

Quantum Mechanics

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Chapter 1

Key Features of Quantum Mechanics

1.1 How it all started

It all started with Max Planck who was trying to understand the black body radiation spectrum. He guessed what the formula for the radiation spectrum was and worked backwards and found the astonishing consequence that the energy of electromagnetic waves were quantized, that is for a given frequency the energy could only have the values $E_n = nh\nu = n\hbar\omega$ where h is Planck's constant and $\hbar = \frac{h}{2\pi}$.

The next to contribute to the theory about electromagnetic waves was Albert Einstein who studied the photo electric effect and explained the observed results by suggesting that the electromagnetic wave consists of particles each having the energy $h\nu$.

It was hard for many physicists to accept the theory, but several years later Arthur Compton made an experiment with x-ray scattering and showed that the results could only be explained by assuming the x-rays being particles with momentum $p = \frac{h\nu}{c}$. This convinced the physicists that the electromagnetic waves really behaved as particles and it led Louis de Broglie to suggest that particles in some situations should be viewed as "matter waves" with energy $E = h\nu$ and momentum $p = \frac{h\nu}{c} = \frac{h}{\lambda}$:

$$\Psi(x, t) = e^{i(kx - \omega t)}$$

where $\hbar k = p$ and $\hbar\omega = E$

The interpretation of the wavefunction is difficult, but after the introduction of the Schrödinger equation it becomes more clear.

1.2 The Schrödinger equation for the free particle

Erwin Schrödinger developed a differential equation with the "matter wave" as a solution. He first suggested the momentum operator:

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

Inserting the wave $\Psi(x, t)$ gives:

$$\hat{p}\Psi(x, t) = \frac{\hbar}{i}(ik)\Psi(x, t) = \hbar k\Psi(x, t) = p\Psi(x, t)$$

Since the operator \hat{p} has the momentum as eigenvalue it is called the momentum operator. Differentiating the wavefunction with respect to time gives:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = i\hbar(-i\omega)\Psi(x, t) = \hbar\omega\Psi(x, t) = E\Psi(x, t)$$

Inserting the non-relativistic expression for the kinetic energy we have:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = \frac{p^2}{2m}\Psi(x, t)$$

By using the expression for the momentum operator we get:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = \frac{1}{2m} \frac{\hbar}{i} \frac{\partial}{\partial x} \frac{\hbar}{i} \frac{\partial \Psi(x, t)}{\partial x} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2}$$

The Schrödinger equation for the free particle is thus:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2}$$

or

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = \hat{H}\Psi(x, t)$$

where \hat{H} is called the energy operator or hamiltonian operator.

By inserting the expression for the wavefunction we get:

$$\hbar\omega = \frac{\hbar^2 k^2}{2m}$$

as expected.

Since the Schrödinger equation is linear the complete solution can be written as a superposition of "matter waves":

$$\Psi(x, t) = \int_{-\infty}^{\infty} \Phi(k) e^{i(kx - \omega t)}$$

Note that $\Phi(k)$ can be complex and that $\Psi(x, t)$ in general is complex.

We now turn to the interpretation of this formula.

1.3 It makes sense

Max Born suggested that the solution to the Schrödinger equation should be interpreted as a probability function where $|\Phi(k)|^2 dk$ is the probability of finding the particle with energy $E = \hbar\omega = \frac{\hbar^2 k^2}{2m}$ and the momentum in the interval $[k, k + dk]$. $|\Psi(x, t)|^2 dx$ is the probability of finding the particle in the interval $[x, x + dx]$

This makes sense if:

$$\int_{-\infty}^{\infty} \Psi(x, t) \Psi^*(x, t) dx = 1$$

since the sum of probabilities should sum up to 1.

The integral can be shown to be finite if $\Psi(x, t)$ vanish for $x \rightarrow \pm\infty$ and $\frac{\partial \Psi}{\partial x}$ is bounded for

$x \rightarrow \pm\infty$ and the wavefunction can thus be normalized. It is not necessary to normalise if we are only interested in e.g. the energy.

Note that it is meaningless to talk about the probability of finding the particle at a specific location or of a specific momentum, but this is no different from other continuous probability functions.

If $\Phi(k)$ only has a significant value in an interval Δk around k_0 $\Psi(x, t)$ becomes a wave packet and the location x can be known with an uncertainty of Δx and it can be shown that:

$$\Delta k \Delta x > 1/2$$

or

$$\Delta p \Delta x > \hbar/2$$

This is the Heisenberg uncertainty principle.

