Quantum Mechanics II - Lecture Notes

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

Syllabus

- Recap of QM & 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
- Electromagnetic in quantum mechanics
- Quantization of the electromagnetic 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. Scheck, Quantum Mechanics I + II
- Griffiths, Quantum Mechanics
- Hellwig, Sopher, and Stiti, "Stadium"
Chapter 4: Principles of Non-Relativistic Quantum Mechanics (Recap)

1.1 State Vectors, Hilbert Space, and Operators

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

- Inner Notation (but vector): \( |\psi\rangle \rightarrow \text{vector in dim } n; \text{linear vector space } \mathbb{C}^n \) (\( \sim \text{Hilbert space} \))

Properties: \( (|\psi_1\rangle, |\psi_2\rangle, \ldots \in \mathbb{C}^n) \)

- \(|\psi_1\rangle, |\psi_2\rangle \in \mathbb{C} \rightarrow |\psi_1\rangle + |\psi_2\rangle \in \mathbb{C} \)
- There exists a null vector \( |0\rangle \) with \( |0\rangle + |0\rangle = |0\rangle \) for all \( |0\rangle \in \mathbb{C} \)
- To each state \( |\psi\rangle \in \mathbb{C}^n \) there is an inverse state \( |\psi\rangle \) with \( |\psi\rangle + |\psi\rangle = 0 \)
- \(|\psi\rangle + |\psi\rangle = |\psi\rangle \rightarrow |0\rangle \) (addition commutes)
- \(|\psi\rangle + |\psi\rangle + |\psi\rangle = |\psi\rangle + |\psi\rangle \) (associative law for addition)
- \( \alpha |\psi\rangle + \alpha |\psi\rangle = \alpha |\psi\rangle + \beta |\psi\rangle \) (associative law for multiplication)
- \( \alpha (|\psi\rangle + |\psi\rangle) = \alpha |\psi\rangle + \beta |\psi\rangle \) (distribution law for multiplication)
- \( \alpha (|\psi\rangle + |\psi\rangle) = \alpha |\psi\rangle + \beta |\psi\rangle \) (distribution law for addition)
- For each state \( |\psi\rangle \), there is a dual state \( \langle \psi | \) that is physically equivalent and with which one can define a scalar product
- Dual vector property: \( \langle \psi | \phi \rangle = \langle \psi | \phi \rangle \)
- The scalar product has the properties:
  \[ \langle \psi | \psi \rangle = \langle \psi | \phi \rangle \in \mathbb{C} \]
  \[ \langle \psi | (\alpha |\phi\rangle + \beta |\phi\rangle) = \langle \psi | \phi \rangle + \beta \langle \psi | \phi \rangle \]
  \[ \langle \psi | \phi \rangle = \langle \phi | \psi \rangle \]
  \[ \langle \psi | \psi \rangle = 0 \text{ (0 if and only if } |\psi\rangle = |\psi\rangle \text{)} \]
  \[ \langle \psi | \psi \rangle \text{ (Schwarz's inequality)} \]

The scalar product is used to define:
- norm of state \( \psi \): \( \|\psi\| = \langle \psi | \psi \rangle^{1/2} \)
- orthogonality: \( |\phi\rangle \) and \( |\psi\rangle \) (both non-null vectors) are orthogonal if \( \langle \phi | \psi \rangle = 0 \)
- 0 = \( |\phi\rangle \perp |\psi\rangle \text{ and they are physically independent} \)

\[ \text{Note: The ground (vacuum) state of the harmonic oscillator is frequently also denoted as } |0\rangle \text{ (for } n=0 \text{), but it is not a null state.} \]
Orthogonal basis (0003):

A basis for the Hilbert space $\mathcal{H}$ is a set of basis vectors $\{ |n\rangle \}$, where

$|n\rangle = \begin{cases} |\text{state}\rangle & \text{if} n = \text{counting variable} \\ |\text{state}\rangle |\text{basis}\rangle & \text{otherwise} \end{cases}$

and the property $\sum |n\rangle \langle n| = \mathbb{1}$ (completeness relation).

