Quantum and Solid State Physics

Aakash Jog

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Part I

Quantum Physics

1 Lecturer Information

Asia Shapira

E-mail: asiasapi@gmail.com

2 Required Reading

1. Griffiths, D. Introduction to quantum mechanics

3 Additional Reading

1. Tang: Fundamentals of quantum mechanics, Cambridge press.
2. Miller, Quantum mechanics for scientists and engineers.

4 Waves

Waves

Mechanical | Electromagnetic
Need medium for propagation | Do not need medium for propagation

4.1 1D Wave Equation

Definition 1 (1D wave equation)**.** The equation

$$\frac{\partial^2 \psi}{\partial t^2} = v^2 \frac{\partial^2 \psi}{\partial x^2}$$

where ψ is a function of x and t, and v is the velocity of the wave, is called a 1D wave equation.

5 Harmonic Waves

Definition 2 (Harmonic waves)**.** If a wave satisfies the equation

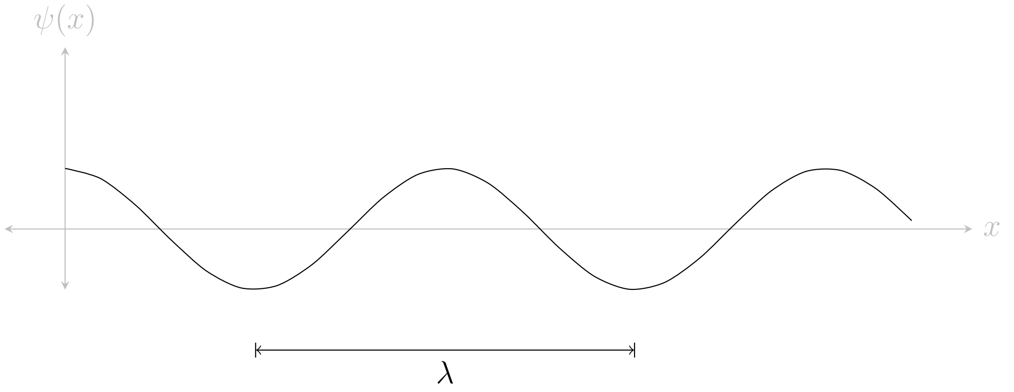
$$\psi(x, t) = A \cos(kx - \omega t + \varphi)$$

it is called a harmonic wave.
A is called the amplitude of the wave.
k is called the wave number, or spatial frequency of the wave.
ω is called the angular frequency of the wave.

Definition 3 (Wavelength)**.** For a harmonic wave, a number λ, such that

$$\psi(x) = \psi(x + \lambda)$$

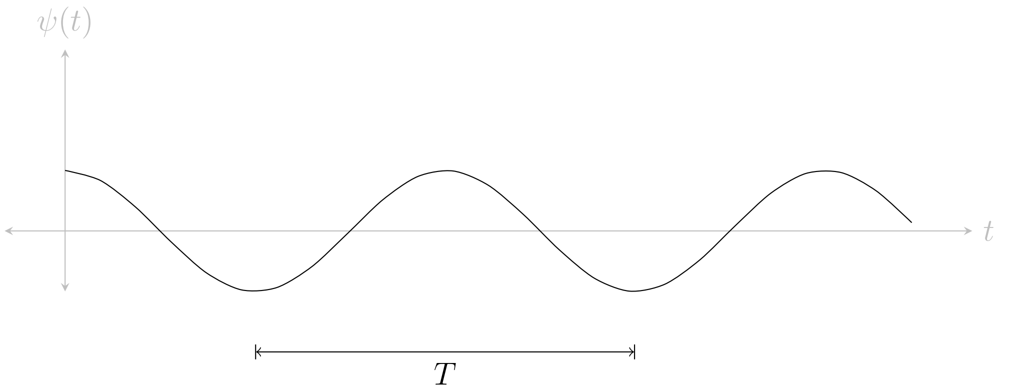
is called the wavelength of the wave.



Definition 4 (Time period)**.** For a harmonic wave, a number T, such that

$$\psi(t) = \psi(t + T)$$

is called the time period of the wave.



Theorem 1.

$$k = \frac{2\pi}{\lambda}$$

where k is the wave number, and λ is the wavelength.

Proof. If $t = 0$,

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

By the definition of wavelength,

$$\begin{aligned} \psi(x) &= \psi(x+\lambda) \\ \therefore A\cos(kx) &= A\cos\left(k(x+\lambda)\right) \\ \therefore k\lambda &= 2\pi \\ \therefore k &= \frac{2\pi}{\lambda} \end{aligned}$$

□

Theorem 2.

$$\omega = \frac{2\pi}{T}$$

where ω is the angular frequency, and T is the time period.

Proof. If $x = 0$,

$$\psi(t) = A\cos(\omega t)$$

By the definition of wavelength,

$$\begin{aligned} \psi(t) &= \psi(t+T) \\ \therefore A\cos(\omega t) &= A\cos\left(\omega(t+T)\right) \\ \therefore \omega T &= 2\pi \\ \therefore \omega &= \frac{2\pi}{T} \end{aligned}$$

□

5.1 Complex Representation of Waves

Let

$$\widetilde{\psi} = Ae^{i(kx-\omega t+\varphi)}$$

Then,

$$\psi = \Re\{\widetilde{\psi}\}$$

5.2 Interference of Waves

Theorem 3. *Wave equations are linear, i.e. if ψ_1 and ψ_2 are solutions to the equation, then $\psi_1 + \psi_2$ is also a solution to the equation.*

5.2.1 Interference of Waves with a Phase Difference

Let

$$\psi_1 = A\cos(kx - \omega t + \varphi)$$
$$\psi_2 = A\cos(kx - \omega t)$$

Therefore,

$$\begin{aligned}
\psi_3 &= \psi_1 + \psi_2 \\
&= A\cos(kx - \omega t + \varphi) + A\cos(kx - \omega t) \\
&= 2A\cos\left(\frac{\varphi}{2}\right)\cos\left(kx + \omega t + \frac{\varphi}{2}\right)
\end{aligned}$$

$\because \cos a + \cos b = 2\cos\left(\frac{a+b}{2}\right)\cos\left(\frac{a-b}{2}\right)$

Therefore, the resultant wave is a wave with amplitude $2A\cos\left(\frac{\varphi}{2}\right)$ and phase $\frac{\varphi}{2}$.

6 Young's Double Slit Experiment (1801)

This experiment provided substantial proof that light behaves like a wave.

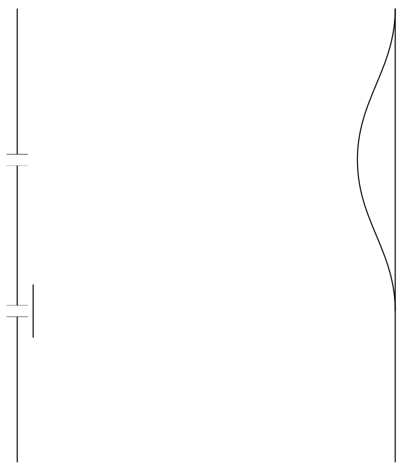


Figure 1: Intensity of light with only first slit open

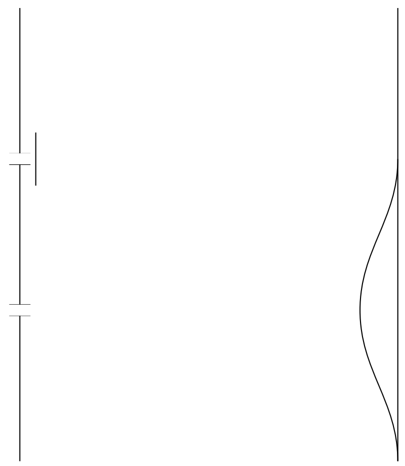


Figure 2: Intensity of light with only second slit open

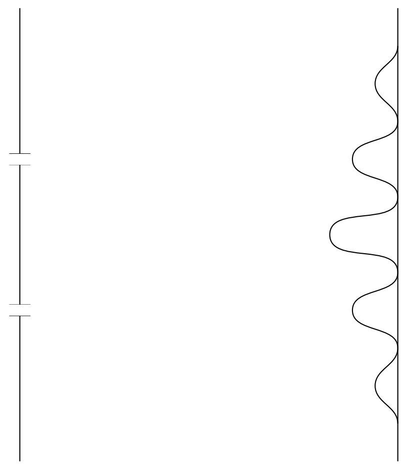


Figure 3: Intensity of light with both slits open

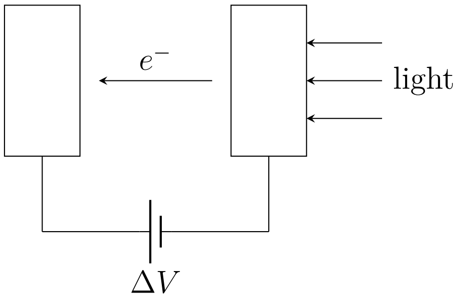
6.1 YDSE with Classical Particles

If the double slit experiment is performed with classical particles, instead of waves, the intensities add up. There is no fringe pattern, as observed in the experiment with waves.

7 The Photoelectric Effect

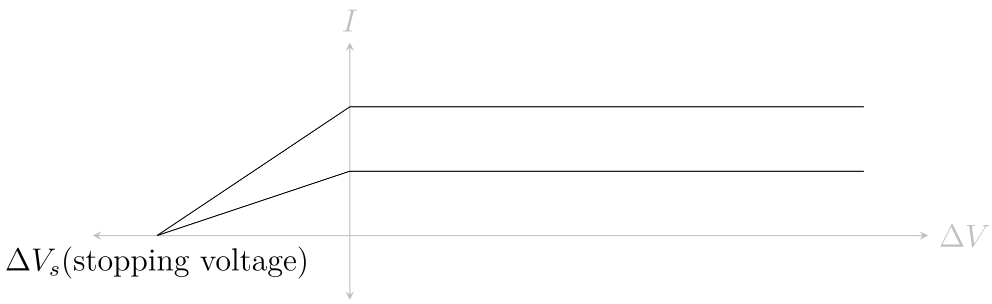
The first experiment in which the photoelectric effect was observed was performed by Hertz in 1887.

Two metallic plates, acting as electrodes were arranged as shown. They were connected to a voltage source ΔV, as shown.



The results observed were as shown.

1. The relationship between ΔV and the current in the wire was observed to be as shown.



The conclusions were as follows.

(a) If the light intensity is constant, a specific amount of electrons is emitted. Therefore, the current is constant, and independent of ΔV.

(b) If $\Delta V >> 0$, all electrons emitted reached the other plate, and hence contributed to the current.
If $\Delta V < 0$, some electrons were unable to reach the other plate, and hence did not contribute to the current.

(c) ΔV_s is not dependent on the intensity of the light.

As the energy of an electron is conserved,

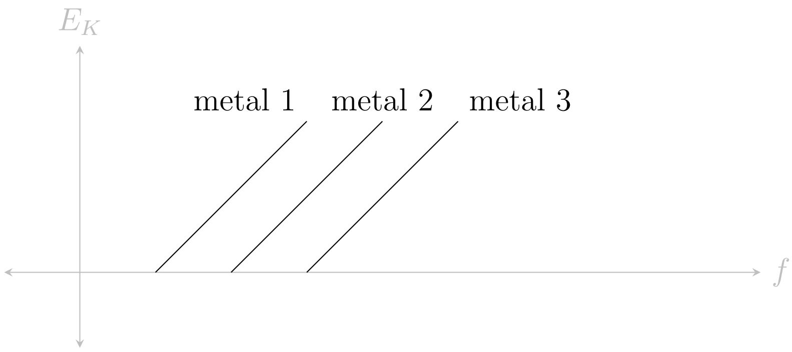
$$E_{K_i} + E_{P_i} = E_{K_f} + E_{P_f}$$

Therefore, if the electron barely reaches the other plate, i.e. if the voltage is ΔV_s

$$E_{K_i} + 0 = (-e)(-\Delta V_s)$$
$$\therefore e\Delta V_s = E_K$$

Therefore, as ΔV_s is independent of the intensity of light, the kinetic energy of the emitted electrons is also independent of the intensity of light.

2. The relationship between the kinetic energy of the emitted electrons, and the frequency of the incident light was observed to be as shown.



The conclusions were as follows.

(a) There is a cutoff frequency, i.e. a frequency below which no electrons are emitted.

(b) The kinetic energy of the emitted electrons is linearly dependent on the frequency of light.

These conclusions were inconsistent with the accepted notion of light being a wave.

7.1 Einstein's Explanation of the Photoelectric Effect (1905)

According to Einstein's explanation, light is a stream of particles, called photons. Each photon has energy equal to hf, where h is Planck's constant, and f is the frequency of the light, which is in fact a property of the wave nature of the light. This theory can explain the conclusions of Hertz's

experiment, which could not be explained by classical theories.
According to the explanation, each material has a property called the work function (W). The fact that there exists a cutoff voltage is justified due to this energy barrier. For an electron to be emitted, it needs to be provided energy to overcome this barrier. The cutoff frequency is such that all energy in a photon of this frequency to be used to overcome the work function. Therefore,

$$hf_{\text{cutoff}} = W$$

Also, as each photon provides all its energy to a single electron, increasing the intensity of light just increases the number of electrons emitted, but does not increase the kinetic energy of the emitted electrons.

8 Quantum Particles

Definition 5 (Momentum of a quantum particle)**.** The momentum of a quantum particle is defined as

$$p = \frac{E}{c}$$

where E is the energy of the particle.

Theorem 4 (Einstein Equation)**.**

$$E = mc^2 + pc$$

Definition 6. The reduced Planck's constant is defined as

$$\hbar = \frac{h}{2\pi}$$

where h is Planck's constant.

Theorem 5.

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

Proof.

$$\begin{aligned} E &= hf \\ &= h\frac{\omega}{2\pi} \\ &= \hbar\omega \end{aligned}$$

$$\begin{aligned} p &= \frac{E}{c} \\ &= \frac{h}{\lambda} \\ &= \frac{h}{2\pi}k \\ &= \hbar k \end{aligned}$$

$\square$

8.1 de Broglie Wavelength

According to de Broglie's theory, particles have waves associated with them. Therefore, according to this theory,

$$\begin{aligned} \lambda &= \frac{h}{p} \\ &= \frac{h}{mv} \\ f &= \frac{E}{h} \end{aligned}$$

where m is the mass of the particle and v is its velocity.
Therefore, according to this theory, particles must exhibit wave-like behaviour. Hence, if the double slit experiment is performed with particles, the pattern observed must be similar to the fringe pattern observed with waves.
If the double slit experiment is performed with a single electron emitted at a time, over a long period of time, a fringe-like pattern, made up of dots corresponding to single electrons, is observed. This is consistent with de Broglie's theory.

Exercise 1.
Find the de Broglie wavelength of an electron moving at $10^7 \frac{\mathrm{m}}{\mathrm{s}}$.

Solution 1.

$$\begin{aligned}\lambda &= \frac{h}{mv}\\ &= \frac{6.63\times 10^{-34}\,\mathrm{J\,s}}{(9.11\times 10^{-31}\mathrm{kg})\left(10^{7}\frac{\mathrm{m}}{\mathrm{s}}\right)}\\ &= 7.27\times 10^{-11}\mathrm{m}\\ &= 72\mathrm{pm}\end{aligned}$$

Exercise 2.
Find the de Broglie wavelength of a rock of 50 g, thrown with a speed of 40 $\frac{\mathrm{m}}{\mathrm{s}}$.

Solution 2.

$$\begin{aligned}\lambda &= \frac{h}{mv}\\ &= \frac{6.63\times 10^{-34}}{(50\times 10^{-3})\,(40)}\\ &= 3.3\times 10^{-34}\,\mathrm{m}\end{aligned}$$

8.2 Impact of Observation on the Result of Experiments

If 100% of the electrons are observed to determine which slit they pass through, the pattern observed is exactly like the pattern observed with classical particles.
If only some electrons are observed, say 70%, then those 70% electrons behave like classical particles, and the rest behave like a wave. Therefore, the effective result is a superposition both of these pattern.

Therefore, the outcome of the experiment is affected by the fact that the particles are being observed.
The reason behind this is that the act of observation involves interacting with the particles, usually in the form of the particle being hit by photons, which are necessary for the observer to make the observations.
Classical particles are not affected by this factor on such a large scale, as their mass is much larger than that of quantum particles.

9 Schrödinger Equation

Theorem 6 (Schrödinger Equation)**.**

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

Proof. Let the wave be given by

$$\psi(x,t) = Ae^{i(kx-\omega t)}$$

Differentiating with respect to time,

$$\begin{aligned}
\frac{\partial\psi(x,t)}{\partial t} &= -i\omega\psi(x,t) \\
&= -i\frac{E}{\hbar}\psi(x,t) && \because \omega = \tfrac{E}{\hbar} \\
&= -\frac{i}{\hbar}\left(\frac{p^2}{2m} + E_P\right)\psi(x,t) && \text{where } E_P = V(x) \text{ is the potential energy of the particle} \\
&= -\frac{i}{\hbar}\left(\frac{p^2}{2m} + V(x)\right)\psi(x,t) && (1)
\end{aligned}$$

Differentiating with respect to x,

$$\begin{aligned}
\frac{\partial\psi(x,t)}{\partial x} &= ik\psi(x,t) \\
\therefore \frac{\partial^2\psi(x,t)}{\partial x^2} &= (ik)(ik)\psi(x,t) \\
&= -k^2\psi(x,t) \\
&= -\frac{p^2}{\hbar^2}\psi(x,t) \\
\therefore -h^2\frac{\partial^2\psi(x,t)}{\partial x^2} &= p^2\psi(x,t) \\
\therefore -\frac{h^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} &= \frac{p^2}{2m}\psi(x,t) && (2)
\end{aligned}$$

Therefore, solving the above equations simultaneously,

$$\begin{aligned}
\frac{\partial\psi(x,t)}{\partial t} &= -\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\right)\psi(x,t) \\
\therefore i\hbar\frac{\partial\psi(x,t)}{\partial t} &= \left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\right)\psi(x,t)
\end{aligned}$$

□

10 Basic Postulates of Quantum Mechanics

1. $\psi(x,t)$ describes the configuration of the system.
2. The probability of finding the particle between x and $x+\mathrm{d}x$ at time t is

   $$|\psi(x,t)|^2 = \psi(x,t)\psi^*(x,t)$$

   where ψ^* is the complex conjugate of of ψ,
3. If $\psi_1(x,t)$ and $\psi_2(x,t)$ are solutions to the Schrödinger equation, then $\alpha\psi(x,t) + \beta\psi(x,t)$ is also a solution to the Schrödinger equation.

11 Properties of $\psi(x,t)$

1. $\displaystyle\int\limits_{-\infty}^{\infty} |\psi(x,t)|^2 \,\mathrm{d}x = 1$

   $|\psi(x,t)|^2$ is the probability of the particle being in the neighbourhood of x. Therefore, the equation is obvious, as the probability of the particle being in the entire universe must be 1.
2. $|\psi(x,t)|$ is a single valued function.
   This is obvious, as the probability of the particle existing at a point in space must have exactly one value.

12 Conservation of Normalization

Definition 7. If

$$\int\limits_{-\infty}^{\infty} |\psi(x,t)|^2 \,\mathrm{d}x = 1$$

Then the equation is said to be normalized.

Theorem 7. *The Schrödinger equation conserves normalization, i.e.,*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{-\infty}^{\infty} |\psi(x,t)|^2 = 0$$

Proof.