It can be shown that the wave packet travels with the group velocity $\frac{p}{m}$ as expected. Note that the wave packet will smear with time.

1.4 The Schrödinger equation with a potential

If the particle is moving in a potential the Schrödinger equation becomes:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) \right) \Psi(x, t)$$

and the hamiltonian operator is given by:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t)$$

The Schrödinger equation can thus again be written:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = \hat{H} \Psi(x, t)$$

There is no general solution to this problem, but since the \hat{H} operator can be shown to be hermitian, see below, the solution is a superposition of the eigenfunctions. For some potentials a solution can be found, see the chapter about stationary states.

1.5 Probability current

The Schrödinger equation is first order in time. This means if a solution is known at time $t = 0$ the solution at later times can be calculated by integration.

As mentioned above the wave equation can be normalized if it vanishes at infinity and moreover it is shown below that the normalization factor is independent of time, that is if:

$$\int_{-\infty}^{\infty} \Psi(x, 0) \Psi^*(x, 0) dx = 1$$

then:

$$\int_{-\infty}^{\infty} \Psi(x, t) \Psi^*(x, t) dx = 1$$

for all t

Let:

$$\rho(x, t) = \int_{-\infty}^{\infty} \Psi(x, t) \Psi^*(x, t) dx$$

then

$$\frac{\partial \rho(x, t)}{\partial t} = \frac{\partial}{\partial t} \int_{-\infty}^{\infty} \Psi(x, t) \Psi^*(x, t) dx = \frac{i}{\hbar} ((\hat{H}\Psi)^* \Psi - \Psi^* (\hat{H}\Psi) + V(x, t) \Psi \Psi^* - \Psi^* V(x, t) \Psi)$$

The contribution from the potential cancel and we have:

$$\frac{\partial \rho(x, t)}{\partial t} = \frac{i}{\hbar} ((\hat{H}\Psi)^* \Psi - \Psi^* (\hat{H}\Psi)) = \frac{\hbar}{2im} \left(\frac{\partial^2 \Psi^*}{\partial x^2} \Psi - \Psi^* \frac{\partial^2 \Psi}{\partial x^2} \right) = -\frac{\partial}{\partial x} \left[\frac{\hbar}{m} \text{Im}(\Psi^* \frac{\partial \Psi}{\partial x}) \right] = \frac{\partial J(x, t)}{\partial x}$$

J is called the probability current and we have:

$$\frac{\partial \rho(x, t)}{\partial x} + \frac{\partial J(x, t)}{\partial x} = 0$$

We now have:

$$\int_{-\infty}^{\infty} \frac{\partial \rho(x, t)}{\partial t} dx = - \int_{-\infty}^{\infty} \frac{\partial J}{\partial x} dx = -J(\infty, t) + J(-\infty, t) = 0$$

since Ψ vanish and $\frac{\partial \psi}{\partial x}$ is limited, showing that the normalizations factor is independent of t .

1.6 Momentum space

As seen above the solution to the Schrödinger equation for a free particle can be written:

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{ikx} dk$$

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(k) e^{ikx} dx$$

Since $\hbar k = p$ we have

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p) e^{ipx/\hbar} dp$$

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) e^{ipx/\hbar} dx$$

Note the symmetry.

1.7 A few words about operators

Linear operators can be added and multiplied:

$$\begin{aligned}(\hat{A} + \hat{B})\phi &= \hat{A}\phi + \hat{B}\phi \\ \hat{A}(\hat{B}\hat{C}) &= (\hat{A}\hat{B})\hat{C} = \hat{A}\hat{B}\hat{C}\end{aligned}$$

But in general the commutative law does not hold:

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}$$

The difference being the commutator of the two operators:

$$[\hat{A}; \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$$

Note that for the \hat{x} operator and the \hat{p} operator we have for arbitrary $\phi(x)$:

$$[\hat{x}; \hat{p}]\phi(x) = i\hbar\phi(x)$$

I am not sure what this means but it can be used to prove the Heisenberg uncertainty principle. An operator is called Hermitian if for arbitrary functions:

$$\int_{-\infty}^{\infty} (\hat{H}\Psi_1)^*\Psi_2 = \int_{-\infty}^{\infty} (\Psi_1^*(\hat{H}\Psi_2))$$

