Quantum Mechanics II

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Lecture Notes

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1. Introduction

Whereas standard introductory courses on quantum mechanics typically spend a lot of effort on developing and understanding the theoretical concepts, interpretation and mathematical formalism (often using standard examples such as the harmonic oscillator and the ideal hydrogen atom), quantum mechanics II prepares the ground for real applications. Chapter 2 can be viewed as an introductory chapter on many-body physics which provides the language of many contemporary challenges of modern physics (such as cold quantum gases, mesoscopic systems, nuclear physics).

The techniques for summing angular momentum pave the way for a realistic description of atomic systems where orbital angular momentum and spin coupling are a crucial ingredient for the

spectral properties of atoms and molecules.

Time-dependent perturbation theory (Chapter 4) and scattering theory (chapter 5) give an introduction into concepts that are essential in particle physics. A similar comment applies the chap. 6 on relativistic quantum mechanics, which represents a first attempt to merge quantum physics and relativity (special). (This attempt will not be fully successful; for this quantum field theory will ultimately be required which goes beyond the scope of the present course).

Also the last section on path integrals can be viewed as an introduction into a modern formalism for later use also in particle physics, statistical or many-body physics, i.e. in systems that are dominated by fluctuations. Many of these advanced applications will not be fully visible in this quantum mechanics II course, but the choice of topics and the

theoretical approach chosen here is inspired by these many challenges of contemporary (theoretical) physics.

1.1 Elements of quantum mechanics I

Let us give a brief reminder of the formalism developed in QM I. (No attempt at conceptual completeness is made here; the rest of the section will merely be a reminder or a guide to what you should look up in a textbook if you are not yet familiar with this language).

The <u>state</u> of a physical system is described by a vector, say $|\psi\rangle$, in Hilbert space

$$|\psi\rangle \in \mathcal{H} \,. \tag{1.1}$$

the latter being a generally complex and possibly infinite dimensional vector space. (Eg. for the description of spin-$\frac{1}{2}$ particles (Stern-Gerlach experiment), $|\psi\rangle$ is a 2-dim complex vector; for the description of states in the harmonic oscillator potential, $|\psi\rangle$ corresponds to

an element of the vector space of real square integrable functions). These state vectors are also called "kets". To each element of the ket vector space there exists a dual vector, a "bra" vector, which maps ket vectors into the complex numbers by means of a scalar product; i.e. for a bra vector $\langle \Phi |$ and a ket $|\Psi\rangle$, we have

$$\langle \Phi | \Psi \rangle \in \mathbb{C} \tag{1.2}$$

A postulate of QM is that

$$\langle \Psi | \Psi \rangle > 0 \tag{1.3}$$

(implying that $\langle \Psi | \Psi \rangle \in \mathbb{R}$)

(1.3) implies that (1) physical states are normalizable:

$$|\hat{\Psi}\rangle := \frac{1}{\sqrt{\langle \Psi | \Psi \rangle}} |\Psi\rangle \tag{1.4}$$

$$\Rightarrow \quad \langle \hat{\Psi} | \hat{\Psi} \rangle = 1 ,$$

and that (2) the metric on the space of physical states is positive definite.

Mappings of kets onto kets are called operators

$$|\psi\rangle \xrightarrow{A} |\phi\rangle = A|\psi\rangle \equiv |A\psi\rangle \tag{1.5}$$

A mapping in the ket space induces a similar mapping in bra space. The associated operator is called the adjoint of A: $A^\dagger$,

$$\langle\psi| \xrightarrow{A^\dagger} \langle\phi| = \langle\psi|A^\dagger \equiv \langle A\psi| . \tag{1.6}$$

Physical observables such as position, momentum, angular momentum, etc. are associated with self-adjoint (hermitean*) operators, satisfying

$$A = A^\dagger \tag{1.7}$$

A ket $|a'\rangle$ satisfying

$$A|a'\rangle = a'|a'\rangle \quad \text{with } a' \in \mathbb{C} \text{ or } \mathbb{R} \tag{1.8}$$

is called eigenket of A with eigenvalue a'.

Eigenvalues of hermitean operators are real

$$a' \in \mathbb{R} \quad \text{if} \quad A = A^\dagger \tag{1.9}$$

In principle, the properties of being self-adjoint and hermitean need not be the same. They can be the same if the domain of validity/definition satisfies suitable properties. In this course, we ignore possible differences.

which corresponds to the fact that measurements of physical observables result in <u>real</u> numbers.

The associated eigenkets are orthogonal

$$\langle a' | a'' \rangle = \delta_{a'a''} \tag{1.10}$$

(or in the case of degeneracy, i.e. two or more eigenvalues being identical, can be orthogonalized to satisfy (1.10)).