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}|\psi(x,t)|^2\,\mathrm{d}x &= \int_{-\infty}^{\infty}\frac{\partial}{\partial t}\left(\psi(x,t)\psi^*(x,t)\right)\mathrm{d}x \\
&= \int_{-\infty}^{\infty}\frac{\partial\psi}{\partial t}\,\psi^* + \psi\,\frac{\partial\psi^*}{\partial t}
\end{aligned}$$

From the Schrödinger Equation,

$$\begin{aligned}
\frac{\partial\psi}{\partial t} &= \frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} - \frac{i}{\hbar}V\psi \\
\therefore \frac{\partial\psi^*}{\partial t} &= -\frac{i\hbar}{2m}\frac{\partial^2\psi^*}{\partial x^2} + \frac{i}{\hbar}V\psi^*
\end{aligned}$$

Therefore,

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}|\psi(x,t)|^2\,\mathrm{d}x &= \int_{-\infty}^{\infty}\left(\frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2}\,\psi^* - \frac{i\hbar}{2m}\frac{\partial^2\psi^*}{\partial x^2}\,\psi\right)\mathrm{d}x \\
&= \int_{-\infty}^{\infty}\left(\frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\psi^*\,\frac{\partial\psi}{\partial x} - \psi\,\frac{\partial\psi^*}{\partial x}\right)\right)\mathrm{d}x \\
&= \frac{i\hbar}{2m}\left(\psi^*\,\frac{\partial\psi}{\partial x} - \psi\,\frac{\partial\psi^*}{\partial x}\right)\Bigg|_{-\infty}^{\infty}
\end{aligned}$$

Therefore,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}|\psi(x,t)|^2\,\mathrm{d}x = 0$$

$$\iff \frac{i\hbar}{2m}\left(\psi^*\,\frac{\partial\psi}{\partial x} - \psi\,\frac{\partial\psi^*}{\partial x}\right)\Bigg|_{-\infty}^{\infty} = 0$$

Therefore, the normalization is conserved if the wave function tapers off at infinity. □

13 Measurements and Operators

13.1 The Collapse of the Wave Function

Consider a probability distribution of finding a particle at x, given by the wave function $\psi(x,t)$. The position of the particle is actually measured, and hence found to be at some position $x = A$, at time t. Therefore, after a small time interval $\mathrm{d}t$ after t, it can be predicted with certainty that the particle is around $x = A$. Hence, the original wave function is no longer valid, and there is a new wave function which describes the particle. This phenomenon is called the collapse of the wave function.

13.2 Momentum

Definition 8 (Observable)**.** A physical parameter which describes a particle, such as position, momentum, energy, velocity, etc., is called an observable.

Definition 9 (Expected value)**.** The average value of the position, measured with the same wave function $\psi(x, t)$ and N particles, is called the expected value. It is denoted as $\langle x \rangle$.

Theorem 8 (Ehrenfest's Theorem)**.** *Expected values obey classical laws, i.e, for example,*

$$\begin{aligned}\langle v \rangle &= \frac{\mathrm{d}}{\mathrm{d}t} \langle x \rangle \\ \langle p \rangle &= m \frac{\mathrm{d}}{\mathrm{d}t} \langle x \rangle\end{aligned}$$

Theorem 9.

$$\langle x \rangle = \int\limits_{-\infty}^{\infty} \psi^* x \psi \, \mathrm{d}x$$

Proof. By definition,

$$\begin{aligned}\langle x \rangle &= \int\limits_{-\infty}^{\infty} x \left|\psi(x, t)\right|^2 \mathrm{d}x \\ &= \int\limits_{-\infty}^{\infty} x \psi(x, t) \psi^*(x, t) \, \mathrm{d}x \\ &= \int\limits_{-\infty}^{\infty} \psi^* x \psi \, \mathrm{d}x\end{aligned}$$

□

Theorem 10.

$$\langle p \rangle = \int\limits_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi \,\mathrm{d}x$$

Proof. By Ehrenfest's Theorem,

$$\begin{aligned}
\langle p \rangle &= m \frac{\mathrm{d}}{\mathrm{d}t} \langle x \rangle \\
&= m \frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{-\infty}^{\infty} x \left| \psi(x,t) \right|^2 \mathrm{d}x \\
&= m \int\limits_{-\infty}^{\infty} x \frac{\partial}{\partial t} (\psi \psi^*) \,\mathrm{d}x \\
&= m \frac{i\hbar}{2m} \int\limits_{-\infty}^{\infty} x \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} \right) \mathrm{d}x \\
&= \frac{i\hbar}{2} \left(\cancelto{0}{\left. x \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \right|_{-\infty}^{\infty}} - \int\limits_{-\infty}^{\infty} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \mathrm{d}x \right) \\
&= -\frac{i\hbar}{2} \int\limits_{-\infty}^{\infty} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \mathrm{d}x \\
&= -\frac{i\hbar}{2} 2 \int\limits_{-\infty}^{\infty} \frac{\partial \psi}{\partial x} \psi^* \,\mathrm{d}x \\
&= -i\hbar \int\limits_{-\infty}^{\infty} \frac{\partial \psi}{\partial x} \psi^* \,\mathrm{d}x \\
&= \int\limits_{-\infty}^{\infty} \psi^* (-i\hbar) \frac{\partial}{\partial x} \psi \,\mathrm{d}x
\end{aligned}$$

□

13.3 Operators

Definition 10 (Operator)**.** A function which acts on a function is called an operator. There exists an operator associated with every observable.

Theorem 11. *Every operator can be written as a function of $\hat{x}$, $\hat{p}$, $Q(\hat{x},\hat{p})$. In general,*

$$\langle Q \rangle = \int\limits_{-\infty}^{\infty} \psi^* \hat{Q} \psi \, \mathrm{d}x$$

where

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

Theorem 12.

$$\begin{aligned} E_k &= \frac{1}{2} m v^2 \\ &= \frac{p^2}{2m} \end{aligned}$$

Therefore,

$$\hat{E}_k = \frac{\hat{p}^2}{2m}$$

Therefore,

$$\begin{aligned} \langle E_k \rangle &= \int\limits_{-\infty}^{\infty} \psi^* \left(\frac{\hat{p}^2}{2m} \right) \psi \, \mathrm{d}x \\ &= \frac{1}{2m} \int\limits_{-\infty}^{\infty} \psi^* \left(-\hbar^2 \right) \frac{\partial^2}{\partial x^2} \psi \, \mathrm{d}x \end{aligned}$$

Exercise 3.
A particle with mass m has wave function

$$\psi(x,t) = A e^{-a\left(\frac{mx^2}{\hbar} + it\right)}$$

where a and A are constants.

1. Find A.

2. Find $V(x)$ which gives $\psi(x,t)$ as a solution of the Schrödinger Equation.

3. Find the expected values of
   (a) x.
   (b) x^2.
   (c) p.
   (d) p^2.

Solution 3.

1.

$$\begin{aligned}
1 &= \int_{-\infty}^{\infty} |\psi(x,t)|^2 \,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} \psi(x,t)\psi^*(x,t)\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} Ae^{-a\left(\frac{mx^2}{\hbar}+it\right)} Ae^{-a\left(\frac{mx^2}{\hbar}-it\right)}\,\mathrm{d}x \\
&= A^2 \int_{-\infty}^{\infty} e^{-2a\frac{mx^2}{\hbar}}\,\mathrm{d}x \\
&= 2A^2 \int_{0}^{\infty} e^{-2a\frac{mx^2}{\hbar}}\,\mathrm{d}x \\
&= 2A^2 \left(\frac{1}{2}\left(\frac{\pi\hbar}{2am}\right)^{\frac{1}{2}}\right) \\
&= A^2 \left(\frac{\pi\hbar}{2am}\right)^{\frac{1}{2}}
\end{aligned}$$

As the function is even, the integral from $-\infty$ to ∞ is twice that of the integral from 0 to ∞.

Therefore,

$$A = \left(\frac{2am}{\pi\hbar}\right)^{\frac{1}{4}}$$

2.

$$\begin{aligned}
\psi(x,t) &= Ae^{-a\left(\frac{mx^2}{\hbar}+it\right)} \\
&= \left(\frac{2am}{\pi\hbar}\right)^{\frac{1}{4}} e^{-a\left(\frac{mx^2}{\hbar}+it\right)}
\end{aligned}$$

Therefore,

$$\begin{aligned}
\frac{\partial \psi}{\partial t} &= (-ia)\psi(x,t) \\
\frac{\partial \psi}{\partial x} &= -\frac{am}{\hbar}2m\psi(x,t) \\
\therefore \frac{\partial^2 \psi}{\partial x^2} &= -\frac{2am}{\hbar}\frac{\partial}{\partial x}\left(x\psi(x,t)\right) \\
&= -\frac{2am}{\hbar}\left(\psi(x,t) - \frac{am}{\hbar}2x^2\psi(x,t)\right)
\end{aligned}$$

Therefore, substituting in the Schrödinger Equation,

$$\begin{aligned}
i\hbar\frac{\partial \psi}{\partial t} &= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi \\
\therefore a\hbar\psi &= a\hbar\left(\psi - \frac{am}{\hbar}2x^2\psi\right) + V(x)\psi \\
\therefore V(x) &= 2a^2mx^2
\end{aligned}$$

3. (a)

$$\begin{aligned}
\langle x \rangle &= \int\limits_{-\infty}^{\infty} \psi^* x \psi \,\mathrm{d}x \\
&= \int\limits_{-\infty}^{\infty} x\left|\psi(x,t)\right|^2 \mathrm{d}x \\
&= \int\limits_{-\infty}^{\infty} xA^2e^{-2a\left(\frac{mx^2}{\hbar}\right)} \mathrm{d}x
\end{aligned}$$

Therefore, as this function is odd, its integral over a symmetric interval is zero.
Therefore,

$$\langle x \rangle = 0$$

(b)

As $\int\limits_{-\infty}^{\infty} x^2 e^{-bx^2}\,\mathrm{d}x = \frac{1}{2b}\sqrt{\frac{\pi}{b}}$

$$\begin{aligned}
\left\langle x^2 \right\rangle &= \int\limits_{-\infty}^{\infty} x^2A^2e^{-2a\left(\frac{mx^2}{\hbar}\right)} \mathrm{d}x \\
&= \frac{\hbar}{4am}
\end{aligned}$$

(c)

$$\begin{aligned}
\langle p\rangle &= \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi \, \mathrm{d}x \\
&= m \frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} \\
&= 0
\end{aligned}$$

(d)

$$\begin{aligned}
\left\langle p^2 \right\rangle &= \int_{-\infty}^{\infty} \psi^* (-\hbar^2) \frac{\partial^2 \psi}{\partial x^2} \, \mathrm{d}x \\
&= -\hbar^2 \int_{-\infty}^{\infty} \psi^* \left(\left(\frac{2am}{\hbar} x\right)^2 - \frac{2am}{\hbar}\right) \psi \, \mathrm{d}x \\
&= -\hbar^2 \int_{-\infty}^{\infty} A^2 e^{-2a\frac{mx^2}{\hbar}} \left(\left(\frac{2am}{\hbar} x\right)^2 - \frac{2am}{\hbar}\right) \mathrm{d}x \\
&= am\hbar
\end{aligned}$$

13.4 Eigenfunctions and Eigenvalues of Operators

Definition 11 (Eigenvalues and eigenfunctions)**.** Let $\hat{O}$ be an operator. The scalar α_n such that

$$\hat{O}(f_n) = \alpha_n f_n$$

is called the eigenvalue corresponding to the eigenfunction f_n.

Definition 12. If the wave function of of a particle is given by

$$\psi(x) = Ae^{ikx}$$

the particle is said to be in a state with definite momentum.

Exercise 4.
Find the eigenvalue of the momentum operator for a particle with definite momentum.

Solution 4.

$$\begin{aligned}
\hat{p}\psi(x) &= \alpha\psi(x) \\
\therefore -i\hbar\frac{\mathrm{d}\psi(x)}{\mathrm{d}x} &= \alpha\psi(x) \\
\therefore \psi(x) &= Ae^{-\frac{\alpha}{\hbar}x}
\end{aligned}$$

As

$$\psi(x) = Ae^{ikx}$$

Therefore,

$$\begin{aligned}
\frac{\alpha}{\hbar} &= k \\
\therefore \alpha &= \hbar k \\
&= p
\end{aligned}$$

Therefore,

$$\begin{aligned}
\hat{p}\psi(x) &= \alpha\psi(x) \\
&= p\psi(x)
\end{aligned}$$

Therefore, the eigenvalue of $\hat{p}$ is p.

Definition 13 (Dirac delta function)**.** The Dirac delta function is defined to be

$$\delta(x-a) = \begin{cases} \infty & ; \quad x = a \\ 0 & ; \quad x \neq a \end{cases}$$

Theorem 13.

$$\int\limits_{-\infty}^{\infty} \delta(x-a)\,\mathrm{d}x = 1$$

Theorem 14.

$$\delta(x-a) = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} e^{ip(x-a)}\,\mathrm{d}p$$

Theorem 15.

$$f(a) = \int\limits_{-\infty}^{\infty} \delta(x-a)f(x)\,\mathrm{d}x$$

13.5 Dirac Delta Function

Theorem 16. *The Dirac delta function is even, i.e.*

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

13.6 Fourier Transform

Definition 14 (Fourier transform)**.** The Fourier transform of $f(x)$ is defined as

$$F(k) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} f(x) e^{-ikx} \, \mathrm{d}x$$
$$f(k) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} F(x) e^{ikx} \, \mathrm{d}x$$

Exercise 5.
Find the Fourier transform of $f(x) = 1$.

Solution 5.

$$\begin{aligned} F(k) &= \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} f(x) e^{-ikx} \, \mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} e^{-ikx} \, \mathrm{d}x \\ &= \sqrt{2\pi}\delta(-k) \\ &= \sqrt{2\pi}\delta(k) \end{aligned}$$

As $\delta(x-a) = \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} e^{ip(x-a)} \, \mathrm{d}p$.
As $\delta(x)$ is even.

Exercise 6.
Find the Fourier transform of $f(x) = e^{iax}$.

Solution 6.

$$\begin{aligned}
F(k) &= \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} f(x) e^{-ikx} \,\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} e^{iak} e^{-ikx} \,\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} e^{-i(k-a)x} \,\mathrm{d}x
\end{aligned}$$

As $\delta(x-a) = \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} e^{ip(x-a)} \,\mathrm{d}p$.

$$= \sqrt{2\pi}\delta\left(-(k-a)\right)$$

As $\delta(x)$ is even.

$$= \sqrt{2\pi}\delta(k-a)$$

14 Heisenberg's Uncertainty Principle

Heisenberg's Uncertainty Principle states that

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

where

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

is the standard deviation of the position of the particle, and

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

is the standard deviation of the momentum of the particle.

14.1 Attempting to Measure both the Position and Momentum of an Electron

Consider a screen with a single slit kept in the path of a beam of electrons as shown.
Let the momentum of the electrons be a known value p_0.
Let the thickness of the slit be $\mathrm{d}y$.
Consider the electrons which pass through the slit.

As the thickness of the slit is $\mathrm{d}y$, the uncertainty in the position of the electrons, which pass through the slit, is $\mathrm{d}y$.

As the probability wave of the electron passes through the slit, it diffracts. Hence, some of the electrons which pass through the slit continue on the original trajectory, and some of them change their trajectory and also move in the y-axis. Hence, there is an uncertainty in the momentum of the electrons. Let the angle that a particular electron deviates with be θ. Therefore, the uncertainty in the momentum of the electron is $p_0 \sin\theta$.

Therefore,

$$\begin{aligned}
\sigma_x \sigma_p &= p_0 \sin\theta \, \mathrm{d}y \\
&= p_0 \frac{\lambda}{\mathrm{d}y} \, \mathrm{d}y \\
&= p_0 \lambda \\
&= p_0 \frac{h}{p_0} \\
&= h \\
&\approx \hbar
\end{aligned}$$

15 Definite Momentum States

Theorem 17. *$\left|\widetilde{\psi}(k)\right|^2 \mathrm{d}k$ is the probability of the momentum of a particle being between $k\hbar$ and $(k + \mathrm{d}k)\hbar$).*

Consider the wave function

$$\psi(x) = Ae^{ikx}$$

Therefore, using Fourier transformation,

$$\widetilde{\psi}(k) = A\sqrt{2\pi}\delta(k + k_1)$$

Therefore,

$$\left|\psi(x)\right|^2 = A^2$$
$$\left|\widetilde{\psi}(k)\right|^2 = \delta(k + k_1)$$

Therefore, the probability distributions are as shown in Figure 4, and Figure 5.

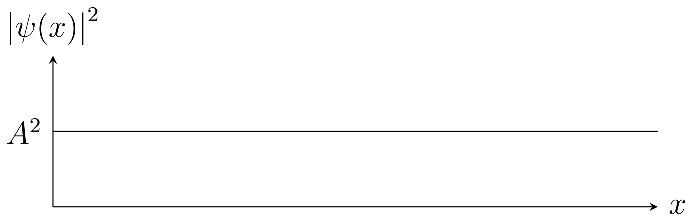


Figure 4: Probability distribution of x for a definite momentum state

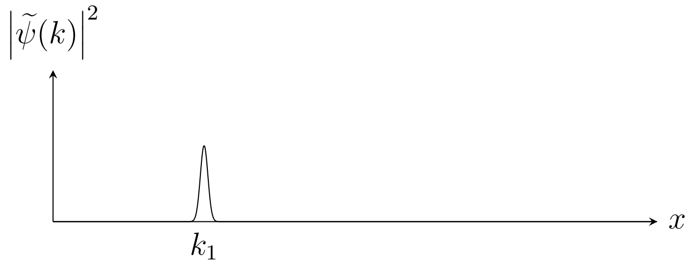


Figure 5: Probability distribution of k for a definite momentum state

Hence, σ_x is high, and σ_p is low.

16 Definite Position States

Consider the wave function

$$\psi(x) = \delta(x - x_1)$$

Therefore, using Fourier transformation,

$$\widetilde{\psi}(k) = \frac{e^{ikx_1}}{\sqrt{2\pi}}$$

Therefore,

$$
\begin{aligned}
|\psi(x)| &= \delta(x - x_1) \\
\left|\widetilde{\psi}(k)\right| &= \frac{1}{2\pi}
\end{aligned}
$$

Therefore, the probability distributions are as shown in Figure 6, and Figure 7.

Figure 6: Probability distribution of x for a definite position state

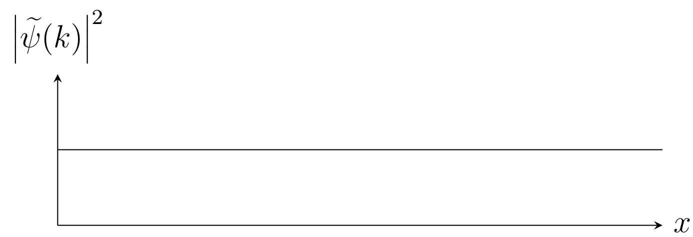


Figure 7: Probability distribution of k for a definite position state

Hence, σ_x is low, and σ_p is high.

Theorem 18. *The eigenstates or eigenfunctions of the momentum operator form a basis. Therefore, if*

$$\hat{A}\varphi_a = a\varphi_a$$

for discrete variables,

$$\psi(x) = \sum_a c_a \varphi_a(x)$$

for continuous variables,

$$\psi(x) = \int c_a \varphi_a(x) \, \mathrm{d}a$$

Proof.

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} \widetilde{\psi}(x) e^{ikx} \, \mathrm{d}k$$

Therefore, any value of $\psi(x)$ can be written in terms of the corresponding $\widetilde{\psi}(k)$ and e^{ikx}. Hence, the eigenstates of the momentum operator form a basis. □

Theorem 19. *If*

$$\hat{A}\varphi_a = a\varphi_a$$

then, for discrete variables,

$$\psi(x) = \sum_a c_a \varphi_a(x)$$

then, for continuous variables,

$$\psi(x) = \int c_a \varphi_a(x) \, \mathrm{d}a$$

Then, the probability of the observable A having value a is

$$P(A = a) = |c_a|^2$$

17 Description of Physical State by Eigenstates

Let the particle be in a state of definite momentum.
Therefore,

$$\psi(x) = A e^{ik_1 x}$$

Therefore, the total probability over the entire space is

$$\begin{aligned}
\int\limits_{-\infty}^{\infty} |\psi|^2 \, \mathrm{d}x &= \int\limits_{-\infty}^{\infty} A e^{ik_1 x} A^* e^{ik_2 x} \, \mathrm{d}x \\
&= \int\limits_{-\infty}^{\infty} |A|^2 \, \mathrm{d}x \\
&\to \infty
\end{aligned}$$

Therefore, as this integral cannot be finite, irrespective of A, this state does not represent a physical state.
Let

$$\begin{aligned}\varphi_n &= Ae^{ik_n x}\\ \varphi_m &= Ae^{ik_m x}\end{aligned}$$

be eigenfunctions of $\hat{p}$.
Therefore, as they are eigenfunctions, they are orthonormal to each other.
Therefore,

$$\begin{aligned}\int\limits_{-\infty}^{\infty} {\varphi_n}^* \varphi_m \,\mathrm{d}x &= |A|^2 \int\limits_{-\infty}^{\infty} e^{i(k_m - k_n)x} \,\mathrm{d}x\\ &= |A|^2 \cdot 2\pi\delta(k_m - k_n)\end{aligned}$$

As the eigenfunctions are orthonormal, and not just orthogonal to each other, the coefficient of the delta function must be 1. Therefore,

$$\begin{aligned}1 &= |A|^2 \cdot 2\pi\\ \therefore |A|^2 &= \frac{1}{2\pi}\\ \therefore |A| &= \frac{1}{\sqrt{2\pi}}\end{aligned}$$

Hence, a single eigenstate cannot describe the physical state of the particle, but if more that one eigenstates are known, then together they can describe the physical state of the particle

18 The Commutator

Definition 15 (Commutator)**.** The commutation of two functions $\hat{A}$ and $\hat{B}$ is defined to be

$$\begin{aligned}\left[\hat{A}, \hat{B}\right] &= \hat{A}\hat{B} - \hat{B}\hat{A}\\ \therefore \left[\hat{A}, \hat{B}\right] f(x) &= \hat{A}\left(\hat{B}\left(f(x)\right)\right) - \hat{B}\left(\hat{A}\left(f(x)\right)\right)\end{aligned}$$

The operator which gives the commutation of two functions is called the commutator.