The Hermitian conjugate is defined by:

$$\int_{-\infty}^{\infty} (\Psi_1^*(\hat{T}\Psi_2)) = \int_{-\infty}^{\infty} (\hat{T}^\dagger\Psi_1)^*\Psi_2$$

An operator is Hermitian if:

$$T^\dagger = T$$

The distributive law is as follows:

$$\begin{aligned}[A; BC] &= [A; B]C + B[A; C] \\ [AB; C] &= A[B; C]C + [A; C]B \\ [A; [B; C]] + [B; [C; A]] + [C; [A; B]] &= 0\end{aligned}$$

1.8 Expectation values of operators

The expected value of a random variable Q is:

$$\langle Q \rangle = \sum_{i=1}^n Q_i p_i$$

It can be shown that the expected value of \hat{p} is:

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \hat{p} \Psi(x, t) dx$$

where:

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

This motivates the formula for any operator \hat{Q} : The expected value of an operator \hat{Q} is:

$$\langle \hat{Q} \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \hat{Q} \Psi(x, t) dx$$

Derivative of expected value:

$$i\hbar \frac{d}{dt} \langle \hat{Q} \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \hat{Q} \Psi(x, t) dx$$

Since H is hermitian we have Ehrenfests formula:

$$i\hbar \frac{d}{dt} \langle \hat{Q} \rangle = \langle [\hat{Q}; \hat{H}] \rangle$$

1.9 Observables and hermitian operators

If \hat{Q} is a hermitian operator then:

1. The expected value of \hat{Q} is real.
2. The eigenvalues of \hat{Q} are real.
3. The eigenfunctions of \hat{Q} can be organized to satisfy orthonormality.
4. The eigenfunctions of \hat{Q} form a complete set of basis functions.

$$\Psi(x) = \alpha_1 \psi_1(x) + \alpha_2 \psi_2(x) + \dots = \sum \alpha_i \psi_i(x)$$

If we know the eigenfunctions then:

$$\alpha_i = \int \psi_i^*(x) \Psi(x) dx$$

5. Postulate: If we measure a hermitian operator in the state Ψ , then the possible outcomes for the measurement are the eigenvalues q_1, q_2, \dots . The probability p_i to measure q_i is given by:

$$p_i = |a_i|^2$$

where

$$\Psi(x) = \sum a_i \psi_i(x)$$

After the outcome q_i , the state of the system becomes

$$\Psi(x) = \psi_i(x)$$

This is called the collapse of the wave function. The postulate follows the Copenhagen interpretation of quantum mechanics.

1.10 Uncertainty

If Q is a discrete random variable (similar for continuous) then:

$$\bar{Q} = \sum_i p_i Q_i$$

$$(\Delta Q)^2 = \sum_i p_i (Q_i - \bar{Q})^2 = \overline{Q^2} - \bar{Q}^2$$

For hermitian operators we have:

$$(\Delta \hat{Q})^2 = \langle \hat{Q}^2 \rangle - \langle \hat{Q} \rangle^2$$

giving

$$(\Delta \hat{Q})^2 = \langle (\hat{Q} - \langle \hat{Q} \rangle)^2 \rangle$$

$$(\Delta \hat{Q})^2 = \int_{-\infty}^{\infty} |(\hat{Q} - \langle \hat{Q} \rangle)\psi(x)|^2 dx$$

$$\Delta Q = 0 \iff \Psi \text{ is an eigenstate of } \hat{Q}$$

Chapter 2

Time-independent Schrödinger equation

2.1 Stationary states

Recall the Schrödinger equation:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) \right) \Psi(x, t) = \hat{H} \Psi(x, t)$$

In order to solve partial differential equations it is often useful to try to separate the variables. If possible this will reduce the problem to the solution of ordinary differential equations. The states are called stationary since the observables have no time dependencies.

The wavefunction is written:

$$\Psi(x, t) = g(t)\psi(x)$$

By inserting into the Schrödinger equation we have:

$$i\hbar \frac{\partial g(t)}{\partial t} \psi(x) = g(t) \hat{H} \psi(x)$$

or

$$i\hbar \frac{1}{g(t)} \frac{dg(t)}{dt} = \frac{1}{\psi(x)} \hat{H} \psi(x)$$

Since the left hand side only depends on t and the right hand side only depends on x they must be equal to a constant E . The left hand side now becomes:

$$i\hbar \frac{dg(t)}{dt} = E g(t)$$

The solution is:

$$g(t) = C e^{-iEt/\hbar}$$

where C is an arbitrary constant.