$\langle 1|\langle 1 | = \frac{1}{N} \langle 1 | 1 \langle 1 | = | 1 \rangle \langle 1 | = | 1 \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

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$A|1\rangle = (a_1, a_2, a_3, \ldots)$

1.2 Operators

An operator $A : \mathcal{H} \to \mathcal{H}$ that assigns each vector $\psi \in \mathcal{H}$ the vector $A\psi \in \mathcal{H}$ is a linear operator if:

$A(\alpha|1\rangle + \beta|2\rangle) = \alpha A|1\rangle + \beta A|2\rangle \quad \forall \psi \in \mathcal{H} \text{ and } \alpha, \beta \in \mathbb{C}$

Let $\{|n\rangle\}$ be an orthonormal basis:

$A|n\rangle = \sum_{m=1}^{N} A_{mn}|m\rangle = \sum_{m=1}^{N} \langle m|A|n\rangle |m\rangle$

$A_{mn} = \langle m|A|n\rangle \quad \text{operator matrix elements}$

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

$\langle 1|A^\dagger|2\rangle = \langle 2|A|1\rangle \quad \forall \psi_1, \psi_2 \in \mathcal{H}$

$A = \begin{pmatrix} a_1 & a_2 & \cdots \\ a_3 & a_4 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$

The following rules apply:

$(\alpha A + \beta B)^\dagger = \alpha^* A^\dagger + \beta^* B^\dagger$,

$(\alpha A^\dagger)^\dagger = \alpha^* A$,

$(AB)^\dagger = B^\dagger A^\dagger$,

Hermitian (or self-adjoint) operator: A linear operator $A$ is called Hermitian if $A = A^\dagger$.

Unitary operator: A linear operator is called unitary if $A A^\dagger = A^\dagger A = \mathbb{1}$.
4.2. Observables

Correspondence Theorem: Each observable (measurable) in quantum mechanics is the set of measurable values of an observable in position.

Example: An observable $A$ in position is represented by a position operator.

$L^2$ Hilbert space: $a |i\rangle = |\psi_i\rangle$

The set of observables (eigenvalues) of the position operator is represented by an observable in position.

$A = A_x = a |i\rangle \langle i|$

Central Limit Theorem: For each observable $A$, there is a $\sigma^2$ for $k$. 

$\sigma^2 \approx \hbar$ in quantum mechanics.

Spectral Theorem: $A$ is a Hermitian operator in $L^2$ Hilbert space.

Proof: $\langle \psi \mid A^2 \psi \rangle = \langle \psi \mid A \psi \rangle \langle \psi \mid A \psi \rangle$

1. $A$ is self-adjoint.
3. $A^2$ is self-adjoint.
4. $A$ is a bounded operator.
5. $A$ is a bounded operator.
6. $A^2$ is a bounded operator.
7. $A$ is a bounded operator.
8. $A$ is a bounded operator.

Equivalence and classification: If $\mathcal{H}$ is a C*-algebra generated by the linear operator $A$, then the equivalence class.

$A = a |i\rangle \langle i| + a^* |j\rangle \langle j|$

$A^2 = a^2 |i\rangle \langle i| + a^2 |j\rangle \langle j|$

$A^*A = a^* a |i\rangle \langle i| + a a^* |j\rangle \langle j|$

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$A^*A = a^* a |i\rangle \langle i| + a a^* |j\rangle \langle j|$
Average of using repeated measurements on identical system in the state $|\psi\rangle$:

$$\sum a_i |\psi_i\rangle = \frac{1}{N} \sum a_i (a_i |\psi_i\rangle) = \frac{1}{N} \sum a_i (a_i |\psi_i\rangle + |\psi_i\rangle) = \frac{1}{N} |\psi\rangle = |\psi\rangle$$

Variance of these measurements: $(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$

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

Collapse of the state: If the measurement does not minimally destroy the system, the system is also measured of value $a_i$ in the (still unnormalized) state

$$|\psi_i\rangle = \frac{1}{\sqrt{|a_i|}} |\psi_i\rangle = \frac{1}{\sqrt{|a_i|}} b_i |\psi_i\rangle$$

**Complete Set of Physical Observables**

A sufficiently large set of commuting (Hermitian) operators $\{A_i, A_j \ldots, A_n\}$ such that each eigenvalue of their common (and unique) eigenstate can be unambiguously identified by the eigenvalue set to these operators

$$A_i |\psi\rangle = a_i |\psi\rangle \rightarrow |\psi\rangle = |a_1, a_2, \ldots, a_n\rangle$$

The set $\{a_1, a_2, \ldots, a_n\}$ are called the quantum numbers of state $|\psi\rangle$.