Theorem 20. *If*

$$\left[\hat{A}, \hat{B}\right] = 0$$

then $\hat{A}$ and $\hat{B}$ have some eigenfunctions in common.

Proof. Let a be an eigenvalue of $\hat{A}$, and let φ_a be an eigenfunction of $\hat{A}$.
Therefore,

$$\hat{A}\varphi_a = a\varphi_a$$

Therefore, applying $\hat{B}$ on the LHS, as the commutation is zero,

$$\hat{B}\hat{A}\varphi_a = \hat{A}\hat{B}\varphi_a$$

Therefore, applying $\hat{B}$ on the RHS,

$$\hat{B}a\varphi_a = a\hat{B}\varphi_a$$

Therefore,

$$\hat{A}\left(\hat{B}\varphi_a\right) = a\left(\hat{B}\varphi_a\right)$$

This equation is of the form

$$\hat{A}\varphi = a\varphi$$

Therefore, $\hat{B}\varphi_a$ is also an eigenfunction of $\hat{A}$ with eigenvalue a.
Hence, assuming there is no degeneracy in eigenvalues, i.e. every eigenvalue has a single corresponding eigenfunction, $\hat{B}$ cannot change φ_a, except by a constant.
Therefore,

$$\hat{B}\varphi_a = b\varphi_a$$

Therefore, φ_a is an eigenfunction of $\hat{B}$ corresponding to the eigenvalue b.
Hence there is a common eigenfunction for $\hat{A}$ and $\hat{B}$. $\square$

Exercise 7.
Find the commutation of $\hat{x}$ and $\hat{p}$.

Solution 7.

$$
\begin{aligned}
[\hat{x}, \hat{p}]\, f(x) &= \hat{x}\hat{p} f(x) - \hat{p}\hat{x} f(x) \\
&= (x)\left(-i\hbar \frac{\mathrm{d}}{\mathrm{d}x}\, f(x)\right) + i\hbar \frac{\mathrm{d}}{\mathrm{d}x}\,(x f(x)) \\
&= -i\hbar x f'(x) + i\hbar f(x) + i\hbar x f'(x) \\
&= i\hbar f(x)
\end{aligned}
$$

Therefore,

$$[\hat{x}, \hat{p}] = i\hbar \hat{I}$$

where $\hat{I}$ is the identity operator.

Exercise 8.
Can a wave function be an eigenfunction of both $\hat{x}$ and $\hat{p}$?

Solution 8.

$$
\begin{aligned}
\hat{x} f(x) &= x f(x) \\
\hat{p} f(x) &= -i\hbar \frac{\partial}{\partial x}\, f(x) \\
&= \hbar k f(x)
\end{aligned}
$$

Therefore, as the two equations cannot be solved simultaneously, the two operators cannot have a common eigenfunction.

Exercise 9.
Can any wave function be written as a superposition of momentum eigenstates?

Solution 9.
Therefore, as

$$f(x) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} F(k) e^{ikx}\, \mathrm{d}k$$

every $f(x)$ can be written in terms of e^{ikx}.
Hence, any wave function can be written as a superposition of momentum eigenstates.

Exercise 10.

It is impossible to demonstrate the wave-like behaviour of macroscopic objects as λ is too small. True of false?

Solution 10.

$$\lambda = \frac{h}{p}$$

Therefore, as the p for macroscopic objects is very large, the λ is very small. Hence, the statement is true.

Exercise 11.

If

$$\langle x \rangle = 0$$

then σ_p is infinite.
True of false?

Solution 11.

The standard deviation of the position, σ_x, is not known, and cannot be calculated using the given data. Therefore, as nothing is known about σ_x, nothing can be said about σ_p. Hence, the statement is false.

19 Schrödinger Equation in 1D for Separable Wave Functions

Let the wave function $\Psi(x,t)$ be separable, i.e. let is be expressible in the form

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

Let the potential V be independent of time, i.e. let it be a function of x only. Therefore, the Schrödinger equation is

$$\begin{aligned}
i\hbar\frac{\partial \Psi}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \\
&= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi \\
\therefore \left(i\hbar\frac{\partial}{\partial t}\right)\Psi &= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)(\psi(x)\varphi(t)) \\
\therefore i\hbar\left(\psi(x)\varphi'(t)\right) &= -\frac{\hbar^2}{2m}\psi''(x)\varphi(t) + V(x)\psi(x)\varphi(t) \\
\therefore i\hbar\frac{\varphi'(t)}{\varphi(t)} &= -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + V(x)
\end{aligned}$$

For both sides of the equation to be satisfied, they need to be constant.
Let this constant be E.
Therefore,

$$\begin{aligned}
\frac{\varphi'(t)}{\varphi(t)} &= \frac{E}{i\hbar} \\
&= -i\frac{E}{\hbar} \\
\therefore \varphi(t) &= c_1 e^{-\frac{iEt}{\hbar}}
\end{aligned}$$

The RHS of the equation is

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

Definition 16. The operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

is called the Hamiltonian or the energy operator.

Therefore,

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

Therefore, the E is the eigenvalue of $\hat{H}$ corresponding to $\psi(x)$.
Therefore,

$$\begin{aligned}
\Psi(x,t) &= \psi(x)\varphi(t) \\
&= \sum_n c_n\psi_n(x)e^{-\frac{iE_nt}{\hbar}}
\end{aligned}$$

Therefore, $\psi_n(x)$ is an eigenfunction of $\hat{H}$ with eigenvalue E_n.

Theorem 21.

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

20 Stationary States

Definition 17. A state with definite energy, $\psi(x)e^{-\frac{iEt}{\hbar}}$, is called a stationary state.

Theorem 22. *Any state can be expressed as a superposition of stationary states.*

$$\begin{aligned}\Psi(x,t) &= \psi(x)\varphi(t) \\ &= \sum_n c_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}}\end{aligned}$$

Theorem 23. *For a particle in a stationary state, the probability of finding the particle at some x is independent of time.*

Theorem 24. *For a particle in a stationary state, the expected value of x is independent of time.*

Theorem 25. *For a particle in a stationary state, the expected value of p is independent of time.*

Theorem 26. *For a particle in a stationary state, the expected value of any operator Q is independent of time.*

Theorem 27. *A definite state is a state of definite energy.*

Definition 18 (Kronecker delta function)**.** The Kronecker delta function is defined as

$$\delta_{ij} = \begin{cases} 1 & ; \quad i = j \\ 0 & ; \quad i \neq j \end{cases}$$

Theorem 28. *The coefficients in*

$$\Psi(x) = \sum_{m=1}^{\infty} c_m \psi_m(x)$$

are given by

$$c_m = \int_{-\infty}^{\infty} {\psi_m}^*(x) \Psi(x) \, \mathrm{d}x$$

Proof.

$$\int_{-\infty}^{\infty} \psi_m * (x)\Psi(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} \psi_m{}^*(x) \sum_{n=1}^{\infty} c_n \psi_n(x)\,\mathrm{d}x$$
$$= \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} c_n \psi_m{}^*(x)\psi_n(x)\,\mathrm{d}x$$
$$= \sum_{n=1}^{\infty} c_n \delta_{nm}$$
$$= c_m$$

As $\psi_m{}^*(x)$ and $\psi_n(x)$ are eigenfunctions of the Hamiltonian operator, their product is either 0 or 1 depending on the combination of m and n. If $m = n$, then the product is 1, otherwise the product is 0. Therefore, the product can be expressed as the Kronecker delta function. $\square$

Theorem 29. *For a general state*

$$\psi(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

the expected value of the Hamiltonian operator is

$$\langle H \rangle = \sum_{n=1}^{\infty} P(E = E_n) E_n$$

Proof.

$$\begin{aligned}
\langle H \rangle &= \int_{-\infty}^{\infty} \psi^*(x) \hat{H} \psi(x) \,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} \left(\sum_{n=1}^{\infty} {c_n}^* {\psi_n}^*(x) \right) \hat{H} \left(\sum_{n=1}^{\infty} c_n \psi_n(x) \right) \mathrm{d}x \\
&= \int_{-\infty}^{\infty} \sum_{n=1}^{\infty} {c_n}^* {\psi_n}^*(x) \sum_{m=1}^{\infty} c_m E_m \psi_m(x) \,\mathrm{d}x \\
&= \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} {c_n}^* c_m E_m \int_{-\infty}^{\infty} \psi_n(x) \psi_m(x) \,\mathrm{d}x \\
&= \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} {c_n}^* c_n E_n \delta_{nm} \\
&= \sum_{n=1}^{\infty} {c_n}^* c_n E_n \\
&= \sum_{n=1}^{\infty} |c_n|^2 E_n \\
&= \sum_{n=1}^{\infty} P(E = E_n) E_n
\end{aligned}$$

□

21 Infinite Potential Wells

Consider an infinite square well, from $x = 0$ to $x = a$, with the potential given by

$$V(x) = \begin{cases} \infty & ; \quad x < 0 \\ 0 & ; \quad 0 < x < a \\ \infty & ; \quad a < x \end{cases}$$

Consider a particle with mass m, under this potential.
Therefore,

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

Therefore,

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + V(x)\psi(x) = E\psi(x)$$

For $x < 0$,

$$V(x) = \infty$$

Therefore,

$$\psi(x) = 0$$

For $a < x$,

$$V(x) = \infty$$

Therefore,

$$\psi(x) = 0$$

For $0 < x < a$,

$$V(x) = 0$$

Therefore,

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = E\psi(x)$$
$$\therefore \frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = -\frac{2mE}{\hbar^2}$$

Let

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

Therefore, for $0 < x < a$,

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

Therefore, at the boundaries,

$$\psi(x = 0) = 0$$
$$\psi(x = a) = 0$$

Therefore, for $\psi(0) = 0$,

$$\begin{aligned} A\sin(0) + B\cos(0) &= 0 \\ \therefore B &= 0 \end{aligned}$$

Therefore, for $\psi(a) = 0$,

If A is zero, the wave function will not be normalizable. Therefore, A cannot be zero. Hence, $\sin(ka)$ has to be zero.

$$\begin{aligned} A\sin(ka) &= 0 \\ \therefore \sin ka &= 0 \end{aligned}$$

Therefore, for $n \in \mathbb{N}$,

$$ka = n\pi$$

Therefore,

$$k_n = \frac{n\pi}{a}$$

Therefore,

$$\begin{aligned} k &= \sqrt{\frac{2mE}{\hbar^2}} \\ \therefore \frac{n\pi}{a} &= \sqrt{\frac{2mE}{\hbar^2}} \\ \therefore E &= \frac{\pi^2 n^2 \hbar^2}{2ma^2} \end{aligned}$$

Therefore,

$$\begin{aligned} \psi_n(x) &= A\sin(k_n x) \\ &= A\sin\left(\frac{n\pi}{a}x\right) \end{aligned}$$

Therefore, normalizing the wave function,

$$A = \sqrt{\frac{2}{a}}$$

Therefore,

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

Therefore,

$$\begin{aligned}\psi(x) &= \sum_{n=1}^{\infty} c_n \psi_n(x) \\ &= \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)\end{aligned}$$

Therefore, the probability distribution of x is as shown in Figure 8 and Figure 9.

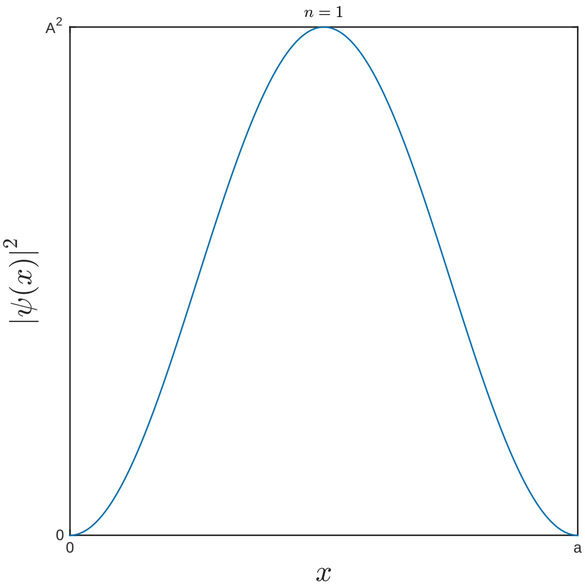


Figure 8: Probability distribution of x, with $n = 1$, in an infinite square well

Therefore, as these states are stationary

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-\frac{iE_n t}{\hbar}}$$

Exercise 12.
The wave function of a particle of mass m in an infinite square well from $x = 0$ to $x = a$, at time $t = 0$ is given by

$$\psi(x,0) = Ax(a-x)$$

for $0 < x < a$.

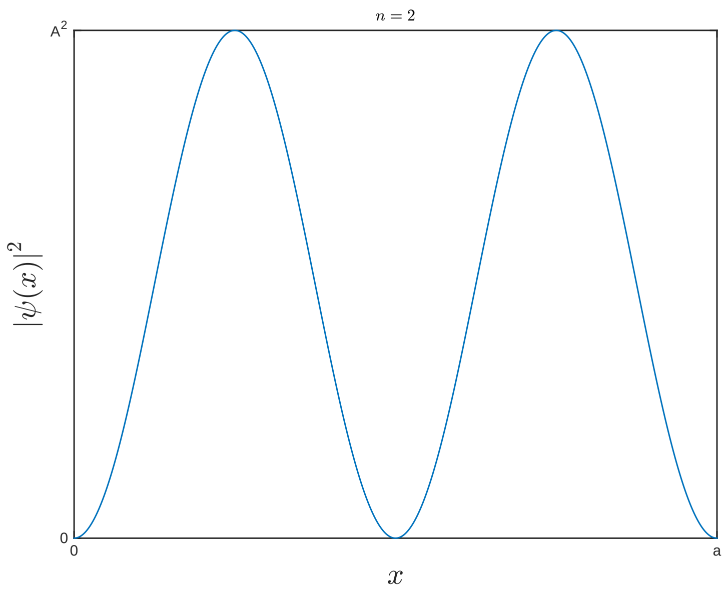


Figure 9: Probability distribution of x, with $n = 2$, in an infinite square well

1. Find the general wave function $\psi(x,t)$.

2. What is the probability of measuring the following energies at time $t = 0$?

   (a) $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$

   (b) $E_2 = \frac{4\pi^2\hbar^2}{2ma^2}$

   (c) $E_3 = \frac{9\pi^2\hbar^2}{2ma^2}$

Solution 12.

1.

$$1 = \int_0^a A^2 x^2 (a-x)^2 \, \mathrm{d}x$$

Therefore, solving,

$$A = \sqrt{\frac{30}{a^5}}$$

Therefore,

$$Ax(a-x) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

Therefore,

$$\begin{aligned} c_n &= \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) Ax(a-x)\,\mathrm{d}x \\ &= \sqrt{\frac{2}{a}} Aa \int_0^a \sin\left(\frac{n\pi}{a}x\right) \mathrm{d}x - \sqrt{\frac{2}{a}} A \int_0^a \sin\left(\frac{n\pi}{a}x\right) x^2\,\mathrm{d}x \end{aligned}$$

Therefore,

$$c_n = \begin{cases} 0 & ; \quad n \text{ is even} \\ \frac{8\sqrt{15}}{n^3\pi^3} & ; \quad n \text{ is odd} \end{cases}$$

Therefore,

$$\psi(x,t) = \sum_{n=1,3,5,\dots} \sqrt{\frac{2}{a}} \frac{8\sqrt{15}}{n^3\pi^3} \sin\left(\frac{n\pi}{a}x\right) e^{-\frac{iE_n t}{\hbar}}$$

where

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

2. (a)

$$\begin{aligned} P(E=E_1) &= |c_1|^2 \\ &= \left(\frac{8\sqrt{15}}{\pi^3}\right) \\ &= 0.9986 \end{aligned}$$

(b)

$$\begin{aligned} P(E=E_2) &= |c_2|^2 \\ &= 0 \end{aligned}$$

For even n, c_n is zero.

(c)

$$\begin{aligned}P(E=E_3) &= |c_3|^2 \\ &= \left(\frac{8\sqrt{15}}{27\pi^3}\right) \\ &= 0.0014\end{aligned}$$

Exercise 13.
A particle with mass m in an infinite square wall, has initial wave function

$$\psi(x,0) = A\left(\psi_1(x) + \psi_2(x)\right)$$

1. Find A.
2. Find the general wave function $\psi(x,t)$.
3. What is the probability of measuring the following energies at time $t = 0$?
   (a) $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$
   (b) $E_2 = \frac{4\pi^2\hbar^2}{2ma^2}$
4. Find the wave function if the energy is measured to be E_1.
5. Find the expectation value of x.

Solution 13.
1. As the square of the coefficients represents the probability of a particular value,

$$\begin{aligned}1 &= \sum_{n=1}^{\infty} |c_n|^2 \\ &= 2A^2 \\ \therefore \frac{1}{\sqrt{2}} &= A\end{aligned}$$

2.

$$\begin{aligned}\psi(x,t) &= A\left(\psi_1(x)e^{-\frac{iE_1t}{\hbar}} + \psi_2(x)e^{-\frac{iE_2t}{\hbar}}\right) \\ &= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right)e^{-\frac{iE_1t}{\hbar}} + \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x\right)e^{-\frac{iE_2t}{\hbar}}\right)\end{aligned}$$

where

$$
\begin{aligned}
E_1 &= \frac{\pi^2\hbar^2}{2ma^2} \\
E_2 &= \frac{4\pi^2\hbar^2}{2ma^2}
\end{aligned}
$$

3. (a)

$$
\begin{aligned}
P(E = E_1) &= |c_1|^2 \\
&= \left| \frac{1}{\sqrt{2}} e^{-\frac{iE_1 t}{\hbar}} \right|^2 \\
&= \frac{1}{2}
\end{aligned}
$$

(b)

$$
\begin{aligned}
P(E = E_2) &= |c_2|^2 \\
&= \left| \frac{1}{\sqrt{2}} e^{-\frac{iE_2 t}{\hbar}} \right|^2 \\
&= \frac{1}{2}
\end{aligned}
$$

4. If E is measured to be E_1, then the wave function collapsed to

$$
\psi(x) = \psi_1(x) e^{-\frac{iE_1 t}{\hbar}}
$$

5. At time t,

$$
\begin{aligned}
\langle x \rangle_t &= \int_0^a x \left| \psi(x,t) \right|^2 \mathrm{d}x \\
&= A^2 \int_0^a x \left({\psi_1}^*(x) e^{\frac{iE_1 t}{\hbar}} + {\psi_2}^*(x) e^{\frac{iE_2 t}{\hbar}} \right) \left(\psi_1(x) e^{-\frac{iE_1 t}{\hbar}} + \psi_2(x) e^{-\frac{iE_2 t}{\hbar}} \right) \mathrm{d}x \\
&\neq \langle x \rangle_{t=0}
\end{aligned}
$$

22 Free Particles

For a free particle,

$$V(x) = 0$$

Therefore,

$$\begin{aligned}
\hat{H}\psi(x) &= E\psi(x) \\
\therefore -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} &= E\psi(x) \\
\therefore \frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} &= -\frac{2Em\psi(x)}{\hbar^2} \\
&= -k^2\psi(x)
\end{aligned}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

Therefore,

$$\psi(x) = Ae^{ikx}$$

However, this wave function is not normalizable. Hence, a free particle cannot exist in a stationary state.

