiguously) the proper powers of t and c in all formulae.

Note 2: Classical mechanics and non-relativistic kinematics are not "wrong" physical theories but the correct physical theories in certain limits

Classical mechanics $\hat{=}$ leading order in an expansion in t (for classical systems)

Non-relativistic kinematics $\hat{=}$ leading order in an expansion in $\frac{t}{c}$ (for non-rel systems)

- 2 \Rightarrow Classical mechanics, non-rel. kinematics are "effective theories" of more fundamental and more widely applicable theories
- 2 \Rightarrow Basic property of an effective theory: One can (in principle) determine all higher order corrections in the expansion parameter (t, c, \dots)