Theoretical Physics II B – Quantum Mechanics

Lecture 1

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Classical determinism

- Measurements can in principle be performed such that they do not change the state of the system.
- All information can *in principle* be retrieved – measured – simultaneously, and with infinite precision.
- Exact knowledge of state of a system at time t_0 (e.g. for a mass point: its position $\underline{r}$ and momentum $\underline{p}$) yields precise knowledge of the state of the system at any other time (aka Laplace's demon).

Quantum Mechanical probabilities

- Measurements typically will change the dynamical state of a system.
- The uncertainty principle prevents a simultaneous measurement of arbitrary observables with infinite precision.
- Quantum Mechanics (QM) can only predict the probabilities for certain outcomes of a measurement.
- Measurements performed over a statistical ensemble of systems yield averages as outcomes - the **expectation value**.

For this to be realised, QM rests on a number of postulates.

> **Postulate 1:** A wave (state) function can be associated to an ensemble of systems, containing all information that can be known. This function in general is complex, multiplying it with an arbitrary complex number ($\in \mathbf{C}$) does not change its physical significance.

A simple example

- Consider a structureless (= no internal degrees of freedom) single particle in a potential $V(\underline{r})$.
- In classical physics: Can calculate trajectory $\underline{r}(t)$ with arbitrary precision, if $\underline{r}(t_0)$ and $\underline{p}(t_0)$ are exactly known.
- In QM: Have wave function $\psi(\underline{r},\, t)$ in configuration (position) space. It is called *square integrable*, if

$$I = \int \mathrm{d}\underline{r}\, |\psi(\underline{r},\, t)|^2 = \int \mathrm{d}\underline{r}\, \psi^*(\underline{r},\, t)\psi(\underline{r},\, t) = \text{ finite.}$$

- Since a norm can be extracted, can normalise such that $I = 1$. Then $|\psi(\underline{r},\, t)|^2$ is a probability density to find the particle at time t at position $\underline{r}$.
- Note 1: This is invariant under $\psi(\underline{r},\, t) \longrightarrow \psi'(\underline{r},\, t) = e^{i\alpha}\, \psi(\underline{r},\, t)$ (phase invariance)
- Note 2: Generalised for N particles: $\psi = \psi(\underline{r}_1,\, \underline{r}_2,\, \ldots,\, \underline{r}_N,\, t)$.

The superposition principle

Postulate 2: The superposition principle holds true.

- Superposition principle in QM: The state vectors of quantum systems can be written as linear superpositions, i.e. can decompose ψ:

$$\psi(\underline{r},\, t) = c_1\,\psi_1(\underline{r},\, t) + c_2\,\psi_2(\underline{r},\, t)$$

  with constants $c_{1,2} \in \mathbf{C}$ (relative phase matters: calculate $|\psi|^2$!).
- $\psi_{1,2}$ are wave functions for the system to be in states 1 and 2.
- If ψ_1 and ψ_2 are orthogonal

$$\int \mathrm{d}\underline{r}\psi_2^*(\underline{r},\, t)\psi_1(\underline{r},\, t) = \int \mathrm{d}\underline{r}\psi_1^*(\underline{r},\, t)\psi_2(\underline{r},\, t) \stackrel{!}{=} 0$$

  then the probability to measure the system to be in state 1 (2) is proportional to $|c_1|^2$ ($|c_2|^2$).

Momentum space

- Instead of position space can use momentum space for wave-functions:

$$\psi = \psi(\underline{p},\, t)\ :\ \int \mathrm{d}\underline{r} |\psi(\underline{r},\, t)|^2 = 1 \longleftrightarrow \int \mathrm{d}\underline{r} |\psi(\underline{p},\, t)|^2 = 1$$

- In this case $|\psi(\underline{p},\, t)|^2$ is probability density to find system with momentum $\underline{p}$ at time t.
- Relation through Fourier Transform (FT):

$$\psi(\underline{p},\, t) = \frac{1}{\sqrt{(2\pi\hbar)^3}} \int \mathrm{d}\underline{r}\, \exp\left(-\frac{i}{\hbar}\, \underline{p} \cdot \underline{r}\right) \psi(\underline{r},\, t)\,.$$

- Remember: In QM $\boxed{\ \underline{p} = -i\hbar\underline{\nabla}\ }$.

Why state vectors?

- Up to now, used the concept of wave (state) functions as mathematical representations for the state of a system.
- To further analyse properties, need many theorems from the theory of (complex) functions and integral transformations.
- Can formulate these theorems in terminology of vectors and vector calculus. Allows for simple interpretation of many properties of QM in n- or ∞-dimensional vector space.
- Caveat: This vector space is *purely abstract* and has *nothing in common with position space* of three real dimensions.
- However: Will try and represent ideas through sketches in 2-dimensional real space, where possible.

Ket-space as vector space

- Denote vectors by: $|\phi\rangle$, $|\chi\rangle$, $\dots$, $|\uparrow\rangle$, $|\downarrow\rangle$, $\dots$, $|\underline{r}\rangle$, $|\underline{p}\rangle$, $\dots$.
  (use quantum numbers etc. to label them)
- Kets form a *complex vector space $\mathcal{V}$ under addition*,
  if $\forall\,|\phi\rangle, |\chi\rangle, |\psi\rangle, \dots \in \mathcal{V}$ the following properties are fulfilled:
  - Closure: $|\phi\rangle + |\chi\rangle \quad \in \mathcal{V}$.
  - Commutativity: $|\phi\rangle + |\chi\rangle = |\chi\rangle + |\phi\rangle$
  - Associativity: $|(\phi+\chi)\rangle + |\psi\rangle = |\phi\rangle + |(\chi+\psi)\rangle$.
  - Multiplication with a complex number $c \in \mathbf{C}$: $c\,|\phi\rangle = |(c\phi)\rangle$
    is "parallel" with $|\phi\rangle$: $|\phi\rangle \parallel |(c\phi)\rangle$
  - Distributive law: $c\,|(\phi+\chi)\rangle = c\,|\phi\rangle + c\,|\chi\rangle$.
- Introduce a *dual* space $\langle\phi|$, $\langle\chi|$, $\dots$, $\langle\uparrow|$, $\langle\downarrow|$, $\dots$, $\langle\underline{r}|$, $\langle\underline{p}|$, $\dots$
  to define scalar products of vectors: $\langle\phi|\chi\rangle$.

Learning outcomes

- Reminder of classical vs. quantum physics: deterministic vs. probabilistic
- Measurements in classical and quantum physics
- Kets and bras as vectors in a vector space

Control questions

At the end of each lecture, there will be some control questions. Try to solve them as part of your preparation for the next lecture.

1.1 Name the properties of a complex vector space

1.2 With $z = a + bi$, $z^* = a - bi$ and $a, b \in \mathbf{R}$, real numbers, show that

  (a) $zz^* = |z|^2$, with $|z|$ the length of z,
  (b) $z + z^* \in \mathbf{R}$,
  (c) $(z_1 + z_2)^* = z_1^* + z_2^*$,
  (d) $(z_1 z_2)^* = z_1^* z_2^*$,
  (e) $|z_1 z_2| = |z_1||z_2|$.

1.3 When are vectors linearly independent? Are the vectors $|a\rangle = (1 - i,\ 1,\ 0)^T$, $|b\rangle = (1 + i,\ 1,\ 0)^T$ and $|c\rangle = (0,\ 0,\ 1)^T$ linearly independent? What, if $|b\rangle = (1 + i,\ i,\ 0)^T$?