The general solution to the time-dependent Schrödinger equation is a linear combination of separable solutions, i.e.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int\limits_{-\infty}^{\infty} \varphi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} \, \mathrm{d}k$$

This function can be normalized, but it carries a multiple ks, and hence multiple energies and speeds.

Definition 19 (Wave packet)**.** A solution of the form

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int\limits_{-\infty}^{\infty} \varphi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} \, \mathrm{d}k$$

is called a wave packet.

Therefore, for $t = 0$,

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} \varphi(k) e^{ikx} \, \mathrm{d}k$$

Therefore,

$$\varphi(k) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} \, \mathrm{d}x$$

Exercise 14.

A free particle, initially localized as

$$\psi(x,0) = \begin{cases} A & ; \quad x \in (-a,a) \\ 0 & ; \quad x \notin (-a,a) \end{cases}$$

where A and a are real and positive.
Find $\psi(x,t)$.

Solution 14.

$$\begin{aligned} 1 &= \int\limits_{-\infty}^{\infty} |\psi(x,0)|^2 \, \mathrm{d}x \\ &= \int\limits_{-a}^{a} A^2 \, \mathrm{d}x \\ &= 2aA^2 \end{aligned}$$

Therefore,

$$A = \frac{1}{\sqrt{2a}}$$

Therefore, taking the inverse Fourier transform,

$$
\begin{aligned}
\widetilde{\psi}(k) &= \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} \psi(x,0) e^{-ikx} \, \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \int\limits_{-a}^{a} e^{-ikx} \, \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \int\limits_{-a}^{a} e^{-ikx} \, \mathrm{d}x \\
&= \frac{1}{\sqrt{4\pi a}} \, \frac{1}{-ik} e^{-ikx} \Big|_{-a}^{a} \\
&= \frac{1}{\sqrt{4\pi a}} \frac{1}{-ik} \left(e^{-ika} - e^{ika} \right) \\
&= \frac{1}{\sqrt{\pi a}} \frac{1}{k} \frac{e^{ika} - e^{-ika}}{2i} \\
&= \frac{1}{k\sqrt{\pi a}} \sin(ka)
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\psi(x,t) &= \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} \widetilde{\psi}(k) e^{ikx} e^{-\frac{iEt}{\hbar}} \, \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi^2 a}} \int\limits_{-\infty}^{\infty} \frac{\sin(ka)}{k} e^{ikx} e^{-\frac{ik^2\hbar}{2m} t} \, \mathrm{d}k
\end{aligned}
$$

If a is very small,

$$
\begin{aligned}
\widetilde{\psi}(k) &= \frac{\sin(ka)}{k\sqrt{\pi a}} \\
&= \frac{ka}{k\sqrt{\pi a}} \\
&= \sqrt{\frac{a}{\pi}}
\end{aligned}
$$

If a is very large,

$$\begin{aligned}
\widetilde{\psi}(k) &= \frac{\sin(ka)}{k\sqrt{\pi a}} \\
&= \sqrt{\frac{a}{\pi}}\frac{\sin(ka)}{ka} \\
&= \sqrt{\frac{a}{\pi}}\operatorname{sinc}(ka)
\end{aligned}$$

23 Finite Potential Wells

Definition 20 (Bound state)**.** An eigenfunction of $\hat{H}$, which satisfies

$$\begin{aligned}
\lim_{x\to\infty} \psi(x) &= 0 \\
\lim_{x\to-\infty} \psi(x) &= 0
\end{aligned}$$

is called a bound state.

Definition 21 (Scattering state)**.** An eigenfunction of $\hat{H}$, which satisfies

$$\begin{aligned}
\lim_{x\to\infty} \psi(x) &\neq 0 \\
\lim_{x\to-\infty} \psi(x) &\neq 0
\end{aligned}$$

is called a scattering state.

Theorem 30. *A particle in a finite or infinite well is in a bound state.*

Theorem 31. *A free particle is in a scattering state.*

Consider a finite square well such that

$$V(x) = \begin{cases} -V_0 & ; \quad x \in (-a, a) \\ 0 & ; \quad x \notin (-a, a) \end{cases}$$

Consider a particle with energy $-V_0 < E < 0$.
For $x < -a$,

$$V = 0$$

Therefore,

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = -\frac{2mE}{\hbar^2}\psi(x)$$

Let

$$k = \sqrt{-\frac{2mE}{\hbar^2}}$$

Therefore if $E < 0$, k is real.
Therefore,

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = k^2\psi(x)$$

Therefore,

$$\psi(x) = Ae^{kx} + Be^{-kx}$$

For the wave function to be normalizable, $\lim\limits_{x\to\infty} \psi(x)$ must be zero.
Therefore,

$$\begin{aligned} 0 &= \lim_{x\to-\infty} \psi(x) \\ &= \lim_{x\to-\infty} Ae^{kx} + Be^{-kx} \end{aligned}$$

Therefore B must be zero.
Therefore,

$$\psi(x) = Ae^{kx}$$

Similarly, for $x > a$,

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

where

$$k = \sqrt{-\frac{2mE}{\hbar^2}}$$

For $-a < x < a$,

$$\begin{aligned} \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} &= -\frac{2m}{\hbar}\left(E - V(x)\right)\psi(x) \\ &= -\frac{2m}{\hbar}(E + V_0)\psi(x) \end{aligned}$$

Let

$$\beta = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

Therefore,

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = -\beta^2\psi(x)$$

Therefore,

$$\psi(x) = D\cos(\beta x) + F\sin(\beta x)$$

Therefore,

$$\psi(x) = \begin{cases} Ae^{kx} & ; \quad x < -a \\ D\cos(\beta x) + F\sin(\beta x) & ; \quad -a < x < a \\ Ce^{-kx} & ; \quad a < x \end{cases}$$

where

$$k = \sqrt{-\frac{2mE}{\hbar^2}}$$
$$\beta = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

Theorem 32. *If $V(x)$ is an even function, then the eigenfunctions of $\hat{H}$ are either odd or even.*

23.1 Even Wave Functions for Finite Potential Wells

If $\psi(x)$ is even,

$$\psi(x) = \begin{cases} Ae^{kx} & ; \quad x < -a \\ D\cos(\beta x) & ; \quad -a < x < a \\ Ce^{-kx} & ; \quad a < x \end{cases}$$

As $|\psi(x)|^2$ represents probability, $\psi(x)$ must always be continuous.
As the well is finite, the jump in the expression of $V(x)$ is also finite. Hence, $\psi'(x)$ must always be continuous.
Therefore, as $\psi(x)$ is always continuous,

$$Ae^{-ka} = D\cos(-\beta a)$$

Therefore, as $\psi'(x)$ is always continuous,

$$kAe^{-ka} = \beta D \cos(\beta a)$$

Similarly, for $x = a$,

$$\begin{aligned} Ce^{-ka} &= D\cos(\beta a) \\ -kCe^{-ka} &= -\beta D \sin(\beta a) \end{aligned}$$

Therefore,

$$A = C$$

Therefore,

$$k = \beta \tan(\beta a)$$

where

$$\begin{aligned} k &= \sqrt{\frac{-2mE}{\hbar^2}} \\ \beta &= \sqrt{\frac{2m(E+V_0)}{\hbar^2}} \end{aligned}$$

Let

$$\begin{aligned} z &= \beta a \\ y &= ka \end{aligned}$$

Therefore,

$$\begin{aligned} k &= \beta \tan(\beta a) \\ \therefore ka &= \beta a \tan(\beta a) \\ \therefore y &= z \tan(z) \end{aligned}$$

Also,

$$\begin{aligned} \beta^2 + k^2 &= \frac{2mV_0}{\hbar^2} \\ \therefore z^2 + y^2 &= a^2\left(\beta^2 + z^2\right) \\ &= \frac{2mV_0 a^2}{\hbar^2} \end{aligned}$$

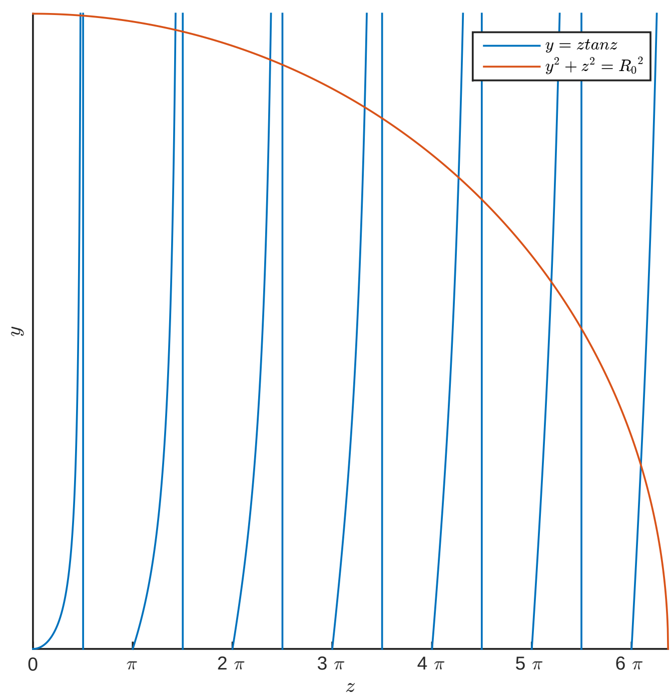
Let

$$R_0{}^2 = \frac{2mV_0a^2}{\hbar^2}$$

Therefore,

$$z^2 + y^2 = R_0{}^2$$

As a, k, and B are real and positive, z and y also must be real and positive. Therefore,



As the two graphs must intersect at least once, the equation has at least one solution.
If $R_0 < \pi$, the graphs intersect exactly once. Hence, if $R_0 < \pi$, there exists a single solution.
If $R_0 \to \infty$, there are infinitely many solutions, $z = \frac{n\pi}{2}$, where n is odd. Hence,

$$z_n = \frac{n\pi}{2}$$
$$\therefore \beta_n = \frac{n\pi}{2a}$$

Exercise 15.
The potential is given by

$$V(x) = \begin{cases} \infty & ; \quad x < 0 \\ 0 & ; \quad 0 < x < L \\ V_0 & ; \quad L < x \end{cases}$$

Solve for the bound states for $E < V_0$.

Solution 15.
For $x < 0$,

$$\psi(x) = 0$$

For $0 < x < L$,

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

For $x > L$,

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

where

$$\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

For ψ to be continuous at $x = L$, and ψ and ψ' to be continuous at $x = 0$,

$$\begin{aligned} B &= 0 \\ A\sin(kL) &= Ce^{-\alpha L} \\ kA\cos(kL) &= -\alpha Ce^{-\alpha L} \end{aligned}$$

Therefore,

$$\begin{aligned} k\cot(kL) &= -\alpha \\ \therefore kL\cot(kL) &= -\alpha L \end{aligned}$$

Let

$$
\begin{aligned}
z &= kL \\
y &= \alpha L
\end{aligned}
$$

Therefore,

$$z\cot(z) = -y$$

Also,

$$
\begin{aligned}
\alpha^2 + k^2 &= \frac{2mV_0}{\hbar^2} \\
\therefore \alpha^2 L^2 + k^2 L^2 &= \frac{2mV_0 L^2}{\hbar^2} \\
\therefore y^2 + z^2 &= \frac{2mV_0 L^2}{\hbar^2}
\end{aligned}
$$

23.2 Odd Wave Functions for Finite Potential Wells

If $\psi(x)$ is odd,

$$
\psi(x) = \begin{cases} Ae^{kx} & ; \quad x < -a \\ F\sin(\beta x) & ; \quad -a < x < a \\ Ce^{-kx} & ; \quad a < x \end{cases}
$$

As $|\psi(x)|^2$ represents probability, $\psi(x)$ must always be continuous.
As the well is finite, the jump in the expression of $V(x)$ is also finite. Hence, $\psi'(x)$ must always be continuous.
Therefore, as $\psi(x)$ is always continuous,

$$Ae^{-ka} = F\sin(-\beta a)$$

Therefore, as $\psi'(x)$ is always continuous,

$$kAe^{-ka} = \beta F\cos(-\beta a)$$

Similarly, for $x = a$,

$$
\begin{aligned}
Ce^{-ka} &= F\sin(\beta a) \\
-kCe^{-ka} &= \beta F\cos(\beta a)
\end{aligned}
$$

Therefore,

$$A = -C$$

Therefore,

$$-k = \beta \cot(\beta a)$$

where

$$\begin{aligned} k &= \sqrt{\frac{-2mE}{\hbar^2}} \\ \beta &= \sqrt{\frac{2m(E+V_0)}{\hbar^2}} \end{aligned}$$

Let

$$\begin{aligned} z &= \beta a \\ y &= ka \end{aligned}$$

Therefore,

$$\begin{aligned} k &= -\beta \cot(\beta a) \\ \therefore ka &= -\beta a \cot(\beta a) \\ \therefore y &= -z \cot(z) \end{aligned}$$

Also,

$$\begin{aligned} \beta^2 + k^2 &= \frac{2mV_0}{\hbar^2} \\ \therefore z^2 + y^2 &= a^2 \left(\beta^2 + z^2\right) \\ &= \frac{2mV_0 a^2}{\hbar^2} \end{aligned}$$

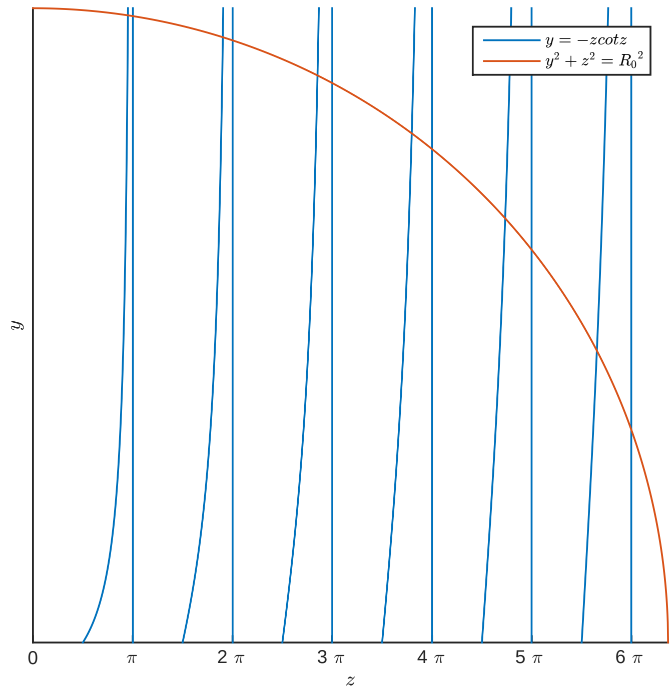
Let

$$R_0{}^2 = \frac{2mV_0 a^2}{\hbar^2}$$

Therefore,

$$z^2 + y^2 = R_0{}^2$$

As a, k, and B are real and positive, z and y also must be real and positive. Therefore,



If $R_0 < \frac{\pi}{2}$, the two graphs do not intersect. Therefore, there is no solution. If $R_0 \to \infty$, there are infinitely many solution, $z = n\pi$, where n is positive.

$$\begin{aligned} z_n &= n\pi \\ \therefore \beta_n &= \frac{n\pi}{a} \end{aligned}$$

24 $\delta(x)$ Potential

Consider a potential

$$V(x) = -V_0 \delta(x)$$

Therefore, for $x < 0$,

$$\begin{aligned} \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} &= -\frac{2m}{\hbar^2}\left(E - V(x)\right)\psi \\ &= -\frac{2mE}{\hbar^2}\psi \end{aligned}$$

Let

$$k = \sqrt{-\frac{2mE}{\hbar^2}}$$

Therefore, for $E < 0$, k is real.
Therefore,

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = k^2\psi$$

Therefore,

$$\psi(x) = Ae^{kx} + Be^{-kx}$$

If $x \to \infty$, as the function is normalizable, $\psi = 0$.
Therefore,

$$B = 0$$

Similarly, for $x > 0$,

$$\psi(x) = Ce^{kx} + De^{-kx}$$

If $x \to -\infty$, as the function is normalizable, $\psi = 0$.
Therefore,

$$C = 0$$

Therefore,

$$\psi(x) = \begin{cases} Ae^{kx} & ; \quad x < 0 \\ Ce^{-kx} & ; \quad x > 0 \end{cases}$$

Therefore, as $\psi(x)$ represents probability, it is continuous at $x = 0$.
Therefore,

$$A = C$$

Therefore,

$$\psi(x) = \begin{cases} Ae^{kx} & ; \quad x < 0 \\ Ae^{-kx} & ; \quad x > 0 \end{cases}$$

Therefore,

$$\psi'(x) = \begin{cases} Ake^{kx} & ; \quad x < 0 \\ -Ake^{-kx} & ; \quad x > 0 \end{cases}$$

By the time independent Schrödinger equation,

$$\psi''(x) = -\frac{2m}{\hbar^2}\left(E + V_0\delta(x)\right)\psi$$

Therefore,

$$\begin{aligned}
\int\limits_{-\varepsilon}^{\varepsilon} \psi''(x)\,\mathrm{d}x &= -\frac{2m}{\hbar^2}\left(E + V_0\delta(x)\right)\psi(x)\,\mathrm{d}x \\
\therefore \psi'(\varepsilon) - \psi'(-\varepsilon) &= -\frac{2m}{\hbar^2}\int\limits_{-\varepsilon}^{\varepsilon} E\psi(x)\,\mathrm{d}x - \frac{2m}{\hbar^2}\int\limits_{-\varepsilon}^{\varepsilon} V_0\delta(x)\psi(x)\,\mathrm{d}x \\
&= -\frac{2m}{\hbar^2}\left(E\psi(0)\cdot 2\varepsilon\right) - \frac{2m}{\hbar^2}V_0\psi(0) \\
&= -\frac{2m}{\hbar^2}V_0\psi(0) \\
\therefore -kA - kA &= -\frac{2m}{\hbar^2}V_0 A \\
\therefore k &= \frac{mV_0}{\hbar^2}
\end{aligned}$$

Therefore,

$$\begin{aligned}
k &= \sqrt{-\frac{2mE}{\hbar^2}} \\
\therefore E &= -\frac{k^2\hbar^2}{2m} \\
&= -\frac{m{V_0}^2}{2\hbar^2}
\end{aligned}$$

Normalizing,

$$\begin{aligned}
A &= \sqrt{k} \\
&= \sqrt{\frac{mV_0}{\hbar^2}}
\end{aligned}$$

25 Tunneling

Consider a potential

$$V(x) = \begin{cases} 0 & ; \quad x < 0 \\ V_0 & ; \quad x > 0 \end{cases}$$

Therefore, for $x < 0$,

$$\begin{aligned} \frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} &= -\frac{2m}{\hbar^2}\left(E - V(x)\right)\psi(x) \\ &= -\frac{2m}{\hbar^2}E\psi(x) \end{aligned}$$

Let

$$k_1 = \frac{2mE}{\hbar^2}$$

Therefore,

$$\psi'' = -{k_1}^2\psi$$

Therefore, for $x > 0$,

$$\begin{aligned} \frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} &= -\frac{2m}{\hbar^2}\left(E - V(x)\right)\psi(x) \\ &= -\frac{2m}{\hbar^2}(E - V_0)\psi(x) \end{aligned}$$

Let

$$k_2 = -\frac{2m(E - V_0)}{\hbar^2}$$

Therefore,

$$\psi'' = {k_2}^2\psi$$

Therefore,

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & ; \quad x < 0 \\ Ce^{k_2x} + De^{-k_2x} & ; \quad x > 0 \end{cases}$$

For the function to be normalizable, for $x \to \infty$, $\psi = 0$.
Therefore,

$$C = 0$$

Therefore,

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & ; \quad x < 0 \\ De^{-k_2x} & ; \quad x > 0 \end{cases}$$

25.1 Finite Barrier

Consider a potential

$$V(x) = \begin{cases} 0 & ; \quad x < 0 \\ V_0 & ; \quad 0 < x < a \\ 0 & ; \quad a < x \end{cases}$$