If A acts on the complete Hilbert space of a given problem, the eigenkets are also complete:

$$\sum_{a'} |a'\rangle\langle a'| = \mathbb{1}. \tag{1.11}$$

Here, we used the notion of an exterior product of bras and kets $|a'\rangle\langle a'|$ which forms an operator itself. This operator

$$P_{a'} = |a'\rangle\langle a'| \tag{1.12}$$

can be viewed as a projection operator, satisfying

$$P_{a'}^2 = P_{a'}$$

$$P_{a'} P_{a''} = \delta_{a'a''} P_{a'} \tag{1.13}$$

$$\sum_{a'} P_{a'} = \mathbb{1}$$

provided that $|a'\rangle$, $|a''\rangle$, etc. are normalized.

Dynamics: if a system is in a state $|\psi, t_0\rangle$ at a time t_0, it evolves into a state $|\psi, t\rangle$ at $t > t_0$ by means of the time evolution operator

$$U(t, t_0): \tag{1.14}$$

$$|\psi, t\rangle = U(t, t_0)\,|\psi, t_0\rangle ,$$

that satisfies

(1) unitarity $\quad U^+ = U^{-1}$

(2) identity $\quad U(t_0, t_0) = \mathbb{1}$

(3) group multiplication $\quad U(t_2, t_1)\,U(t_1, t_0) = U(t_2, t_0)$

(4) Schrödinger's equation

$$i\hbar\,\underbrace{\partial_t}_{\equiv \frac{\partial}{\partial t}}\,U(t, t_0) = H\,U(t, t_0) , \tag{1.15}$$

where H denotes the Hamilton-Operator of a system. Specifying H defines a system and its time evolution.

If H is time-independent, (1.15) is solved by

$$U(t, t_0) = e^{-\frac{i}{\hbar} H (t - t_0)} \tag{1.16}$$

The Schrödinger equation for $\mathcal{U}$ can also be rewritten in terms of the dynamics of a state

$$i\hbar\, \partial_t |\psi, t\rangle = H |\psi, t\rangle \tag{1.17}$$

(all these formulas apply to the "Schrödinger picture" where states are time-dependent and operators are time-independent; a "vice-versa" formulation in terms of the "Heisenberg picture" is alternatively possible).

An eigenket of the Hamiltonian

$$H |\psi_n\rangle = E_n |\psi_n\rangle \tag{1.18}$$

with energy eigenvalue E_n is called a stationary state, as it evolves in time with a pure phase

$$|\psi_n, t\rangle = e^{-\frac{i}{\hbar} E_n (t - t_0)} |\psi_n, t_0\rangle \tag{1.19}$$

Measurement process:

In contrast to classical physics, a quantum mechanical measurement process does not ignore the backreaction of

this process onto the system, but is rather defined in terms of this back-reaction:

Measuring a state $|\psi\rangle$ by means of an observable A "throws" the system into an eigenstate of A:

$$|\psi\rangle \xrightarrow[A]{\text{measurement}} |a'\rangle \tag{1.20}$$

The value of the measurement thus is a'.

As the eigenbasis of A is complete (and) we assume it to be orthonormalized $\mathbb{1} = \sum_{|a'} |a'\rangle\langle a'|$, we can span $|\psi\rangle$ in terms of this basis:

$$|\psi\rangle = \mathbb{1}\,|\psi\rangle = \sum_{a'} |a'\rangle\langle a'|\psi\rangle$$

$$= \sum_{a'} c_{a'}\,|a'\rangle \quad , \; c_{a'} = \langle a'|\psi\rangle \tag{1.21}$$

The "coordinate" $c_{a'}$ of $|\psi\rangle$ along the $|a'\rangle$ direction in Hilbert space generally is $\in \mathbb{C}$.

Postulate (Born's rule): the probability to measure $|\psi\rangle$ in the state $|a'\rangle$ (i.e. to measure the value a' for the observable A) is given by

$$|C_{a'}|^2 = |\langle a'|\psi\rangle|^2 \tag{1.22}$$

(for $|a'\rangle$ and $|\psi\rangle$ being normalized.)

Hence, strictly speaking, physical states are fully characterized not by vectors in Hilbert space, but already by "rays" in Hilbert space, i.e.,

$$|\psi\rangle \text{ and } |\phi\rangle = c\cdot|\psi\rangle \text{ with } c\in\mathbb{C} \tag{1.23}$$

characterize the same physical state.