Spinless Particles:

2x Complete Set: $\{X\} \rightarrow |X\rangle, \langle X|X\rangle = 1$, $\langle X|X\rangle = \frac{1}{2}$ $|\psi\rangle = \langle X|X\rangle$

$|\psi\rangle = \sum |X\rangle \frac{1}{\sqrt{2}} |X\rangle = \frac{1}{\sqrt{2}} |\psi\rangle$ - any function value

Interpretation of $|\psi\rangle$: $\frac{1}{\sqrt{2}} |\psi\rangle$ - probability that particle is found at $X$ certain value, obtained $\langle X|X\rangle$ in a location measurement

Complete Set for Spinless Particles:

$\{ P \} \rightarrow |P\rangle, \langle P|P\rangle = 1$, $\langle P|P\rangle = \frac{1}{2}$

$|\psi\rangle = \langle X|X\rangle |P\rangle = \frac{1}{\sqrt{2}} |\psi\rangle$ - meaningless wave function

$\langle X|X\rangle = \frac{1}{2}$ $|\psi\rangle = |P\rangle e^{i\theta}$

$\langle X|P\rangle = \langle X|P\rangle e^{i\theta} \langle X|X\rangle = \frac{1}{\sqrt{2}} |\psi\rangle = |X\rangle$ $\langle X|X\rangle = \frac{1}{2}$ $\langle P|P\rangle = \frac{1}{2}$ $\langle P|X\rangle = \frac{1}{\sqrt{2}} |\psi\rangle$ $\langle X|P\rangle = \frac{1}{\sqrt{2}} |\psi\rangle$ $\langle X|P\rangle = \frac{1}{\sqrt{2}} |\psi\rangle$ $\langle P|X\rangle = \frac{1}{\sqrt{2}} |\psi\rangle$
1.4 Temporal Dynamics

Schrödinger Picture (S)

\[ \text{Schrödinger Equation: } \frac{i\hbar}{\partial t} \psi(t) = H \psi(t) \]

- widely used for time-independent, stationary problems
- broad class, many methods possible
- standard picture for construction of observable operators
- using the correspondence principle

\[ H = T + V + \ldots \]

- Hamiltonian operator (i.e., functional of time)
- derived from the total energy and the correspondence principle

\[ E = \frac{P^2}{2m} + V \]

- observables: time-independent
- states: time-dependent

special case: \( H \) time-independent \( \Rightarrow \) \( \psi(t) = \psi(x) e^{-iEt/\hbar} \)

2. There is no one of energy \( E \) associated to it.

- limiting time evolution operator: \( U(t, t_0) \)

Separation ansatz: \[ \psi(x, t) = f(x) T(t) \]

- \( i \hbar \frac{\partial}{\partial t} f(x) T(t) = H(x) f(x) T(t) \)

- eigenfunction to some energy eigenvalue \( E \)
\[ i \hbar \frac{1}{\hbar} \frac{\partial \phi(x)}{\partial t} = \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} \phi(x) = E = \text{const} \]

\[ \text{indep. of } \frac{1}{\hbar} \quad \text{indep. of } t \]

\[ \phi(x) = e^{-i \frac{\hbar}{2m} H_0 x^2} \quad \text{H} \phi(x) = \varepsilon \phi(x) \quad \text{time-independent Schrödinger equation} \]

\[ \psi(x,t)^2 = \phi(x,t)^2 \quad \text{stationary} \]

See Stern-Fertig equipment.