Therefore, this potential can be considered to be

$$V(x) = V_1(x) - V_2(x)$$

where

$$V_1(x) = \begin{cases} 0 & ; \quad x < 0 \\ V_0 & ; \quad x > 0 \end{cases}$$

$$V_2(x) = \begin{cases} 0 & ; \quad x < a \\ V_0 & ; \quad x > a \end{cases}$$

Hence, due to tunnelling, a quantum particle can go through this barrier, and the wave function is

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x} & ; \quad x < 0 \\ De^{-k_1 x} & ; \quad 0 < x < a \\ Fe^{ik_1 x} + Ge^{-ik_1 x} & ; \quad a < x \end{cases}$$

25.2 δ Barrier

Consider a potential

$$V(x) = V_0 \delta(x)$$

Consider a single particle approaching the δ barrier from the left.
Therefore, solving the time independent Schrödinger equation,

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & ; \quad x < 0 \\ Ce^{ikx} + De^{-ikx} & ; \quad 0 < x \end{cases}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

Therefore, Ae^{ikx} represents the incident wave, Be^{-ikx} represents the reflected wave, and Ce^{ikx} represents the transmitted wave.
As a single particle approaches the barrier from the left, the wave represented by De^{-ikx} does not exist. Hence,

$$D = 0$$

Therefore,

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & ; \quad x < 0 \\ Ce^{ikx} & ; \quad 0 < x \end{cases}$$

As $\psi(x)$ is continuous at $x = 0$,

$$A + B = C$$

Therefore, solving,

$$\psi(x) = \begin{cases} ik\left(Ae^{ikx} - Be^{-ikx}\right) & ; \quad x < 0 \\ ikCe^{ikx} & ; \quad 0 < x \end{cases}$$

As the barrier is a Dirac Delta function,

$$\psi'(\varepsilon) - \psi'(-\varepsilon) = \frac{2mv_0}{\hbar^2}\psi(0)$$

Therefore,

$$(ikC) - (ikA - ikB) = \frac{2mv_0}{\hbar^2}\psi(0)$$

Let

$$\beta = \frac{mv_0}{\hbar^2 k}$$

Therefore,

$$\frac{B}{A} = \frac{i\beta}{1 + i\beta}$$
$$\frac{C}{A} = \frac{1}{1 - i\beta}$$

Similarly, if

$$V(x) = -V_0\delta(x)$$

then,

$$\psi'(\varepsilon) - \psi'(-\varepsilon) = -\frac{2mv_0}{\hbar^2}\psi(0)$$

Therefore,

$$(ikC) - (ikA - ikB) = -\frac{2mv_0}{\hbar^2}\psi(0)$$

Let

$$\beta = \frac{mv_0}{\hbar^2 k}$$

Therefore,

$$\frac{B}{A} = -\frac{i\beta}{1+i\beta}$$
$$\frac{C}{A} = \frac{1}{1+i\beta}$$

25.3 Double δ Barrier

Consider a potential

$$V(x) = -\alpha\left(\delta(x+a) + \delta(x-a)\right)$$

Therefore,

$$\psi(x) = \begin{cases} Ae^{kx} & ; \quad x < -a \\ Be^{kx} + Ce^{-kx} & ; \quad -a < x < a \\ De^{-kx} & ; \quad a < x \end{cases}$$

where

$$k = \sqrt{-\frac{2mE}{\hbar^2}}$$

Therefore,

$$\psi(-a+\varepsilon) = \psi(-a-\varepsilon)$$
$$\psi(a+\varepsilon) = \psi(a-\varepsilon)$$
$$\psi'(-a+\varepsilon) - \psi'(-a-\varepsilon) = -\frac{2m\alpha}{\hbar^2}\psi(-a)$$
$$\psi'(a+\varepsilon) - \psi'(a-\varepsilon) = -\frac{2m\alpha}{\hbar^2}\psi(a)$$

As $V(x)$ is even, the wave function $\psi(x)$ can be split into odd and even parts, i.e. $\psi_{\text{even}}(x)$ and $\psi_{\text{odd}}(x)$
Therefore, for $\psi_{\text{even}}(x)$,

$$\begin{aligned}
A &= D \\
B &= C
\end{aligned}$$

Therefore,

$$\psi_{\text{even}}(x) = \begin{cases} Ae^{kx} & ; \quad x < -a \\ B\left(e^{kx} + e^{-kx}\right) & ; \quad -a < x < a \\ Ae^{-kx} & ; \quad a < x \end{cases}$$

Therefore,

$$\psi'(x) = \begin{cases} kAe^{kx} & ; \quad x < -a \\ kB\left(e^{kx} - e^{-kx}\right) & ; \quad -a < x < a \\ -kAe^{-kx} & ; \quad a < x \end{cases}$$

Therefore,

$$\begin{aligned}
\psi(-a+\varepsilon) &= \psi(-a-\varepsilon) \\
\therefore Ae^{-ka} B &\left(e^{-ka} + e^{ka}\right) \\
\psi'(-a+\varepsilon) - \psi'(-a-\varepsilon) &= -\frac{2m\alpha}{\hbar^2}\psi(-a) \\
\therefore kB\left(e^{-ka} - e^{ka}\right) - kAe^{-ka} &= -\frac{2m\alpha}{\hbar^2}Ae^{-ka}
\end{aligned}$$

Therefore, solving,

$$\begin{aligned}
A &= B\left(e^{2ka} + 1\right) \\
B\left(e^{2ka} - 1\right) &= A\left(\frac{2m\alpha}{\hbar^2 k} - 1\right)
\end{aligned}$$

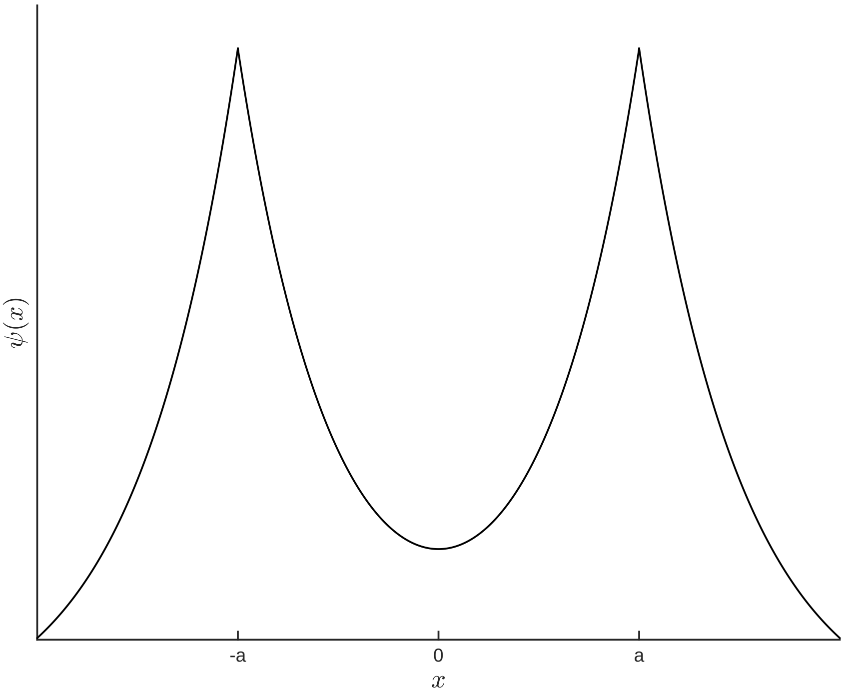
Let

$$\begin{aligned}
z &= 2ka \\
c &= \frac{\hbar^2}{2am\alpha}
\end{aligned}$$

Therefore,

$$
\begin{aligned}
e^{-2ka} &= \frac{\hbar^2 k}{m\alpha} - 1 \\
\therefore e^{-z} &= cz - 1
\end{aligned}
$$

Therefore, this equation has exactly one solution.



Therefore, for $\psi_{\text{odd}}(x)$,

$$
\begin{aligned}
A &= -D \\
B &= -C
\end{aligned}
$$

Therefore,

$$
\psi_{\text{even}}(x) = \begin{cases} -Ae^{kx} & ; \quad x < -a \\ B\left(e^{kx} - e^{-kx}\right) & ; \quad -a < x < a \\ Ae^{-kx} & ; \quad a < x \end{cases}
$$

26 Probability Current

Definition 22 (Probability current)**.** The rate at which the probability distribution passes through the position x is defined to be the probability current. It is denoted as

$$J(x,t) = \frac{i\hbar}{2m}\left(\psi\,\frac{\partial\psi^*}{\partial x} - \psi^*\,\frac{\partial\psi}{\partial x}\right)$$

Part II

Solid State Physics

1 Lecturer Information

Tammy Ben-Yaacov

E-mail: tammybenyaacov@gmail.com

2 Required Reading

1. Streetman, B. Solid State Electronic Devices

3 Additional Reading

1. Kittel, Introduction to solid state physics, John Wiley & Sons.
2. Pierret. Advanced semiconductor Fundamentals, Prentice Hall.
3. Ashcroft, Solid State Physics, Harcourt college publishers.

4 Electrons

Definition 23 (Particle nature of electrons)**.** An electron behaves as a negatively charged charge carrying particle.
The magnitude of the charge on it is

$$q = 1.602 \times 10^{-19}\,\mathrm{C}$$

Its mass is

$$m_0 = 9.11 \times 10^{-31}\,\mathrm{kg}$$

Definition 24 (Wave nature of electrons)**.** Electrons exhibit wave-like properties, in addition to particle-like properties.
The energy transmitted by a wave is

$$\begin{aligned} E &= h\nu \\ &= \frac{hc}{\lambda} \end{aligned}$$

where

$$\begin{aligned} h &= \text{Planck's constant} \left(6.626 \times 10^{-34}\right) \\ \nu &= \text{frequency} \\ c &= \text{speed of light} \\ \lambda &= \text{wavelength} \end{aligned}$$

5 Semiconductors

Law 1 (Ohm's Law)**.** *The voltage across two points on a conductor is directly proportional to the current through the conductor. The constant of proportionality is called the resistance of the conductor.*

$$\frac{V}{I} = R$$

Law 2 (Microscopic Ohm's Law)**.**

$$\overrightarrow{J} = \sigma \overrightarrow{E}$$

where $\overrightarrow{J}$ is the current density, σ is the conductivity, $\overrightarrow{E}$ is the electric field in the resistor.

Definition 25 (Resistivity)**.** If

$$R = \rho \frac{L}{A}$$

where R is the resistance of the resistor, L is the length of the resistor, and A is the cross-sectional area of the resistor, then ρ is called the resistivity of the resistor.
$\sigma = \frac{1}{\rho}$ is called the conductivity of the resistor.
They are constant for a particular material.

5.1 Control Factors

The major factors which affect the conductivity of a material are

1. Temperature
2. Chemical composition
   (a) Atomic bonding
   (b) Crystal structure
   (c) Charge carriers in the crystal
3. Optical effects
4. Doping

5.2 Chemical Makeup

II	III	IV	V	VI
	B	C	N	O
	Al	Si	P	S
Zn	Ga	Ge	As	
Cd	In			

Silicon is usually used as a semiconductor, as it

1. is easily available, hence economical
2. performs better at higher temperatures
3. can be converted to silica on heating

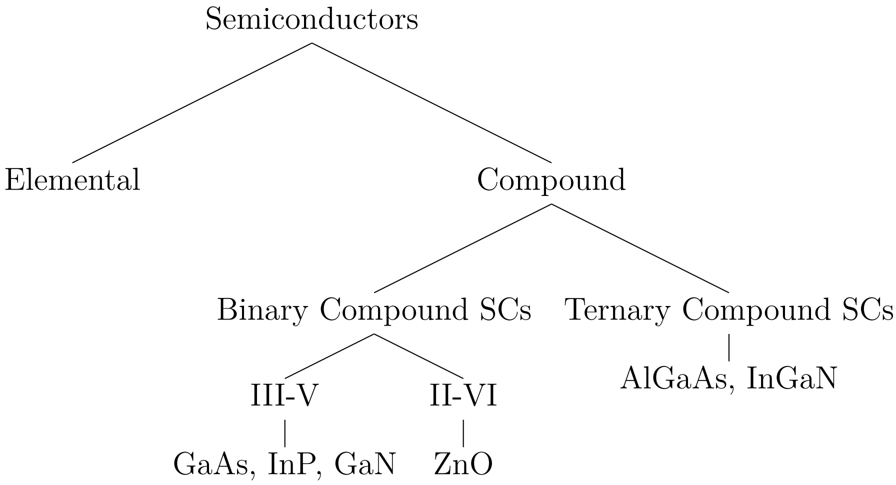


Figure 10: Classification of Semiconductors

Exercise 16.
A sample of Germanium has resistivity $\rho = 0.46\Omega\,\text{m}$. The dimensions of the sample are

$$\begin{aligned} l &= 50\text{µm} \\ h &= 0.2\text{µm} \\ w &= 1\text{µm} \end{aligned}$$

Find the resistance of the sample and the conductivity of the material.

Solution 16.

$$\begin{aligned} \rho &= 0.46\Omega\,\text{m} \\ &= 46\Omega\,\text{cm} \end{aligned}$$

Therefore,

$$\begin{aligned} \sigma &= \frac{1}{\rho} \\ &= \frac{1}{46\Omega\,\text{cm}} \\ &= 0.022\frac{1}{\Omega\,\text{cm}} \end{aligned}$$

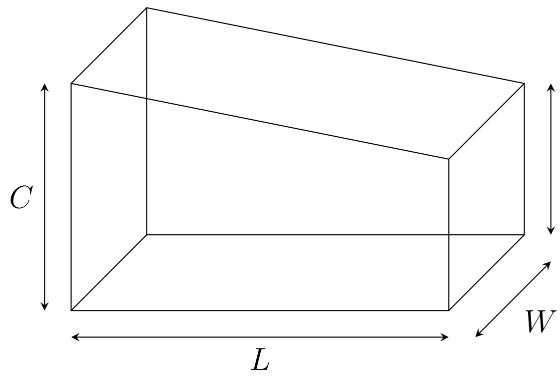
Therefore,

$$
\begin{aligned}
l &= 50\,\mu\mathrm{m} \\
&= 50 \times 10^{-4}\,\mathrm{cm}
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
R &= \rho \frac{l}{A} \\
&= 11500 \times 10^{-4}\Omega
\end{aligned}
$$

Exercise 17.
A sample of Germanium has resistivity σ. The dimensions of the sample are as shown.



Find the relationship between R and σ.

Solution 17.
Consider a slice with height h, width w, and thickness $\mathrm{d}x$. Therefore, the cross-sectional area of the elemental slice is

$$
\begin{aligned}
\mathrm{d}A &= wh \\
&= w\left(\frac{B-C}{L}x + C\right) \\
&= w\left(\frac{Bx - C(L-x)}{L}\right)
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\mathrm{d}R &= \frac{\mathrm{d}x}{\sigma w h} \\
&= \frac{L\,\mathrm{d}x}{\sigma w\left(Bx - C(L-x)\right)}
\end{aligned}
$$

6 Types of Materials

Atoms tend to arrange themselves in such a way that the resultant energy is minimized.

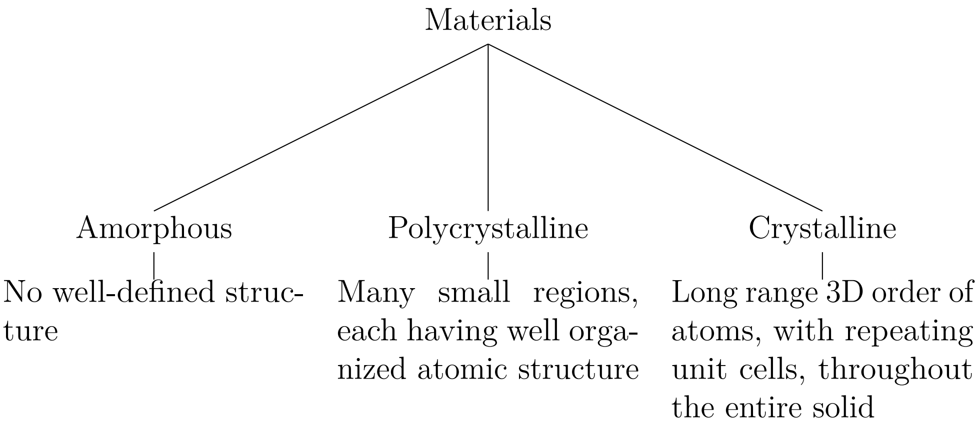


Figure 11: Classification of Materials

Semiconductor devices can use all of these types of materials.

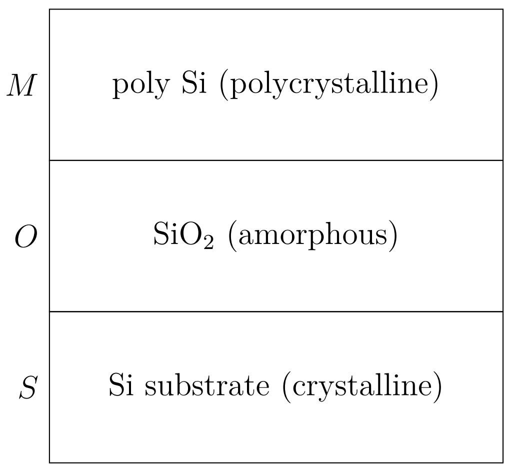


Figure 12: MOS which uses all three types of materials

7 Bohr's Model

According to Bohr's model of the atom, electrons can have discrete energy levels only. The electrons in an atom are arranged in the order of filling

electronic shells, given by the Aufbau Principle.
The energy of a free electron is called E_{vac}. This is used as a reference energy.

8 Atomic Bonding

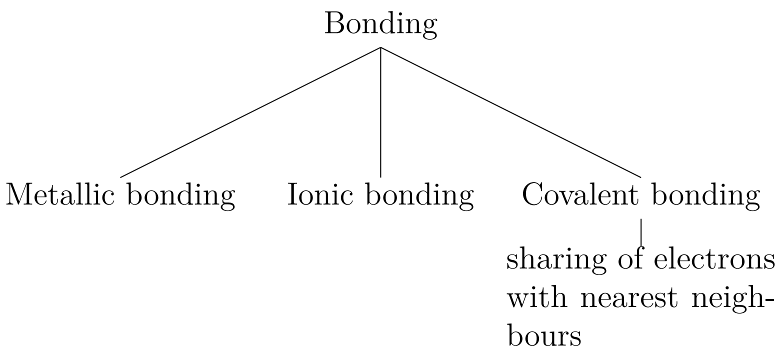


Figure 13: Types of Atomic Bonds

8.1 Covalent Bonds in Silicon

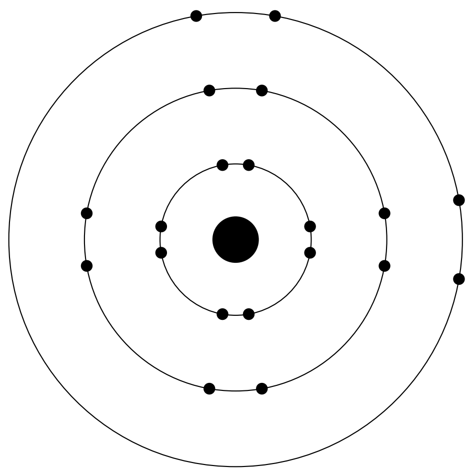


Figure 14: Arrangement of electrons in a silicon atom, in shells according to Bohr's model

In a silicon crystal, the silicon atoms are packed tightly and periodically, i.e. in a repeating pattern. The atomic density for silicon is approximately 10^{23} atoms per cm^3.
This arrangement of silicon atoms in crystalline form acts as a conductor only

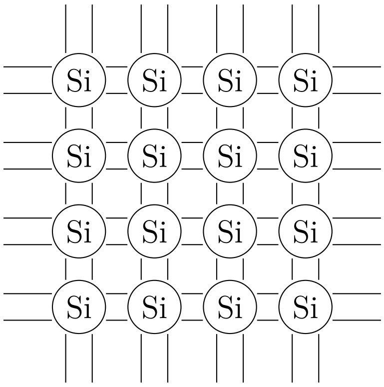


Figure 15: 2D model of bonding in silicon

at certain temperatures. At low temperatures, i.e. around 0 K, the electrons are tightly bound, and hence the crystal behaves as an insulator. However, at higher temperatures, the additional thermal energy may be sufficient to break bonds, and hence produce free electrons.
This property of silicon and other semiconductors makes it possible to control their conductivity.

