Part IB — Quantum Mechanics
Definitions

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

Schrödinger equation and solutions
De Broglie waves. Schrödinger equation. Superposition principle. Probability interpretation, density and current. [2]

Stationary states. Free particle, Gaussian wave packet. Motion in 1-dimensional potentials, parity. Potential step, square well and barrier. Harmonic oscillator. [4]

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]

Contents

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

$$i\hbar\frac{\partial \Psi}{\partial t} = H\Psi. \tag{$*$}$$

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 ψ 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

$$(\phi, \psi) = \int_{-\infty}^{\infty} \phi(x)^* \psi(x)\ \mathrm{d}x.$$

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

$$\|\psi\|^2 = (\psi, \psi) = \int_{-\infty}^{\infty} |\psi(x)|^2\ \mathrm{d}x.$$

Definition (Expectation value)**.** The *expectation value* of any observable H on the state ψ 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 ϕ, ψ, we have

$$(\phi, Q\psi) = (Q\phi, \psi).$$

In other words, we have

$$\int \phi^* Q\psi\ \mathrm{d}x = \int (Q\phi)^*\psi\ \mathrm{d}x.$$

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

$$[Q, S] = QS - SQ.$$

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 λ 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

$$\mathbf{L} = \hat{\mathbf{x}} \wedge \hat{\mathbf{p}} = -i\hbar \mathbf{x} \wedge \nabla.$$

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

$$\mathbf{L}^2 = L_i L_i = L_1^2 + L_2^2 + L_3^3.$$

6.4 Joint eigenstates for a spherically symmetric potential

7 The hydrogen atom

7.1 Introduction

7.2 General solution

7.3 Comments