The right hand side reads:

$$\hat{H} \psi(x) = E \psi(x)$$

and we now have the time-independent Schrödinger equation:

$$\hat{H} \psi(x) = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x, t) \right) \psi(x) = E \psi(x)$$

E is real because it is the eigenvalue of the hermitian operator \hat{H} . For a solution to be acceptable we must require:

$$\int_{-\infty}^{\infty} \psi(x)\psi^*(x)dx = 1$$

Since the stationary state is an eigenstate of \hat{H} , the uncertainty $\Delta\hat{H}$ is zero.

1. The expected value of any time-independent operator \hat{Q} on a stationary state Ψ is time-independent
2. The superposition of stationary states with different energies are not stationary.

2.1.1 Solving for energy eigenstates

The eigenstates may be discrete or fall in continuous bands. They form a complete set of orthonormal functions:

$$\int \psi_i(x)^*\psi_j(x)dx = \delta_{ij}$$

There are indeed many solutions for a given potential. For the potential we only consider:

1. Continuous.
2. Piecewise continuous.
3. May contain delta functions in one dimension.
4. May become infinite beyond certain points, hard wall.
5. May fail to be bounded.
6. May not contain powers or derivatives of delta functions.

This leads to the following restrictions on the wavefunction:

1. ϕ , ϕ' and ϕ'' are all continuous.
2. ϕ , ϕ' are continuous and ϕ'' has finite discontinuities.
3. ϕ is continuous, ϕ' has finite discontinuities and ϕ'' contains delta functions.

2.2 Free particle on a circle

2.3 The infinite square well

In this case the potential is defined by:

$$V(x) = \begin{cases} 0, & 0 \leq x \leq a \\ \infty, & x < 0, x > a \end{cases}$$

and the Schrödinger equation becomes:

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

where $x \in [0, a]$

The wavefunction vanishes for $x \leq 0$ and $x \geq a$.

For $x > 0$ and $x < a$ the wavefunction is given by:

$$\psi(x) = c_1 \cos(kx) + c_2 \sin(kx)$$

Due to boundary conditions $c_1 = 0$ $c_2 = \sqrt{\frac{2}{a}}$ and $k = \frac{n\pi}{a}$, $n = 1, 2, \dots$

$$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

2.4 The finite square well

In this case the potential is defined by:

$$V(x) = \begin{cases} -V_0, & \text{for } |x| \leq a \\ 0, & \text{for } |x| > a \end{cases}$$

If $E < -V_0$ we are in an impossible situation.

If $E > 0$ we get reflections, see later.

If $-V_0 < E < 0$:

It is known that for a symmetrical potential the bound states are either even or odd.

Even solutions We must study the differential equation in two regions.

$|x| < a$

The Schrödinger equation becomes:

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(V_0 - |E|)\psi$$

where $x \in [-a, a]$

Since $V_0 - |E| > 0$ we can define a real k :

$$k^2 = \frac{2m}{\hbar^2}(V_0 - |E|) > 0$$

The solution becomes:

$$\psi(x) = \cos(kx)$$

$|x| > a$ The Schrödinger equation becomes:

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}|E|\psi$$

Since the right hand side is positive a real κ :

$$\kappa^2 = \frac{2m|E|}{\hbar^2}$$

and the solution becomes:

$$\psi(x) = Ae^{-\kappa x}$$

Due to boundary conditions:

$$k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2}$$

By introducing unit free variables, a good thing to do in general, we have

$$\eta \equiv ka > 0$$

$$\xi \equiv \kappa a > 0$$

$$z_0^2 \equiv \frac{2mV_0 a^2}{\hbar^2}$$

$$\eta^2 + \xi^2 = z_0^2, \quad \xi = \eta \tan \eta$$

Odd solutions The wavefunction is now on the form:

$$\psi(x) = \begin{cases} \sin kx, & |x| < a \\ Ae^{-k|x|}, & |x| > a \end{cases}$$
$$\eta^2 + \xi^2 = z_0^2, \quad \xi = -\eta \cot \eta$$

2.5 General properties

2.5.1 Real potentials

1. For a one-dimensional potential there are no degenerate bound states.
2. If the potential is real ψ can be chosen to be real.
3. Any bound state $\psi(x)$ of a one-dimensional potential is real, up to an overall constant phase.
4. if $V(-x) = V(x)$, the energy eigenstates can be chosen to be either even or odd.
5. If $V(-x) = -V(x)$ there is not much to say.