9 Basics of Crystal Structure

Definition 26 (Crystal lattice)**.** The periodic arrangement of atoms in a crystal is called crystal lattice.

Definition 27 (Lattice constant)**.** The distance between two adjacent atoms in a crystal lattice is called the lattice constant.
It is denoted by a.
It is determined by the attractive and repulsive forces acting on the atoms.
The lattice constant corresponds to the lowest energy in the crystal.

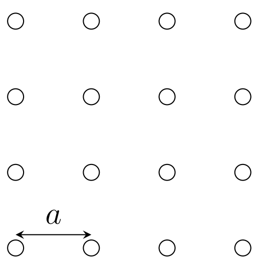
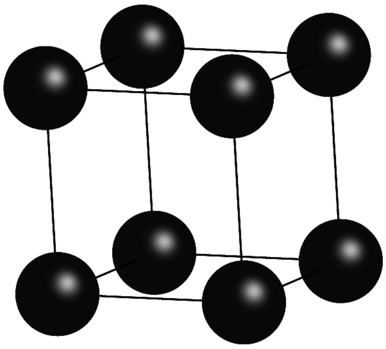


Figure 16: Crystal lattice and lattice constant

Definition 28 (Unit cell)**.** A volume which is repeated throughout the crystal is called the unit cell. It is used to represent the entire crystal lattice.



Definition 29. The atomic packing factor defined to be

$$\text{APF} = \frac{\text{volume filled by atoms}}{\text{total volume of unit cell}}$$

9.1 Simple Cubic Lattice

The number of atoms per unit cell are

$$\begin{aligned}\text{atoms per unit cell} &= \underbrace{\frac{1}{8}}_{\text{atoms per corner}} \times \underbrace{8}_{\text{number of corners}}\\ &= 1\end{aligned}$$

The atomic packing factor is

$$\begin{aligned}\text{APF} &= \frac{\overbrace{\frac{4}{3}\pi r^3}^{\text{volume of 1 atom}} \times \overbrace{1}^{\text{number of atoms}}}{\underbrace{a^3}_{\text{volume of unit cell}}} = \frac{\overbrace{\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}^{\text{volume of 1 atom}} \times \overbrace{1}^{\text{number of atoms}}}{\underbrace{a^3}_{\text{volume of unit cell}}}\\ &= \frac{\pi}{6}\end{aligned}$$

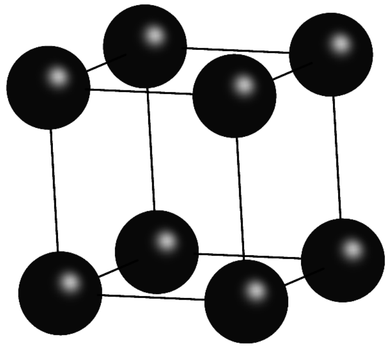


Figure 17: Simple cubic lattice (SC)

9.2 Face Centred Cubic Lattice

The number of atoms per unit cell are

$$
\begin{aligned}
\text{atoms per unit cell} = &\underbrace{\frac{1}{8}}_{\text{atoms per corner}} \times \underbrace{8}_{\text{number of corners}} \\
&+ \underbrace{\frac{1}{2}}_{\text{atoms per face}} \times \underbrace{6}_{\text{number of faces}} \\
&= 4
\end{aligned}
$$

The atomic packing factor is

$$
\begin{aligned}
\text{APF} &= \frac{\overbrace{\frac{4}{3}\pi r^3}^{\text{volume of 1 atom}} \times \overbrace{1}^{\text{number of atoms}}}{\underbrace{a^3}_{\text{volume of unit cell}}} = \frac{\overbrace{\frac{4}{3}\pi\left(\frac{a}{2\sqrt{2}}\right)^3}^{\text{volume of 1 atom}} \times \overbrace{4}^{\text{number of atoms}}}{\underbrace{a^3}_{\text{volume of unit cell}}} \\
&= \frac{\pi}{3\sqrt{2}}
\end{aligned}
$$

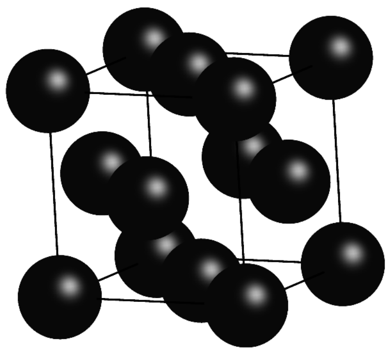


Figure 18: Face centred cubic lattice (FCC)

9.3 Body Centred Cubic Lattice

The number of atoms per unit cell are

$$\text{atoms per unit cell} = \underbrace{\frac{1}{8}}_{\text{atoms per corner}} \times \underbrace{8}_{\text{number of corners}} + \underbrace{1}_{\text{atom at centre}}$$
$$= 2$$

10 Basics of Crystal Growth

Definition 30. Epitaxy is the growth of layers, called epitaxial layers, on top of a thicker substrate layer.
Homoepitaxy is growing an epitaxial layer of the same material as the substrate. Heteroepitaxy is growing an epitaxial layer of a material different from the substrate.

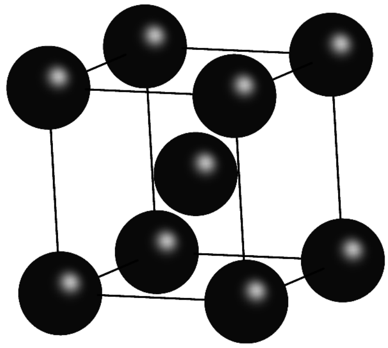


Figure 19: Body centred cubic lattice (BCC)

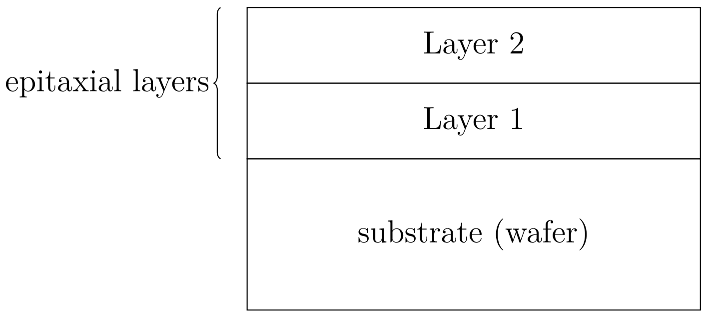


Figure 20: Epitaxial layers

Due to different properties of the materials which make up the substrate and epitaxial layers, there are certain constraints on the possible combinations. These factors include

1. lattice constants

2. crystal structure

10.1 Lattice Matching

If there is a difference between the lattice constants of the materials of two adjacent layers, there is a stress or strain generated, due to the interaction of the different lattices.
To minimize this stress, a technique called lattice matching is used.

Suppose the lattice constants of AlAs, InAs, and GaAs are as shown in the graph.

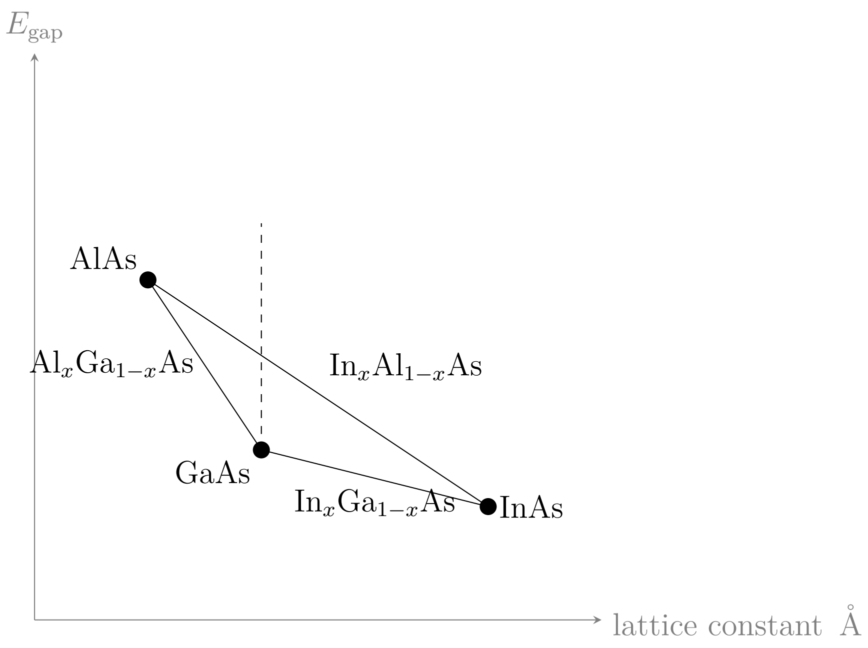


Figure 21: Lattice matching

If the substrate used is GaAs, and the epitaxial layer is made of InAlAs, then the composition of the epitaxial layer of InAlAs can be determined graphically.
The straight line connecting the points representing AlAs and InAs represents all possible values of $In_xAl_{1-x}As$, with x varying from 0 to 1, with 0 corresponding to AlAs, and 1 corresponding to InAs.
Therefore, the ideal material for the epitaxial layer, is the composition of $In_xAl_{1-x}As$ with lattice constant equal to that of GaAs.

11 Thermal Motion

Definition 31 (Ionization energy)**.** The energy needed to break a bond and free an electron is called the binding energy, or the ionization energy.

Definition 32 (Thermal motion)**.** The motion of electrons due to the thermal energy provided, is called thermal motion. This motion is random in nature, with all electrons moving around, rotating, and interacting, i.e. colliding with other electrons.

Theorem 33. *From statistical mechanics, which models the motion of free electrons, the thermal energy of an electron is*

$$E_{\text{thermal}} = \frac{3}{2}kT$$

where k is Boltzmann's constant, and T is the temperature in kelvin.
Hence, the average velocity of an electron is

$$v = \sqrt{\frac{3kT}{m}}$$

11.1 Thermal Generation of Carriers

Definition 33 (EHP)**.** A pair of a free electron, and a positive charge called a hole is called an electron-hole pair, or an EHP. Both the electron and the hole are mobile, and can contribute to conduction.

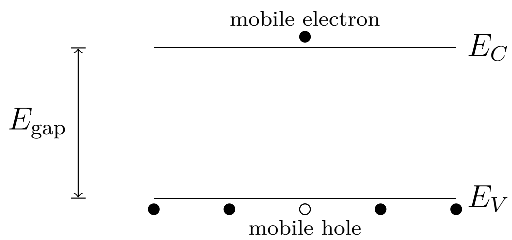


Figure 22: EHP

12 Effective Mass

Definition 34 (Effective mass)**.** To account for influences of the crystal lattice, altered values of particle masses are used.

These values are called effective masses of particles. They indicate how an electron will accelerate in the presence of an external force.
For silicon, the effective masses of electrons and holes are

$$m_n{}^* = 0.25 m_0$$
$$m_p{}^* = 0.5 m_0$$

where m_0 is the real mass of an electron.

13 Intrinsic Semiconductors

Definition 35 (Intrinsic carrier concentration)**.** The concentration of electrons, which is equal to the concentration of holes, in a material is called the intrinsic carrier concentration. It is denoted by n_i.
Therefore,

$$n = p = n_i$$

13.1 Effect of Energy Band Gap on Intrinsic Carrier Concentration

If the energy band gap increases, electrons need more energy to go from the valence band to the conduction band. Therefore, at a specific temperature, the intrinsic carrier concentration decreases as the energy band gap increases.

13.2 Thermal Generation and Recombination

Definition 36 (Generation of an EHP)**.** The process of creation of an EHP, which occurs due to an electron transitioning to the ionization band is called generation of an EHP. The rate of generation of EHPs is denoted by G.

Definition 37 (Recombination)**.** The process of destruction of an EHP, which occurs when an electron transitions back to an empty state, is called recombination. The rate of recombination of EHPs is denoted by R.

For a steady state concentration to be maintained at a given temperature, the recombination of EHPs must take place at the same rate at which they are generated, i.e.,

$$R = G$$

Therefore,

$$
\begin{aligned}
G &= \alpha_i np \\
&= \alpha_i {n_i}^2 \\
&= R
\end{aligned}
$$

where α_i is the recombination coefficient.
At thermal equilibrium,

$$np = {n_i}^2$$

14 Extrinsic Semiconductors

Definition 38 (Doping)**.** The process of introducing atoms into the crystals of a semiconducting material is called doping.
The newly introduced materials are called dopants or impurities.
The dopant atoms either donate or accept electrons, and hence increase the conductivity, as compared to the intrinsic conductivity.

Definition 39 (Dopant concentration)**.** Dopant concentration is defined as the number of donors or acceptors per unit volume.
Typically the values range from 10^{12} to 10^{19} donors or acceptors per cm^3.

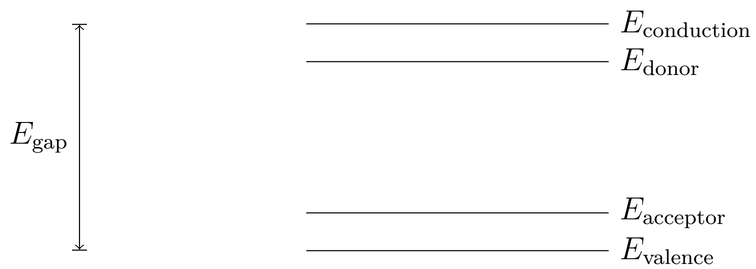


Figure 23: Typical Energy Diagram for Doped Material

14.1 N-type Material

Consider a silicon lattice doped with phosphorus atoms.
Four of the five valence electrons of the phosphorus atoms form covalent bonds with the adjacent silicon atoms. The extra electron, which is loosely bound, is donated to the lattice, and hence is available for conduction.
Such a material is called a N-type material.

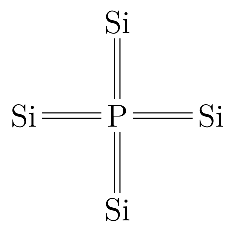


Figure 24: Silicon lattice with phosphorus doping

14.2 P-type Material

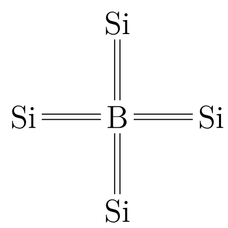


Figure 25: Silicon lattice with boron doping

Consider a silicon lattice doped with boron atoms.
The three valence electrons of the boron atoms form covalent bonds with the adjacent silicon atoms. Therefore, there is one missing electron, as compared to the original lattice. Hence, there is a hole per acceptor atom in the lattice, which is available for conduction.
Such a material is called a P-type material.

14.3 Thermal Equilibrium

Type of Material	Majority Carriers	Minority Carriers
N-type ($N_d >> n_i, p$)	Electrons $n = N_d$	Holes $p = \frac{n_i{}^2}{n}$
P-type ($N_a >> n_i, n$)	Holes $p = N_a$	Electrons $n = \frac{n_i{}^2}{p}$

Table 1: Concentration of charge carriers in N-type and P-type materials

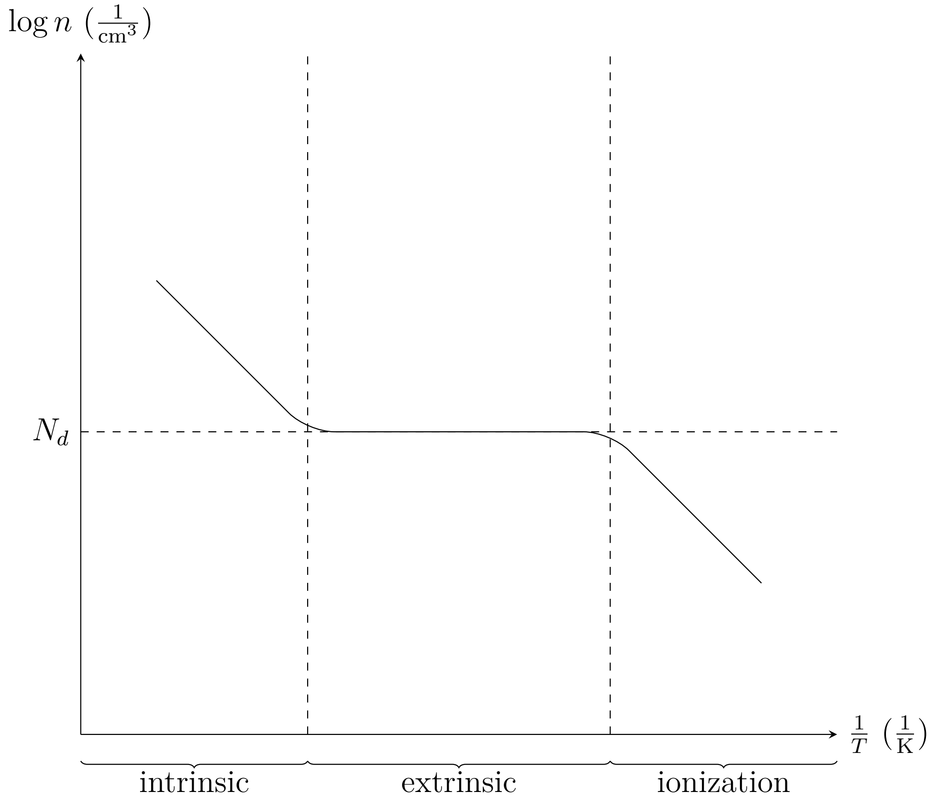


Figure 26: Carrier concentration and temperature regions

14.4 Dependence of Carrier Concentration on Temperature

At very low temperatures, i.e. close to absolute zero, the number of free electrons are almost zero. As the temperature increases, donor atoms start ionizing, and hence the number of free electrons increases. This range of temperature, up to the temperature at which all donor atoms are ionized is called the ionization region.
After the temperature at which all donor atoms are ionized, up to the temperature at which the in the host atoms start ionizing and generating EHPs, is called the extrinsic region. In this region, the number of free electrons is equal to the number of electrons donated by the dopant atoms, i.e. $n = N_d$.
After the temperature at which the host atoms start ionizing, the number of electrons is equal to the sum of the number of electrons donated by the dopant atoms, and the number of thermally generated EHPs. This region is called the intrinsic region.

15 Energy Band Model

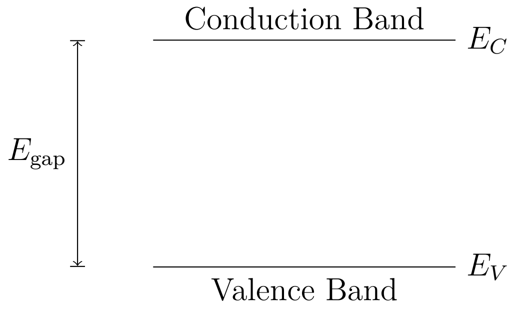


Figure 27: Energy Bands

Definition 40. The energy of a free electron is called E_{vacuum}.

Definition 41. The energy level of the nth shell in an atom is denoted by E_n.

15.1 Splitting of Energy Levels

The energy levels of electrons in an atom can be represented as

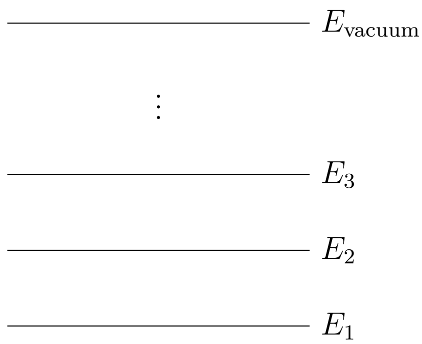


Figure 28: Energy Levels in a Single Atom

According to Pauli's Exclusion Principle, no two electrons can occupy the same energy level. Hence, if two atoms are brought close to each other, the energy levels of the shells split, and form new energy levels, which can be represented as

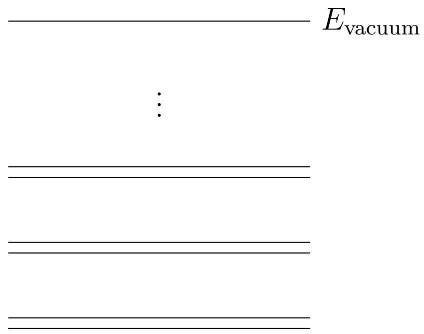


Figure 29: Split Energy Levels in two Atoms

Therefore, in the limiting case, if an infinite number of atoms are brought together to form a crystal, the split energy levels form ranges of energy which can be occupied by electrons. These energy ranges are called energy bands.

