Part IB — Quantum Mechanics

Definitions

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These notes are not endorsed by the lecturers, and I have modified them (often significantly) after lectures. They are nowhere near accurate representations of what was actually lectured, and in particular, all errors are almost surely mine.

Physical background
Photoelectric effect. Electrons in atoms and line spectra. Particle diffraction. [1]

Schrödinger equation and solutions

Observables and expectation values
Position and momentum operators and expectation values. Canonical commutation relations. Uncertainty principle. [2]
Observables and Hermitian operators. Eigenvalues and eigenfunctions. Formula for expectation value. [2]

Hydrogen atom
Spherically symmetric wave functions for spherical well and hydrogen atom.
Orbital angular momentum operators. General solution of hydrogen atom. [5]
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0 Introduction

0.1 Light quanta

0.2 Bohr model of the atom

0.3 Matter waves
1 Wavefunctions and the Schrödinger equation

1.1 Particle state and probability

1.2 Operators

Definition (Time-independent Schrödinger equation). The time-independent Schrödinger equation is the energy eigenvalue equation

\[ H\psi = E\psi, \]

or

\[-\frac{\hbar^2}{2m} \psi'' + V(x)\psi = E\psi.\]

1.3 Time evolution of wavefunctions

Definition (Time-dependent Schrödinger equation). For a time-dependent wavefunction \( \Psi(x,t) \), the time-dependent Schrödinger equation is

\[ i\hbar \frac{\partial \Psi}{\partial t} = H\Psi. \]

Definition (Stationary state). A stationary state is a state of the form

\[ \Psi(x,t) = \psi(x) \exp \left( -\frac{iEt}{\hbar} \right). \]

where \( \psi(x) \) is an eigenfunction of the Hamiltonian with eigenvalue \( E \). This term is also sometimes applied to \( \psi \) instead.
2 Some examples in one dimension

2.1 Introduction

2.2 Infinite well — particle in a box

2.3 Parity

2.4 Potential well

2.5 The harmonic oscillator


3 Expectation and uncertainty

3.1 Inner products and expectation values

**Definition** (Inner product). Let \( \psi(x) \) and \( \phi(x) \) be normalizable wavefunctions at some fixed time (not necessarily stationary states). We define the complex inner product by

\[
(\phi, \psi) = \int_{-\infty}^{\infty} \phi(x)^* \psi(x) \, dx.
\]

**Definition** (Norm). The norm of a wavefunction \( \psi \), written, \( \| \psi \| \) is defined by

\[
\| \psi \|^2 = (\psi, \psi) = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx.
\]

**Definition** (Expectation value). The expectation value of any observable \( H \) on the state \( \psi \) is

\[
\langle H \rangle_{\psi} = (\psi, H \psi).
\]

**Definition** (Uncertainty). The uncertainty in position \( (\Delta x)_{\psi} \) and momentum \( (\Delta p)_{\psi} \) are defined by

\[
(\Delta x)^2_{\psi} = \langle (\hat{x} - \langle \hat{x} \rangle_{\psi})^2 \rangle_{\psi} = \langle \hat{x}^2 \rangle_{\psi} - \langle \hat{x} \rangle^2_{\psi},
\]

with exactly the same expression for momentum:

\[
(\Delta p)^2_{\psi} = \langle (\hat{p} - \langle \hat{p} \rangle_{\psi})^2 \rangle_{\psi} = \langle \hat{p}^2 \rangle_{\psi} - \langle \hat{p} \rangle^2_{\psi},
\]

**Definition** (Hermitian operator). An operator \( Q \) is Hermitian iff for all normalizable \( \phi, \psi \), we have

\[
(\phi, Q \psi) = (Q \phi, \psi).
\]

In other words, we have

\[
\int \phi^* Q \psi \, dx = \int (Q \phi)^* \psi \, dx.
\]

3.2 Ehrenfest’s theorem

3.3 Heisenberg’s uncertainty principle

**Definition** (Commutator). Let \( Q \) and \( S \) be operators. Then the commutator is denoted and defined by

\[
\left[ Q, S \right] = QS - SQ.
\]

This is a measure of the lack of commutativity of the two operators.

In particular, the commutator of position and momentum is

\[
[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar.
\]
4 More results in one dimensions

4.1 Gaussian wavepackets

**Definition** (Wavepacket). A wavefunction localised in space (about some point, on some scale) is usually called a wavepacket.

**Definition** (Gaussian wavepacket). A Gaussian wavepacket is given by

\[ \psi_0(x,t) = \left( \frac{\alpha}{\pi} \right)^{1/4} \frac{1}{\gamma(t)^{1/2}} e^{-x^2/2\gamma(t)}, \]

for some \( \gamma(t) \).

4.2 Scattering

4.3 Potential step

4.4 Potential barrier

4.5 General features of stationary states

**Definition** (Ground and excited states). The lowest energy eigenstate is called the ground state. Eigenstates with higher energies are called excited states.
5 Axioms for quantum mechanics

5.1 States and observables

5.2 Measurements

5.3 Evolution in time

5.4 Discrete and continuous spectra

5.5 Degeneracy and simultaneous measurements

Definition (Degeneracy). For any observable $Q$, the number of linearly independent eigenstates with eigenvalue $\lambda$ is the degeneracy of the eigenvalue. In other words, the degeneracy is the dimension of the eigenspace

$$V_\lambda = \{ \psi : Q\psi = \lambda \psi \}.$$

An eigenvalue is non-degenerate if the degeneracy is exactly 1, and is degenerate if the degeneracy is more than 1.

We say two states are degenerate if they have the same eigenvalue.
6 Quantum mechanics in three dimensions

6.1 Introduction

Definition (Structureless particle). A structureless particle is one for which all observables can be written in terms of position and momentum.

6.2 Separable eigenstate solutions

6.3 Angular momentum

Definition (Angular momentum). The angular momentum is a vector of operators

\[ \mathbf{L} = \mathbf{x} \wedge \mathbf{p} = -i\hbar \mathbf{x} \wedge \nabla. \]

In components, this is given by

\[ L_i = \varepsilon_{ijk} \hat{x}_j \hat{p}_k = -i\hbar \varepsilon_{ijk} x_j \frac{\partial}{\partial x_k}. \]

For example, we have

\[ L_3 = \hat{x}_1 \hat{p}_2 - \hat{x}_2 \hat{p}_1 = -i\hbar \left( x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1} \right). \]

Definition (Total angular momentum). The total angular momentum operator is

\[ \mathbf{L}^2 = L_i L_i = L_1^2 + L_2^2 + L_3^2. \]

6.4 Joint eigenstates for a spherically symmetric potential
7 The hydrogen atom

7.1 Introduction
7.2 General solution
7.3 Comments