2.6 Bound states in slowly varying potentials

You better read the lecture notes.

2.7 Sketching wavefunction

You better read the lecture notes.

2.8 Shooting method

This is a method for numerical solution of the Schrödinger equation.

1. You have to be aware of the boundary conditions.
2. Start with an arbitrary value of the energy, if it diverges change the energy.

2.9 Delta function potential

The potential is given by:

$$V(x) = -\alpha\delta(x)$$

The solution is:

$$\psi(x) = e^{-\kappa|x|}$$
$$\kappa = \frac{m\alpha}{\hbar^2}$$

The form of $\psi(x)$ is as expected looking at the square well for $V_0 \rightarrow \infty$ and $a \rightarrow 0$

2.10 The node theorem

For a potential $V(x)$ where $V(x) \rightarrow \infty$ for $x \rightarrow \infty$ we have a number of bound states $\psi_1, \psi_2, \psi_3, \dots$. The number of nodes of ψ_n is $n - 1$.

2.11 Harmonic oscillator

2.11.1 First method

For the classical harmonic oscillator we have:

$$E_{tot} = \frac{1}{2}mv^2 + \frac{1}{2}kx^2$$

The particle will perform an oscillatory motion with frequency:

$$\omega = \sqrt{\frac{k}{m}} \rightarrow k = m\omega^2$$

This leads to the definition of the quantum harmonic oscillator with a hamiltonian \hat{H} :

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

The potential is here:

$$\frac{1}{2}m\omega^2x^2$$

By changing to dimensionless constants we have:

$$\frac{d^2\psi}{du^2} = (u^2 - \mathcal{E})\psi$$

By substituting:

$$\psi(u) = h(u)e^{-u^2/2}$$

we have:

$$\frac{d^2h}{du^2} - 2u\frac{dh}{du} + (\mathcal{E} - 1)h = 0$$

h is a hermite polynomial and the eigenvalues are given by:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

We then have

$$\psi_n(x) = N_n H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right) e^{-\frac{m\omega}{2\hbar}x^2}, n = 1, 2, \dots$$

2.11.2 Algebraic solution of the oscillator

We can write the hamiltonian as:

$$\hat{H} = \frac{1}{2}m\omega^2(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2})$$

Motivated by the identity $a^2 + b^2 = (a - ib)(a + ib)$ we have:

$$\left(\hat{x} - \frac{p\hat{p}}{m\omega}\right)\left(\hat{x} + \frac{p\hat{p}}{m\omega}\right) = \hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} + \frac{i}{m\omega}(\hat{x}\hat{p} - \hat{p}\hat{x}) = \hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} - \frac{\hbar}{m\omega}\mathbf{1}$$

\hat{x} and \hat{p} do not commute.

We now define:

$$\mathbf{V} = \hat{x} + \frac{i\hat{p}}{m\omega}$$

and we have since \hat{x} and \hat{p} hermitian:

$$\mathbf{V}^\dagger = \hat{x} - \frac{i\hat{p}}{m\omega}$$

and \hat{H} can be written:

$$\hat{H} = \frac{1}{2}m\omega^2\mathbf{V}^\dagger\mathbf{V} + \frac{1}{2}\hbar\omega\mathbf{1}$$

Changing to unit-free operator we have:

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) = \hbar\omega\left(\hat{N} + \frac{1}{2}\right), \quad \hat{N} \equiv \hat{a}^\dagger\hat{a}$$

Note that:

$$\langle\hat{H}\rangle_\psi = (\psi, \hat{H}\psi) = \hbar\omega(\hat{a}\psi, \hat{a}\psi) + \frac{1}{2}\hbar\omega \geq \frac{1}{2}\hbar\omega$$

If $\hat{a}\psi_0 = 0$ then ψ_0 is an eigenfunction of \hat{H} and it must be the ground state. This leads to:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}$$

2.11.3 Operator manipulation and the spectrum

By recursion you get the other eigenfunction. It's a long story.