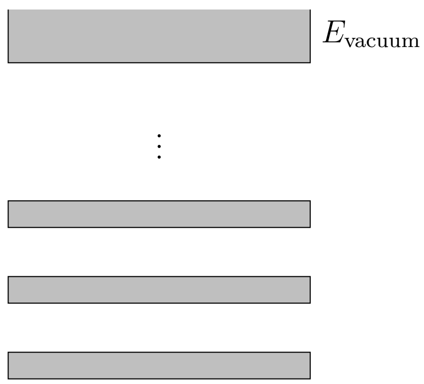


Figure 30: Energy Bands in a Crystal

For a semiconductor, the energy bands can be represented as

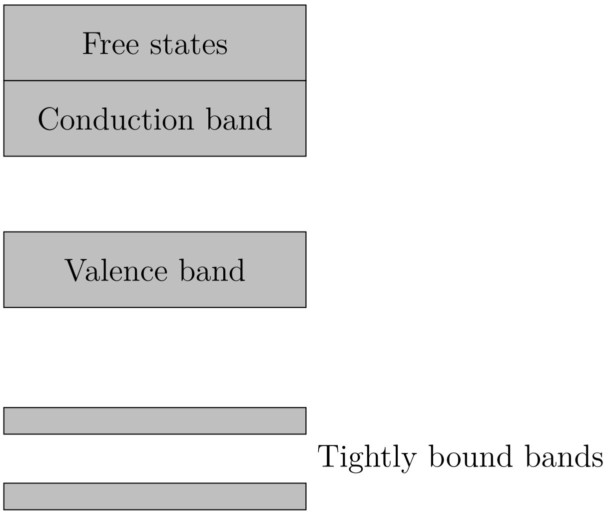


Figure 31: Energy Bands in a Semiconductor Crystal

Definition 42. The energy gap between E_{vacuum} and $E_{\text{conduction}}$ is called the electron affinity for that particular material. It is denoted by $q\chi$.

Definition 43. The intrinsic energy level is denoted by E_i.

Figure 32: Energy Gaps for a Perfect Semiconductor

16 Presence of an Electric Field in the Energy Band Model

Suppose a voltage V is applied across a semiconductor.
Therefore,

$$\begin{aligned}\overrightarrow{E} &= -\frac{\mathrm{d}V}{\mathrm{d}x}\\ &= \frac{1}{q}\frac{\mathrm{d}E_i}{\mathrm{d}x}\end{aligned}$$

where E_i is the intrinsic energy level.
Due to the electric field generated, the electrons move towards the positive terminal and the holes towards the negative terminal.
Let the potential difference be applied such that the electric field generated is directed towards the left.
Hence, the energy bands are modified, and a slope is generated in the bands.
Therefore, the energy bands which were originally represented as in Figure 33, will now be represented as in Figure 34. Hence, the electrons in the energy

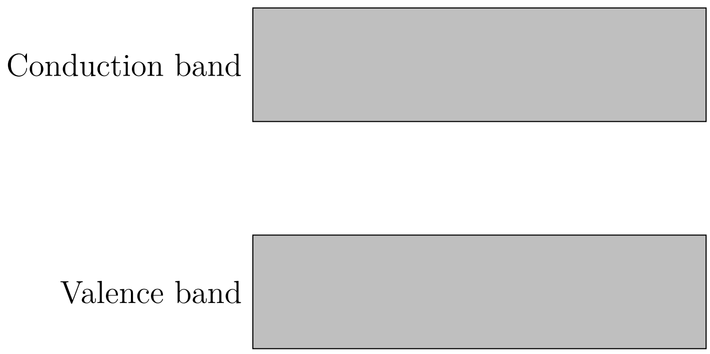


Figure 33: Energy Bands for a Perfect Semiconductor

bands tend to move to the right.
This behaviour is analogous to the behaviour of water in tilted pipes, with the water representing the electrons and the air representing the holes.
In general, the direction of the electric field is the same as the slope of the energy bands.

Exercise 18.
Given an electric field

$$\overrightarrow{E}(x) = -c\frac{\frac{\mathrm{d}n}{\mathrm{d}x}}{n}$$

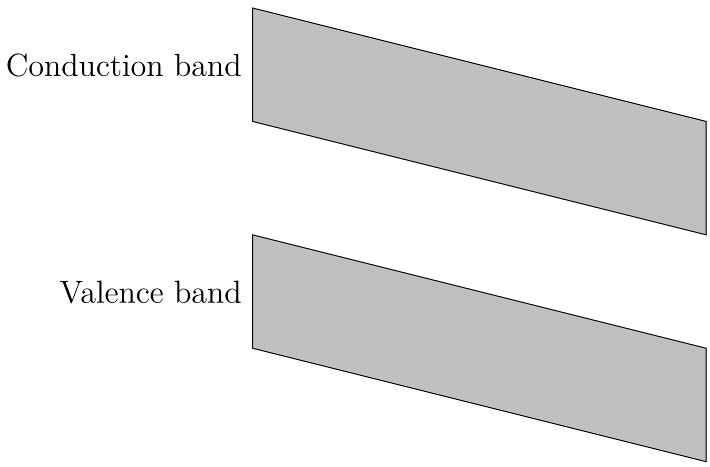


Figure 34: Energy Bands for a Perfect Semiconductor in Presence of an Electric Field

where

$$\begin{aligned} c &= \frac{kT}{q} \\ &= 0.026\,\text{eV}(\text{at room temperature}) \end{aligned}$$

The doping profile is given to be

$$\begin{aligned} n(x) &= N_d(x) \\ &= N_0 e^{-\alpha x} \end{aligned}$$

1. Find $\overrightarrow{E}(x)$.

2. If $\alpha = 1\frac{1}{\mu\text{m}}$, what is $\overrightarrow{E}(x)$?

3. Sketch the energy band diagram.

Solution 18.

1.

$$\begin{aligned} \frac{\mathrm{d}n}{\mathrm{d}x} &= N_0 \frac{\mathrm{d}e^{-\alpha x}}{\mathrm{d}x} \\ &= -N_0 \alpha e^{-\alpha x} \end{aligned}$$

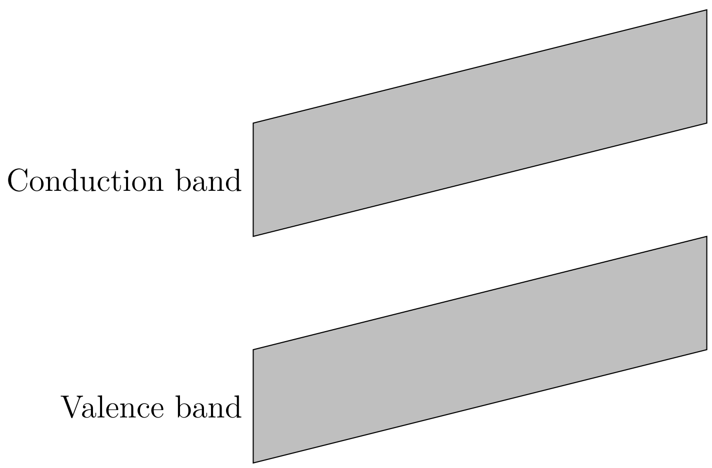
Therefore,

$$
\begin{aligned}
\overrightarrow{E}(x) &= -c\frac{-N_0\alpha e^{-\alpha x}}{N_0 e^{-\alpha x}} \\
&= \frac{cN_0\alpha e^{-\alpha x}}{N_0 e^{-\alpha x}} \\
&= c\alpha
\end{aligned}
$$

2.

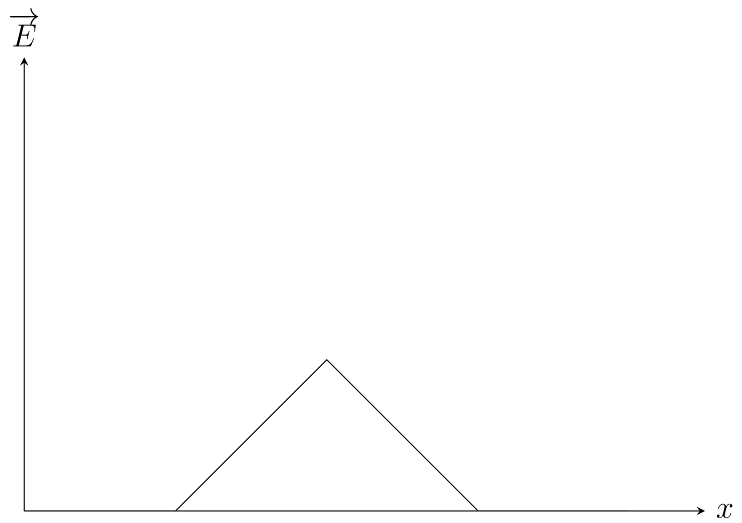
$$
\begin{aligned}
\overrightarrow{E}(x) &= c\alpha \\
&= (0.026\mathrm{V})(1\frac{1}{\mu\mathrm{m}}) \\
&= 260\frac{\mathrm{V}}{\mathrm{cm}}
\end{aligned}
$$

3. As the electric field is positive, the slope of the energy bands also must be positive. As the electric field is constant, the energy bands must be linear. Therefore, the energy band diagram is



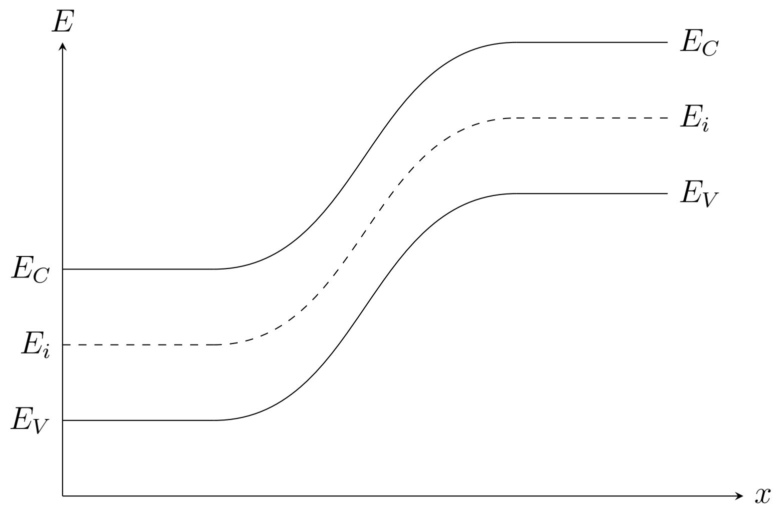
Exercise 19.

The electric field through a sample is given to be as shown.



Sketch the energy levels with respect to x.

Solution 19.



17 Movement of Carriers in Semiconductor Crystals

The motion of charge carriers in a semiconductor crystal is affected by the interactions within the crystal. The collisions between the charge carriers affects their movement.

Definition 44 (Scattering processes)**.** The change in direction of movement of charge carriers, due to collisions is called scattering processes.

Definition 45 (Mean free path)**.** The average distance between collision is called the mean free path. It is denoted by l_m.

Definition 46 (Time between collisions)**.** The average time between collision is called the mean free path. It is denoted by τ_m.

17.1 Drift

Consider an electric field $\overrightarrow{E}$ applied on a sample. Therefore the net motion of the electrons is in the direction opposite to that of the electric field, and the net motion of the holes is in the direction of the electric field.

Definition 47 (Drift)**.** The motion of charge carriers which is driven by electric fields is called drift.

The acceleration of the charge carriers due to the external electric field is balanced by the deceleration of the charge carriers due to collisions.
Therefore, on a microscopic level, the motion of the charge carriers is random, and on a macroscopic level, the charge carriers move with a constant velocity.

Definition 48 (Average drift velocity)**.** The average velocity of charge carriers, on a macroscopic scale, is called the average drift velocity.

The force on a charge carrier is given by

$$\overrightarrow{F} = q\overrightarrow{E}$$

Therefore,

$$\begin{aligned}
\overrightarrow{F}\tau_m &= q\overrightarrow{E}\tau_m \\
&= m^* v_d \\
\therefore v_d &= \frac{q\tau_m}{m^*}\overrightarrow{E}
\end{aligned}$$

Definition 49 (Mobility)**.** The ease with which electrons and holes can flow through the crystal is called mobility. It is denoted by μ. It is defined to be

$$\mu = \frac{q\tau}{m^*}$$

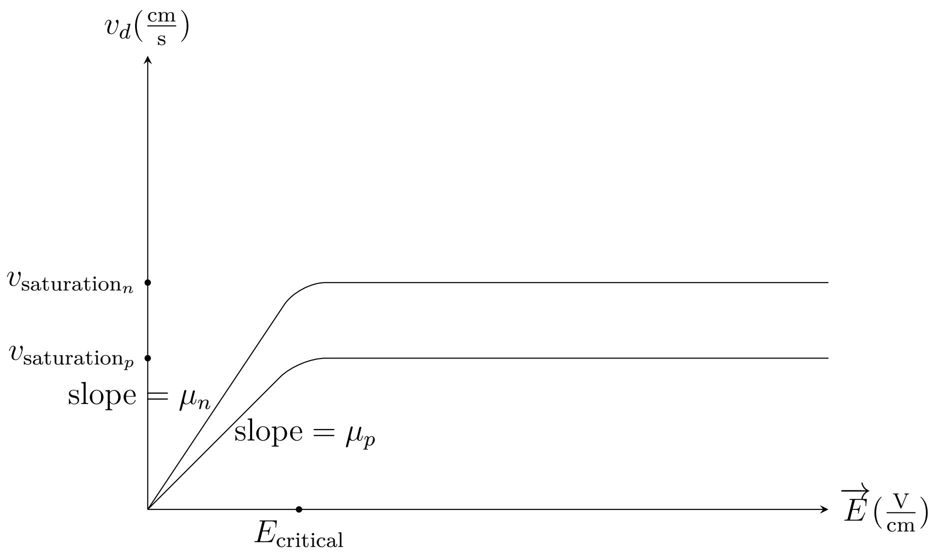
where q is the charge on the particle, τ is the average time between collisions, and m^* is the effective mass.
Mobility is the ratio between the drift velocity of electrons or holes, and the electric field acting on them.

Therefore,

$$\mu = \frac{q\tau_m}{m^*}$$

As the effective mass of an electron is less than that of a hole, the mobility of an electron is more than that of a hole.
For silicon, at room temperature, the mobilities of electrons and holes are

$$\mu_n = 1000\frac{\text{cm}^2}{\text{V s}}$$
$$\mu_p = 400\frac{\text{cm}^2}{\text{V s}}$$



17.1.1 Current Density due to Net Drift

Definition 50 (Direction of current due to drift of electrons)**.** The direction of the current generated due to the net drift of electrons is defined to be in the direction opposite to the drift velocity of the electrons.

Definition 51 (Direction of current due to drift of holes)**.** The direction of the current generated due to the net drift of holes is defined to be in the direction of the drift velocity of the holes.

Theorem 34 (Current density due to net drift)**.** *The current density due to the drift of electrons is*

$$\begin{aligned} J_{drift_n} &= -qnv_{d_n} \\ &= qn\mu_n\overrightarrow{E} \end{aligned}$$

The current density due to the drift of holes is

$$\begin{aligned} J_{drift_p} &= qpv_{d_p} \\ &= qp\mu_p \overrightarrow{E} \end{aligned}$$

Therefore, the net current density is

$$\begin{aligned} J_{drift_{total}} &= J_{drift_n} + J_{drift_p} \\ &= qn\mu_n \overrightarrow{E} + qn\mu_p \overrightarrow{E} \\ &= q(n\mu_n + p\mu_p) \overrightarrow{E} \end{aligned}$$

Theorem 35.

$$\sigma = q(n\mu_n + p\mu_p)$$

Proof.

$$\begin{aligned} J &= \sigma \overrightarrow{E} \\ &= q(n\mu_n + p\mu_p) \overrightarrow{E} \end{aligned}$$

Therefore,

$$\sigma = q(n\mu_n + p\mu_p)$$

□

Theorem 36. *For a N-type material,*

$$\begin{aligned} \sigma &= \sigma_n \\ &= qn\mu_n \end{aligned}$$

Proof. For a N-type material, $n >> p$.
Therefore,

$$\begin{aligned} \sigma &= q(n\mu_n + p\mu_p) \\ &= qn\mu_n \end{aligned}$$

□

Theorem 37. *For a P-type material,*

$$\begin{aligned} \sigma &= \sigma_p \\ &= qp\mu_p \end{aligned}$$

Proof. For a P-type material, $p >> n$.
Therefore,

$$\begin{aligned}\sigma &= q(n\mu_n + p\mu_p)\\ &= qp\mu_p\end{aligned}$$

$\square$

Exercise 20.
A sample of a P-type material with length $l = 10\,\mu\mathrm{m}$ is connected to a voltage of $V = 10\,\mathrm{V}$. The dopant concentration in the material is $N_a = 10^{17}\frac{1}{\mathrm{cm}^3}$. Find the drift velocity of the holes and the current density.

Solution 20.

$$\begin{aligned}\mu_p &= \frac{q\tau}{m^*}\\ &= \frac{\left(1.6\times 10^{-19}\,\mathrm{C}\right)\left(10^{-13}\,\mathrm{s}\right)}{0.5\times 9.11\times 10^{-31}\,\mathrm{kg}}\\ &= 0.035\frac{\mathrm{m}^2}{\mathrm{V\,s}}\end{aligned}$$

Therefore,

$$\begin{aligned}v_{\mathrm{drift}_p} &= \mu_p E\\ &= \mu_p\frac{V}{l}\\ &= \left(350\frac{\mathrm{cm}^2}{\mathrm{V\,s}}\right)\left(10^4\frac{\mathrm{V}}{\mathrm{cm}}\right)\\ &= 3.5\times 10^6\frac{\mathrm{cm}}{\mathrm{s}}\end{aligned}$$

As the material is P type,

$$\begin{aligned}J_{\mathrm{drift}} &= J_{\mathrm{drift}_p}\\ &= qp\mu_p E\\ &= qpv_{\mathrm{drift}_p}\\ &= \left(1.6\times 10^{-19}\,\mathrm{C}\right)\left(10^{17}\frac{1}{\mathrm{cm}^3}\right)\left(3.5\times 10^6\frac{\mathrm{cm}}{\mathrm{s}}\right)\\ &= 5.6\times 10^4\frac{\mathrm{A}}{\mathrm{cm}^2}\end{aligned}$$

17.2 Scattering Mechanisms that Influence Electron and Hole Mobility

Definition 52 (Lattice scattering)**.** The scattering of charge carriers due to interaction with atoms in the crystal lattice is called lattice scattering.

In this scattering, there are collisions of moving carriers due to disturbances in the semiconductor. Therefore, as the velocity of the moving carriers increases with temperature, lattice scattering dominates the mobility at high temperature.

Definition 53 (Impurity scattering)**.** The scattering of charge carriers due to crystal defects is called impurity scattering.

In this scattering, the fixed charges dispersed throughout the crystal exert forces on the charge carriers.
A slow moving carrier is likely to be scattered more strongly due to interaction, than a fast moving carrier. Therefore, impurity scattering dominates the mobility of the charge carriers at low temperature.

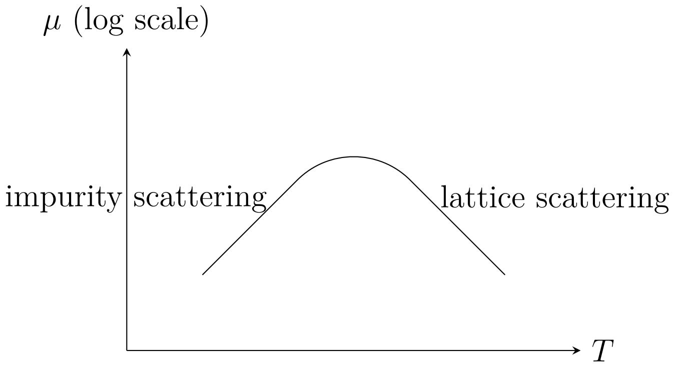


Figure 35: Effect of Temperature on Mobility

The temperature range for the graph in Figure 35 is in the extrinsic region corresponding to the graph in Figure 26. Therefore, the graph of $n\mu$ with respect to $\frac{1}{T}$ is as in Figure 36. Hence, as J and σ are directly proportional to $n\mu$, they exhibit a similar relation to the temperature.