The fact that a measurement of A throws the system into an eigenstate of A has important consequences: simultaneous (i.e. sharp and persistent) measurements of observables are only possible, if observables $A, B, \ldots$ are <u>compatible</u>, i.e. commute

$$[A,B] = AB - BA = 0 \tag{1.24}$$

Incompatible observables $[A,B]\neq 0$ cannot be measured simultaneously. Their measurement values satisfy an <u>uncertainty principle</u>

$$(\Delta A)^2\,(\Delta B)^2 \geq \frac{1}{4}\,|\langle[A,B]\rangle|^2 \tag{1.25}$$

Here $\langle (\ldots) \rangle$ denotes the expectation value (mean measured value) of an observable $(\ldots)$ with respect to a certain state

$$\langle (\ldots) \rangle_\psi = \langle \psi | (\ldots) | \psi \rangle \tag{1.26}$$

Coordinate (Position) & Momentum space

We associate an operator $\vec{x}$ (a vector operator $(x_1, x_2, x_3)^T$) with the position observable of a particle. As a physical observable, we have

$$x_i^+ = x_i \,, \tag{1.27}$$

and the associated eigenkets form a complete orthonormalizable basis. As the eigenvalues can acquire continuous values, the orthogonality and completeness relations now read

$$\langle \vec{x}' | \vec{x}'' \rangle = \delta^{(3)}(\vec{x}' - \vec{x}'')$$

$$\mathbb{1} = \int d^3\vec{x}' \; | \vec{x}' \rangle \langle \vec{x}' | \tag{1.28}$$

The eigenvalue/vector equation reads

$$\vec{x} \, | \vec{x}' \rangle = \vec{x}' \, | \vec{x}' \rangle \,, \tag{1.29}$$

implying that each position of a particle in space

is associated with a different state. Using the completeness of these position states, we can span a general ket $|\psi\rangle$ with these base vectors:

$$|\psi\rangle = \mathbb{1}\,|\psi\rangle = \int d^3x' \; |\vec{x}'\rangle \underbrace{\langle \vec{x}' | \psi \rangle}_{=: \psi(\vec{x}')}$$

$$= \int d^3x' \; \psi(\vec{x}') \; |\vec{x}'\rangle \qquad (1.30)$$

The "coordinates" $\psi(\vec{x})$ of the state $|\psi\rangle$ with respect to the position basis $|\vec{x}\rangle$ is called the wave function in coordinate space. Provided that $|\psi\rangle$ and $|\vec{x}'\rangle$ are properly normalized,

$|\psi(\vec{x}')|^2$ is a measure for the probability to detect the particle at $\vec{x}'$ in position space. (More properly: $|\psi(\vec{x}')|^2 d^3x'$ is a measure to detect the particle in a volume d^3x' attached to the point $\vec{x}'$).

Similar properties hold for the momentum operator $\vec{p}$

$$p_i^{\dagger} = p_i \quad \text{(hermitean)} \qquad (1.31)$$

momentum basis:

$$\vec{p}\,|\vec{p}'\rangle = \vec{p}'\,|\vec{p}'\rangle$$

$$\langle\vec{p}'|\vec{p}''\rangle = \delta^{(3)}(\vec{p}'-\vec{p}'') \qquad (1.32)$$

$$\mathbb{1} = \int d^3p' \; |\vec{p}'\rangle\langle\vec{p}'|$$

A fundamental property of QM is that the position and momentum operators are generally incompatible.

$$[x_i, p_j] = i\hbar\,\delta_{ij} \qquad (1.33)$$

Postulating (1.33) for a Hamiltonian system is often referred to as "quantizing" the system.

As a consequence, in a basis where x_i is diagonal (position basis), p_i cannot be diagonal. Instead p_i in such a basis can be represented by a derivative operator:

$$p_i = -\frac{i}{\hbar}\frac{\partial}{\partial x_i} \equiv -\frac{i}{\hbar}\partial_i \qquad (1.34)$$

For one-particle systems with a Hamiltonian of the form

$$H = \frac{p^2}{2m} + V(\vec{x}) \qquad (1.35)$$

(QM particle in a potential),

the Schrödinger equation (1.17)

$$i\hbar\, \partial_t |\psi, t\rangle = H |\psi, t\rangle$$

in position space then becomes

$$\langle \vec{x}' | i\hbar\, \partial_t |\psi, t\rangle = \langle \vec{x}' | H | \psi, t\rangle$$

$$\Rightarrow i\hbar\, \partial_t \psi(\vec{x}, t) = -\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi(\vec{x}, t) + V(\vec{x})\, \psi(\vec{x}, t) \qquad (1.36)$$

a partial differential equation for the wave function $\psi(\vec{x}, t)$ in position space. This was to a large extent subject to the QM I course.