Chapter 3

Scattering

3.1 The step potential

The potential is given by:

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x \geq 0 \end{cases}$$

3.1.1 Step potential with $E > V_0$

For $x < 0$ we get a transmitted wave and a reflected wave. For $x > 0$ we get a transmitted wave.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ Ce^{i\bar{k}x}, & x > 0 \end{cases}$$

$$k^2 = \frac{2mE}{\hbar^2}, \quad \bar{k}^2 = \frac{2m(E - V_0)}{\hbar^2}$$

ψ and ψ' are continuous:

$$\frac{B}{A} = \frac{k - \bar{k}}{k + \bar{k}}$$
$$\frac{C}{A} = \frac{2k}{k + \bar{k}}$$

Current to left and right the same:

$$J_A - J_B = J_C$$

Gives reflection and transmission coefficient:

$$R = \frac{J_B}{J_A} = \left(\frac{k - \bar{k}}{k + \bar{k}}\right)^2 \leq 1$$

$$T = \frac{J_C}{J_A} = \frac{4k\bar{k}}{(k + \bar{k})^2}$$

For $E = V_0$ $\bar{k} = 0$ and everything is reflected.

3.1.2 Step potential with $E < V_0$

$x > 0$ is a forbidden region classically and we expect an exponential decay. For $x < 0$ we expect reflected and transmitted wave

$$\psi(x) = Ce^{-\kappa x}$$

and we get:

$$\frac{B}{A} = -\frac{\kappa + ik}{\kappa - ik} = -e^{2i\delta(E)}$$

where

$$\delta(E) = \tan^{-1}\left(\frac{k}{\kappa}\right) = \tan^{-1}\left(\sqrt{\frac{E}{V_0 - E}}\right)$$

For future use

$$\delta'(E) = \frac{1}{2} \sqrt{\frac{1}{E(V_0 - E)}}$$

Becomes infinity for $E = 0$ and $E = V_0$

3.2 Wavepacket in the step potential

Looking at wave packets instead of waves we get for $E < V_0$ that the reflected wavepacket is delayed $2\hbar\delta'(E)$. As seen in the previous section the delay is particularly large for E small and E near V_0 . The wavepacket travels into the forbidden region but it can't be measured due to uncertainty.

3.3 Resonant transmission in a square well

We look at the situation where $E > 0$. We have an incoming wave, a reflected wave and also over the well but with a different wave number and an outgoing wave.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < -a \\ Ce^{ik_2x} + De^{-ik_2x}, & |x| < a \\ Fe^{ikx}, & x > a \end{cases}$$

$$k^2 = \frac{2mE}{\hbar^2} \quad k_2^2 = \frac{2m(E + V_0)}{\hbar^2}$$

We define the transmission coefficient:

$$T = \frac{|F|^2}{|A|^2}$$

and get

$$\frac{1}{T} = 1 + \frac{1}{4e(1+e)} \sin^2(2z_0\sqrt{1+e})$$

where

$$e = \frac{E}{V_0} \quad z_0^2 = \frac{2ma^2V_0}{\hbar^2}$$

The well becomes transparent for $T = 1$ that is:

$$2z_0\sqrt{1+e} = n\pi$$

$$E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

Same energy levels as infinite square well. Remember double with here.

3.4 The Ramsauer-Townsend effect

The effect of resonance and transmission = 1, can be observed when scattering low energy particles.

3.5 Scattering in one dimension

Physicists learn a lot from scattering. It can say a lot about the potential. We assume we have a wall and a finite range potential in front of it. The range is R . In polar coordinates r cannot be less than zero and is similar to the one-dimensionally case covered here. There will be bound states for $0 < x < R$. In general we have for any potential:

$$\text{Incomming wave: } e^{ikx}$$

$$\text{Outgoing wave: } e^{2i\delta}e^{-ikx}$$

The outgoing wave is delayed compare to the situation with no potential.

$$\Delta t = 2\hbar\delta'(E)$$

3.5.1 Time delay

TO DO

3.6 An example

Square potential

3.7 Levinson's theorem

Levinson's theorem relates the number N_b of bound states of a given potential to the excursion of the phase shift $\delta(E)$ as the energy goes from zero to infinity:

$$N_b = \frac{1}{\pi}(\delta(0) - \delta(\infty))$$

As the potential is turned on, we can track each energy eigenstates and no state can disappear. If we loose some positive eigen states those states must now appear as negative eigenstates or bound states.

3.8 Resonances

We can have arbitrary large positive time delay. If the wavepacket is trapped for a long time we have a resonance.

3.9 Modeling the resonance

May be we have complex wave numbers like complex frequencies.