17.3 Diffusion

Definition 54 (Diffusion)**.** The motion of charge carriers from regions of higher concentration to regions of lower concentration, is called diffusion. It is a gradient driven motion.

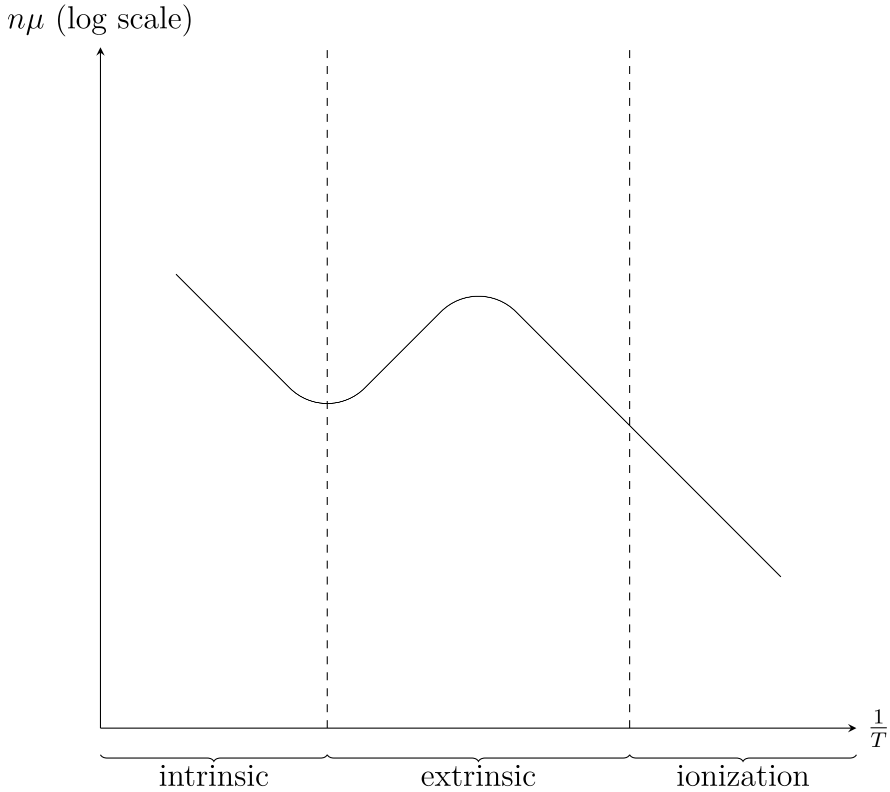


Figure 36: Effect of Doping Concentration and Temperature on Mobility

Definition 55 (Direction of current due to diffusion of electrons)**.** The direction of the current generated due to the diffusion of electrons is defined to be in the direction opposite to the movement of the electrons.

Definition 56 (Direction of current due to diffusion of holes)**.** The direction of the current generated due to the diffusion of electrons is defined to be in the direction of the movement of the holes.

17.3.1 Current Density due to Net Diffusion

Definition 57 (Direction of current due to diffusion of electrons)**.** The direction of the current generated due to the diffusion of electrons is defined to be opposite to the direction of the movement of electrons, and hence in the direction of increase in concentration of electrons with respect to position.

Definition 58 (Direction of current due to diffusion of holes)**.** The direction of the current generated due to the diffusion of holes is defined to be in the direction of the movement of holes, and hence opposite to the direction of increase in concentration of holes with respect to position.

Theorem 38 (Current density due to diffusion)**.** *The current density due to the diffusion of electrons is*

$$J_{diffusion_n} = qD_n \frac{\mathrm{d}n}{\mathrm{d}x}$$

The current density due to the diffusion of holes is

$$J_{diffusion_p} = -qD_p \frac{\mathrm{d}p}{\mathrm{d}x}$$

where D_n and D_p are positive constants.

Theorem 39.

$$D_n = \frac{1}{3} v_{thermal_n} l$$

where the motion of electrons is from $x = l$ to $x = -l$.

Proof. Consider a N-type sample with some doping profile. The flux through a cross-section at $x = 0$ is

The $\frac{1}{6}$ is due to the fact that an electron can move through 3 spatial dimensions, with 2 directions of flow each.

$$F = \frac{1}{6} v_{\text{thermal}} \left(n(-l) - n(l)\right)$$

where electrons move from $x = l$ to $x = -l$.
Therefore,

$$\begin{aligned} J_{\text{diffusion}_n} &= -qF \\ &= (-q)\left(-\frac{1}{3} v_{\text{thermal}} l \frac{\mathrm{d}n}{\mathrm{d}x}\right) \\ &= q\left(\frac{1}{2} v_{\text{thermal}} l\right) \frac{\mathrm{d}n}{\mathrm{d}x} \end{aligned}$$

Therefore,

$$D_n = \frac{1}{3} v_{\text{thermal}_n} l$$

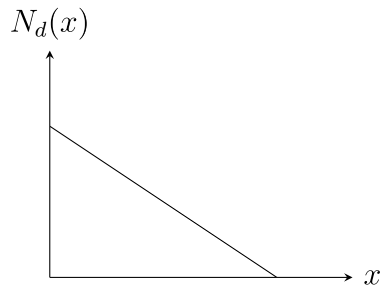
□

Theorem 40.

$$D_p = \frac{1}{3} v_{thermal_p} l$$

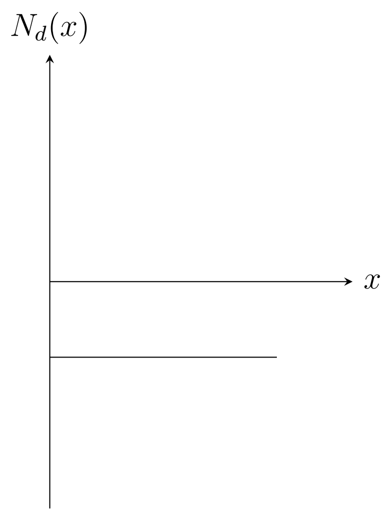
where the motion of holes is from $x = l$ to $x = -l$.

Exercise 21.
A sample of N-type material has doping profile as shown.

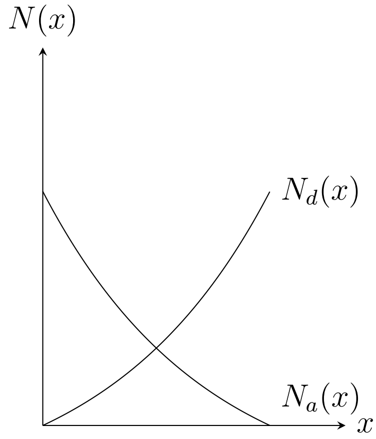


Sketch the graph of the current density with respect to x.

Solution 21.

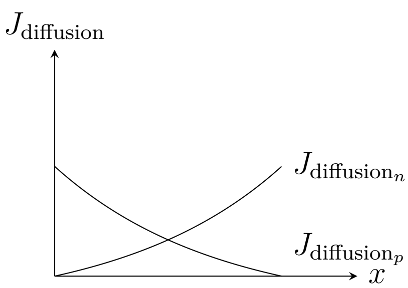


Exercise 22.
A sample has doping profile as shown.

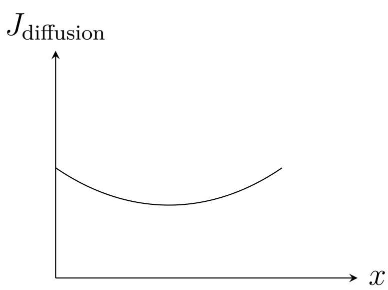


Sketch the graph of the current density with respect to x.

Solution 22.
The current densities due to the diffusion of electrons and holes are



Therefore, the net diffusion current density is



17.4 Transport Equations

The total current densities due to the net motion of electrons and holes is

$$
\begin{aligned}
J_{\text{total}_n} &= J_{\text{drift}_n} + J_{\text{diffusion}_n} \\
&= qn\mu_n \overrightarrow{E} + qD_n \frac{\mathrm{d}n}{\mathrm{d}x}
\end{aligned}
$$

$$
\begin{aligned}
J_{\text{total}_p} &= J_{\text{drift}_p} + J_{\text{diffusion}_p} \\
&= qp\mu_p \overrightarrow{E} + qD_p \frac{\mathrm{d}p}{\mathrm{d}x}
\end{aligned}
$$

17.5 Einstein's Relation

Theorem 41 (Einstein's Relation)**.**

$$\frac{D}{\mu} = \frac{kT}{q}$$

At room temperature,

$$\frac{D}{\mu} = 0.026\,\mathrm{V}$$

Proof.

$$
\begin{aligned}
\frac{D}{\mu} &= \frac{\frac{1}{3}v_{\text{thermal}}l}{\mu} && v_{\text{thermal}} = \frac{l}{\tau} \\
&= \frac{\frac{1}{3}{v_{\text{thermal}}}^2\tau}{\mu} \\
&= \frac{\frac{1}{3}{v_{\text{thermal}}}^2\tau}{\frac{q\tau}{m^*}} \\
&= \frac{1}{3}\frac{m^*{v_{\text{thermal}}}^2}{q} && \frac{1}{2}m^*{v_{\text{thermal}}}^2 = \frac{3}{2}kT \\
&= \frac{1}{3}\frac{3kT}{q} \\
&= \frac{kT}{q}
\end{aligned}
$$

□

Exercise 23.
Find D_n for a sample of silicon at room temperature, if the mobility of electrons in the sample is $1000\frac{\mathrm{cm}^2}{\mathrm{V\,s}}$.

Solution 23.
By Einstein's Relation,

$$\begin{aligned}\frac{D_n}{\mu_n} &= 0.026\,\mathrm{V}\\ \therefore D_n &= 0.026\mu_n\frac{\mathrm{cm}^2}{\mathrm{s}}\\ &= 26\frac{\mathrm{cm}^2}{\mathrm{s}}\end{aligned}$$

Exercise 24.
Find D_n for a sample of silicon at 450 K, if the mobility of electrons in the sample is $800\frac{\mathrm{cm}^2}{\mathrm{V\,s}}$.

Solution 24.
By Einstein's Relation,

$$\begin{aligned}\frac{D_n}{\mu_n} &= \frac{kT}{q}\\ \therefore D_n &= \frac{kT}{q}\mu_n\\ &= 49.7\frac{\mathrm{cm}^2}{\mathrm{s}}\end{aligned}$$

18 Quantum Wells

Consider a sample made with one semiconductor sandwiched between two samples of another semiconductor. The energy bands in this composite material is as in Figure 37. Hence, there are quantum wells created in the energy bands.

19 Optical Absorption

Let a sample be illuminated with light of photon energy greater than the energy band gap of the material of the sample.

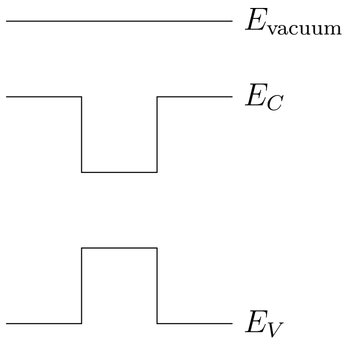


Figure 37: Quantum Wells due to Varying Energy Band Gaps

Therefore, the electrons in the valence band absorb this energy, and move to the conduction band. Such electrons are called hot electrons. Hot electrons then lose energy till they reach E_C. Thereafter, they recombine with holes in the valence band, and in the process give out photons corresponding to the energy band gap of the material.
This emitted light can be observed, and used to find the energy band gap of the material.

20 Optical Generation of Carriers

Consider a sample illuminated by light with photons of energy greater than the energy gap of the material of the sample. This extra energy will lead to generation of EHPs.
Let n_0 and p_0 be the concentrations of electrons and holes, at thermal equilibrium. Let $\hat{n}$ and $\hat{p}$ be the concentrations of electrons and holes, from the optically generated EHPs.
Therefore,

$$n = n_0 + \hat{n}$$
$$p = p_0 + \hat{p}$$

20.1 Carrier Generation Dependent on Illumination

Consider a sample such that

$$N_d = 10^{16} \frac{1}{\text{cm}^3}$$

Therefore the intensity of light affects the concentration of charge carriers. For no light,

$$
\begin{aligned}
n &= n_0 \\
&= N_d \\
&= 10^{16} \frac{1}{\mathrm{cm}^3} \\
p &= p_0 \\
&= \frac{{n_i}^2}{N_d} \\
&= 10^4 \frac{1}{\mathrm{cm}^3}
\end{aligned}
$$

For low level injection, i.e. $p_0 < \hat{n} = \hat{p} < n_0$, say $\hat{n} = \hat{p} \approx 10^{14} \frac{1}{\mathrm{cm}^3}$,

$$
\begin{aligned}
n &= n_0 + \hat{n} \\
&= 10^{16} + 10^{14} \\
&\approx 10^{16} \frac{1}{\mathrm{cm}^3} \\
p &= p_0 + \hat{p} \\
&= 10^4 + 10^{14} \\
&\approx 10^{14} \frac{1}{\mathrm{cm}^3}
\end{aligned}
$$

For high level injection, i.e. $p_0 < \hat{n} = \hat{p} < n_0$, say $\hat{n} = \hat{p} \approx 10^{20} \frac{1}{\mathrm{cm}^3}$,

$$
\begin{aligned}
n &= n_0 + \hat{n} \\
&= 10^{16} + 10^{20} \\
&\approx 10^{20} \frac{1}{\mathrm{cm}^3} \\
p &= p_0 + \hat{p} \\
&= 10^4 + 10^{20} \\
&\approx 10^{20} \frac{1}{\mathrm{cm}^3}
\end{aligned}
$$

Therefore, the concentrations are as shown in Figure 38.

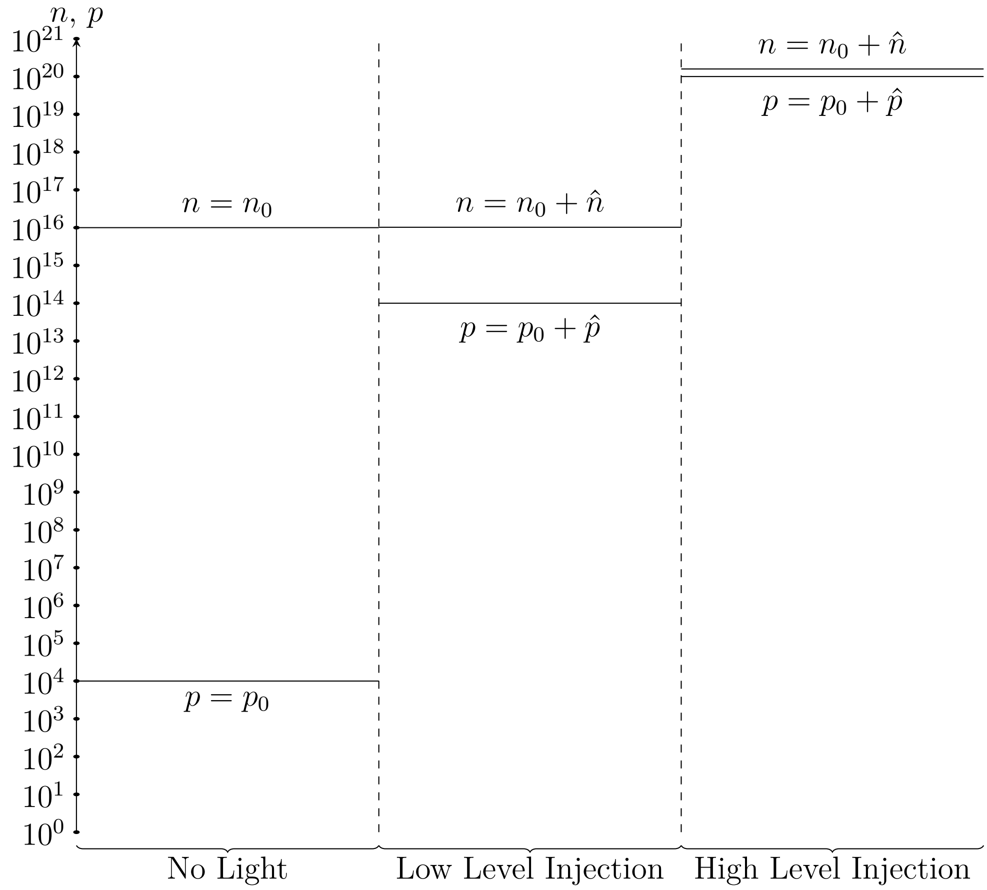


Figure 38: Carrier Concentration in N-type Material under Different Light Conditions

20.2 Minority Carrier Concentration in Illuminated Materials

Consider a N-type material which is illuminated from $t = 0$ onwards.
The rate of recombination is defined to be

$$R = \alpha_r np$$

Therefore, in case of low level injection,

$$
\begin{aligned}
R &= \alpha_r np \\
&= \alpha_r (n_0 + \hat{n}) (p_0 + \hat{p}) \\
&= \alpha_r (n_0 p_0 + n_0 \hat{p} + p_0 \hat{n} \hat{p} \hat{n}) \\
&= \alpha_r \left({n_i}^2 + n_0 \hat{p} \right) \\
&= \alpha_r {n_i}^2 + \alpha_r n_0 \hat{p} \\
&= R_{\text{thermal}} + R_{\text{optical}}
\end{aligned}
$$

As $p_0 \hat{n}$ and $\hat{p} \hat{n}$ are small compared to $n_0 p_0$ and $n_0 \hat{p}$.

Therefore,

$$
\begin{aligned}
G - R &= G_{\text{thermal}} + G_{\text{optical}} - R_{\text{thermal}} + R_{\text{optical}} \\
&= G_{\text{optical}} - R_{\text{optical}}
\end{aligned}
$$

In the steady state, the generation of EHPs is balanced by recombination. Therefore,

$$
\begin{aligned}
G &= R \\
\therefore G_{\text{optical}} &= R_{\text{optical}}
\end{aligned}
$$

As the rate of recombination cannot increase instantaneously, $\hat{p}$ must be a function of time.

Definition 59 (Lifetime of minority carriers)**.**

$$
\tau_p = \frac{1}{\alpha_r n_0}
$$

is called the lifetime of the minority carriers

Therefore,

$$
\begin{aligned}
R &= \alpha_r n_0 \hat{p} \\
&= \frac{\hat{p}}{\tau_p}
\end{aligned}
$$

Therefore, at steady state,

$$
\begin{aligned}
G_{\text{optical}} &= R_{\text{optical}} \\
&= \frac{\hat{p}}{\tau_p}
\end{aligned}
$$

Therefore,

$$\hat{p} = G_{\text{optical}}\tau_p$$

Therefore, before the steady state,

$$\begin{aligned} G - R &= \frac{\mathrm{d}\hat{p}}{\mathrm{d}t} \\ \therefore G_{\text{optical}} - \frac{\hat{p}(t)}{\tau_p} &= \frac{\mathrm{d}\hat{p}}{\mathrm{d}t} \end{aligned}$$

Therefore, solving,

$$\hat{p}(t) = G_{\text{optical}}\tau_p \left(1 - e^{-\frac{t}{\tau_p}}\right)$$

Similarly, for a sample which is stopped being illuminated at $t = 0$,

$$\hat{p}(t) = G_{\text{optical}}\tau_p e^{-\frac{t}{\tau_p}}$$

20.3 Conductivity of Illuminated Materials

When a sample is not illuminated,

$$J = \sigma_0 E$$

When the sample has light shined on it,

$$J = (\sigma_0 + \hat{\sigma}) E$$

Therefore,

$$\begin{aligned} \Delta\sigma &= \hat{\sigma} \\ &= \sigma_{\text{light}} - \sigma_{\text{dark}} \\ &= \Big(q\mu_n (n + \hat{n}) + q\mu_p (p + \hat{p})\Big) - \Big(q\mu_n n + q\mu_p p\Big) \\ &= q\mu_p\hat{p} + q\mu_n\hat{n} \\ &= qG_{\text{optical}}\tau_p(\mu_p + \mu_n) \end{aligned}$$