Chapter 5.6. Obs.-lecture

**Heisenberg Picture** \((\mathcal{H})\)

\[ \rightarrow \text{very useful to calculate time-evolution of quantum states in "almost" closed problems} \]

\[ \rightarrow \text{does not involve determination of eigenfunctions of } \mathcal{H} \]

Observables:

\[ A_H(x) = \mathcal{W}(x) A \mathcal{W}^\dagger \]

\[ \mathcal{W}(x) = \exp\left( \frac{i}{\hbar} \mathcal{H} t \right) \quad \text{(number true for } t = \infty) \]

Observables in the Schrödinger picture

4. Heisenberg equation:

\[ \frac{\partial}{\partial t} A_H(t) = \frac{i}{\hbar} \left[ \mathcal{H}_t, A_H(t) \right] \]

\[ \mathcal{H}_t = \mathcal{H}_0 \quad \text{(always!)} \]

States:

\[ |\psi(t)\rangle = \mathcal{W}(x) |\psi(0)\rangle = |\psi(x)\rangle \]

**Interaction Picture** \((\Sigma)\)

\[ \mathcal{H} = H_0 + \delta H(x) \quad \rightarrow \text{For time-dependent problem where the time-dependent part } \delta H(x) \text{ cannot be solved exactly, but leads to "small" effects which can be treated perturbatively.} \]

\[ A_\Sigma(t) = \mathcal{W}(x) A \mathcal{W}^\dagger \quad \rightarrow \text{operator acquires "trivial" time-dependence from } \mathcal{H}_t \]

\[ \psi(x,t)^2 = e^{\frac{i}{\hbar} \left( \mathcal{H}_0 t + \delta H(x) t \right)} \psi(x,0)^2 = \delta H(x) \psi(x,t)^2 \quad \text{(for linear time evolution)} \]

\[ \frac{\partial}{\partial t} A_\Sigma(t) = \frac{i}{\hbar} \left[ H_0, A_\Sigma(t) \right] + \frac{\partial}{\partial t} A_\Sigma(t) \]

\[ \rightarrow \text{Law in action for determining time-dependent processes that are not linear.} \]
1.5. Units

The fundamental constants of universe

\[ h = \frac{\hbar}{\pi} = 6.626 \times 10^{-34} \text{ eV} \cdot \text{s} \quad \text{(reduced Planck constant)} \]

\[ c = 299,792,458 \frac{\text{m}}{\text{s}} \quad \text{(speed of light)} \quad \text{in vacuum} \]

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

Intrinsic connection of the quantities distance, time, energy, momentum, speed, temperature.

1 eV = kinetic energy a particle with one electric elementary charge e (e.g., proton, p+; electron, e−) acquires from when going through a potential difference of 1 V (V^s).

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

2. are unrelated quantities, can be measured using independent conventions

Quantum mechanics: quantum fluctuations and dynamics determined by particles

Energy \times Time (E \cdot t) and Distance \times Momentum (p \cdot x) is units of T:

\[ E = \frac{p^2}{2m} \]

\[ E(x,t) = e^{-\frac{p^2}{2m}} \]

2. We can adopt units such that \([E] = [x]^4, [p] = [x]^3 \rightarrow \text{t} = 1\]

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

2. are unrelated quantities, can be measured using independent conventions

Relativistic physics: speed of light c (in vacuum) universal, independent of relative source

\[ c \text{ is just another form of energy: } E = mc^2 \]

2. We can adopt units such that \([E] = [x]^4, [E] = [u] \rightarrow \text{c} = 1\]


2. "Natural units" \(x + c = 1\) → All quantities can be measured \(\rightarrow\) Simplifies all calculations.

e.g. in units (eV) joule power.
Note 1: One can always recover (unambiguously) the proper powers of $\hbar$ and $c$ in all formulas.

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

Classical mechanics $\rightarrow$ leading order in an expansion in $\hbar$ (for classical systems)

Non-relativistic kinematics $\rightarrow$ leading order in an expansion in $\frac{1}{c}$ (for non-relativistic systems)

2. Classical mechanics, quantized kinematics are "effective theories" of more fundamental and more widely applicable theories.

2. Basic property of an effective theory: One can (in principle) determine all higher order corrections in the expansion parameter (e.g., $c$, $\hbar$, ...)