Chapter 4

Schrödinger in 3D

4.1 Schrödinger equation in 3D and angular momentum

In spherical coordinates the Laplacian is:

$$\nabla^2\psi = (\nabla \cdot \nabla)\psi = \frac{1}{r} \frac{\partial^2}{\partial r^2}(r\psi) + \frac{1}{r^2} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right) \psi$$

And the Schrödinger equation for a particle in a central potential becomes:

$$-\frac{\hbar^2}{2m} \left[\frac{1}{r} \frac{\partial^2}{\partial r^2}(r\psi) + \frac{1}{r^2} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right) \right] \psi + V(r)\psi = E\psi$$

The angular dependency can be identified as the magnitude squared of the angular momentum operator:

$$\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} = -\frac{\mathbf{L}^2}{\hbar^2}$$

4.2 The angular momentum operator

TO DO

4.3 Eigenstates of angular momentum

TO DO

4.4 The radial wave equation

After some transformations we get:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 u_{El}}{\partial r^2} + \left(V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \frac{1}{r^2} \right) u_{El} = E u_{El}$$

This is called the radial equation. The decomposition of the wavefunction is:

$$\psi(r, \theta, \phi) = R_{El}(r)Y_{l,m}(\theta, \phi) = \frac{u_{El}}{r}Y_{l,m}(\theta, \phi)$$

where Y_{lm} are the spherical harmonics.

We have

$$u_{El} \sim cr^{l+1}, \quad \text{as } r \rightarrow 0$$

4.5 The hydrogen atom

TO DO

4.6 Hydrogen atom spectrum

TO DO

Chapter 5

Spin

5.1 Stern Gerlach experiment

Silver atoms are sent to an inhomogeneous magnetic field pointing in the z-direction and are thereby split into two rays as shown in Figure 5.1.

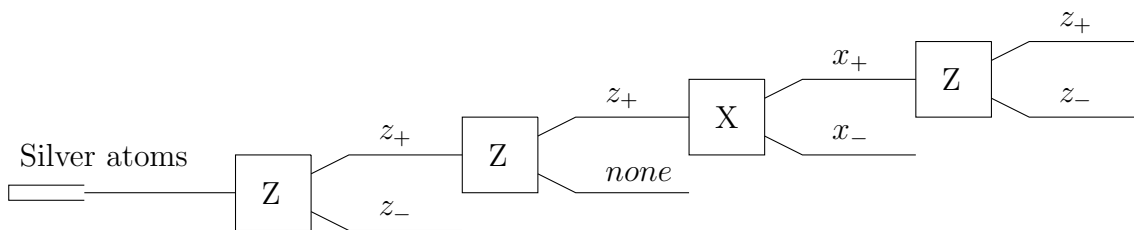


Figure 5.1: Stern - Gerlach setup

The spin seems to have two orthogonal basis states:

$$\begin{aligned} & |z_+\rangle \quad |z_-\rangle \\ & \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned}$$

The eigenvalues are $\pm \frac{\hbar}{2}$ and they are the eigenvectors of a hermitian operator:

$$\hat{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Any two-dimensional complex hermitian matrix can be written:

$$\begin{pmatrix} \alpha_1 + \alpha_2 & \alpha_3 - i\alpha_4 \\ \alpha_3 + i\alpha_4 & \alpha_1 - \alpha_2 \end{pmatrix} = \alpha_1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \alpha_2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \alpha_3 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \alpha_4 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

We therefore chose:

$$\hat{S}_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

with eigenvectors:

$$\begin{aligned} & |x_+\rangle \quad |x_-\rangle \\ & \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \end{aligned}$$

and

$$\hat{S}_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

with eigenvectors:

$$\begin{aligned} & |y_+\rangle \quad |y_-\rangle \\ & \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \end{aligned}$$

we have

$$\begin{aligned} x_+ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(z_+ + z_-) \\ x_- &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(z_+ - z_-) \end{aligned}$$

and

$$\begin{aligned} x_+ &= \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(x_+ + x_-) \\ x_- &= \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} - \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(x_+ - x_-) \end{aligned}$$

Note that we have as for angular momentum:

$$[\hat{S}_z; \hat{S}_x] = i\hbar\hat{S}_y;$$

$$[\hat{S}_x; \hat{S}_y] = i\hbar\hat{S}_z;$$

$$[\hat{S}_y; \hat{S}_z] = i\hbar\hat{S}_x;$$

Chapter 6

Linear algebra

6.1 Vector spaces and dimensionality

A vector space is a set, addition is defined as usual, multiplication with an element in a field (real or complex) is defined as usual.

A subspace is a subset that is a vector space.

A list of vectors is a finite number of vectors.

The span of a list, is the set of all linear combinations.

A basis of V is a list of vectors that spans V and are linearly independent.

Any finite dimensional vector space has a basis.

The dimension is m if you can extract m linearly independent vectors but not $m + 1$.

6.2 Linear operators and matrices

A linear map is a function that maps a vector space V to W .

A linear operator is a linear map that maps a vector space to itself.

Operators can be added and scaled by a constant.

Two operators can be multiplied.

The null space is the set of vectors mapped to 0 by T .

A linear operator T is injective if $Tu = Tv$ if $u = v$.

T is injective if and only if $\text{null } T = 0$.

The range of T is the map of V .

A linear operator T is surjective if the range is V .

$$\dim V = \dim(\text{null } T) + \dim(\text{range } T)$$

For a finite vector space:

$$T \text{ is invertible} \iff T \text{ is injective} \iff T \text{ is surjective}$$

For an infinite vector space:

$$T \text{ is invertible} \iff T \text{ is injective and surjective}$$

Matrices are basis dependent.
Trace and determinant are basis independent.
A matrix that change the basis is invertible.

6.3 Eigenvalues an eigenvectors

For a linear operator the eigenvectors are linearly independent.

6.4 Inner product

6.5 Orthonormal basis and orthogonal projectors

6.6 Linear functionals and adjoint operators

6.7 Hermitian an unitary operators

If $\langle v, Tv \rangle = 0$ for all v , then $T = 0$

The eigenvalues of a hermitian operator are real.

The eigenfunctions of a hermitian operator are orthogonal.

Chapter 7

Bra - Ket

7.1 Inner product

$$(u_1^*, u_2^*, \dots, u_n^*) \begin{pmatrix} v_1 \\ v_2 \\ \cdot \\ \cdot \\ v_n \end{pmatrix} \rightarrow \langle u|v \rangle$$

$$\langle u|v \rangle = \langle v|u \rangle^*$$

$$\langle u|c_1 v_1 + c_2 v_2 \rangle = c_1 \langle u|v_1 \rangle + c_2 \langle u|v_2 \rangle$$

$$\langle c_1 u_1 + c_2 u_2|v \rangle = c_1^* \langle u_1|v \rangle + c_2^* \langle u_2|v \rangle$$

$$|v|^2 = \langle v|v \rangle$$

$$|\langle u|v \rangle| \leq |u||v|$$

Given a set of basis vectors:

$$\langle e_i|e_j \rangle = \delta_{ij}$$

and

$$v = \sum_i \alpha_i e_i$$

then

$$\langle e_k|v \rangle = \langle e_k|\sum_i \alpha_i e_i \rangle = \sum_i \alpha_i \langle e_k|e_i \rangle = \alpha_k$$

and

$$v = \sum_i e_i \langle e_i|v \rangle$$

A linear map is an expression of the form:

$$f(v) = \alpha_1^* v_1 + \alpha_2^* v_2 + \dots + \alpha_n^* v_n = \langle \alpha|v \rangle$$

7.2 Operators

An operator Ω operating on a is written:

$$|\Omega a\rangle \equiv \Omega |a\rangle$$

An operator can be written:

$$\Omega = \begin{pmatrix} v_1 \\ v_2 \\ \cdot \\ \cdot \\ v_n \end{pmatrix} (u_1, u_2, \dots, u_n) = |v\rangle \langle u|$$

Adjoint of a linear operator

$$\langle \Omega^\dagger u | v \rangle = \langle u | \Omega v \rangle$$

We have:

$$\langle v | \Omega^\dagger u \rangle^* = \langle u | \Omega v \rangle$$

and

$$\langle v | \Omega^\dagger | u \rangle = \langle u | \Omega | v \rangle^*$$

and

$$\langle v | \Omega^\dagger | u \rangle = \langle \Omega v | u \rangle$$

and

$$\langle v | \Omega^\dagger | \equiv \langle \Omega v |$$

Hermitian operator

$$\Omega^\dagger = \Omega$$

We have:

$$\langle v | \Omega | u \rangle = \langle u | \Omega | v \rangle^*$$

and

$$\langle \Omega u | v \rangle = \langle u | \Omega^\dagger | v \rangle = \langle u | \Omega | v \rangle = \langle u | \Omega v \rangle$$

Unitary operator

$$U^\dagger U = U U^\dagger = \mathbf{1}$$

7.3 Non-denumerable basis

Chapter 8

Uncertainty principle