Engineering Physics (2025)
Course code 25PY101
Unit 2: Quantum mechanics

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October 25, 2025

Unit 2 Plan

1. Introduction to QM
2. Dual nature of radiation
3. de Broglie's concept of matter waves
4. Heisenberg's uncertainty principle
5. Schrödinger's time dependent wave equation

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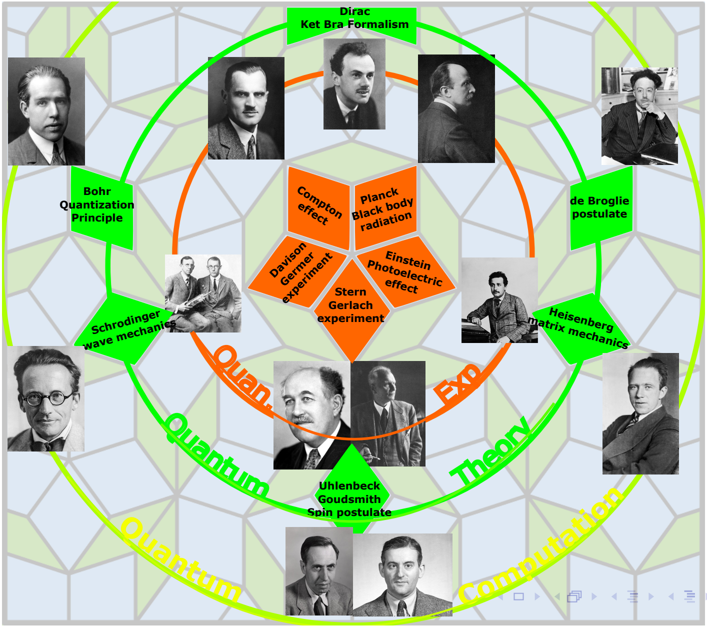
Quantum mechanics jigsaw puzzle



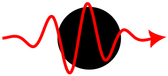
Theories of quantum physics

- Max Planck's postulate of quantization of light energy absorbed or emitted by electron in quanta (plural for quantum)
- Louis de Broglie's postulate of existence of matter waves
- Werner Heisenberg's principle of uncertainty
- Erwin Schrödinger's wave equation

Wave-Particle Duality

de Brogie hypothesis

Any moving particle is associated with a wave. The waves associated with particles are called **de Broglie waves** or **matter waves**.



- Louis de Broglie in 1924 postulated the existence of **matter waves**.
- He suggested since light wave exhibits particle like behaviour, matter particles should be expected to show wave-like properties. This is the hypothesis of **wave-particle duality**.
- The wavelength λ of the matter wave is related to the momentum p of the matter particle by

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

Matter wave: properties

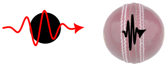
- Matter waves are due to motion of particle and are independent of charge. Therefore, they are neither electromagnetic waves nor acoustic waves. They are a new kind of waves.
- Can propagate/travel through vacuum and do not require any medium for propagation.
- Smaller the mass, longer the de Broglie wavelength.
- Smaller the velocity, longer the de Broglie wavelength.
- Velocity of matter waves depends on velocity of particle and is not a constant quantity.

Estimate: de Broglie wavelength of thermal electron

Estimate at room temperature.

Estimate: de Broglie λ of macroscopic particle

Cricket ball of mass 150 g is bowled at 140 km h^{-1}.



Unit 2 Plan

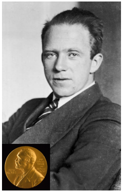
Heisenberg uncertainty principle

Uncertainty principle/hypothesis

Precise values of position and momentum of a particle cannot be determined **simultaneously**. If the uncertainty in position is Δx and uncertainty in momentum is Δp, then

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}, \qquad \text{where} \quad \hbar = \frac{h}{2\pi}$$

where $\hbar$ is the reduced/modified Planck's constant.



- Werner Heisenberg postulated the uncertainty principle in 1927.
- In classical mechanics, position and momentum are **deterministic**. In quantum mechanics, they are not deterministic and are associated with **uncertainties**.
- If position is measured with low uncertainty, then measurement of momentum has high uncertainty and vice versa.

Uncertainty → Probability

- The uncertainty principle relates any pair of **conjugate** variables.
- Position – momentum is a pair of conjugate variables.
- Energy – time is also a conjugate variable pair.
- So the uncertainty in energy ΔE is related to the uncertainty in time by Δt by

$$\Delta E \, \Delta t \geq \frac{\hbar}{2}$$

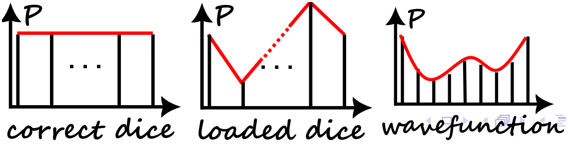
  This is the second statement/corollary of Heisenberg's uncertainty principle.
- Due to the smallness of reduced Planck's constant, the uncertainty principle is significant for subatomic particles.
- The cause of uncertainty is **limitation of measurement**.

Key Insight

Since the position cannot be measured with certainty, we determine the **probability** of finding an electron at a particular position.

Probability: Mapping of Dice $\rightarrow$ position

- The way to deal with uncertainty is to talk in terms of probability.
- If a system has N events, the probability of event A is defined as number of times event A has occured over total number of outcomes.
- A coin is a "2-sided polyhedron/dice". The probability of coin having heads is $\frac{1}{2}$. Similarly for N-sided dice the probability is $\frac{1}{N}$.
- A "loaded" dice can different probability for each outcome.
- In the limit of ∞-sided dice, the probability of a outcome becomes a function.



Uncertainty in function of variable

- If uncertainty in variable x is Δx, then the uncertainty in variable $f(x)$ is given by

$$\Delta f = \frac{\mathrm{d}f}{\mathrm{d}x}\Delta x$$

- Kinetic energy E is related to momentum p by

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

- If uncertainty in momentum is Δp, then uncertainty in kinetic energy E is given by

$$\Delta E = \frac{\mathrm{d}E}{\mathrm{d}p}\Delta p = \frac{p}{m}\Delta E$$

Problem

- *Uncertainity in position of electron is* $12\,\text{Å}$*.*
- *Nominal energy of electron is* $16\,\mathrm{eV}$*.*
- *Determine the uncertainty in momentum and kinetic energy*

Unit 2 Plan

Schrödinger's wave equation

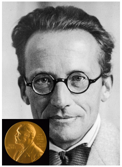
Wave equation hypothesis

If the **wave function** of a particle of mass m is $\Psi(x,t)$, then it satisfies the **wave equation** given by

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

where $V(x)$ is the potential function[a] and j is the imaginary constant $\sqrt{-1}$.

[a] Potential energy and not electric potential difference



- Erwin Schrödinger postulated the wave equation in 1926 that incorporated principles of quanta introduced by Planck and wave-particle duality introduced by de Broglie.
- The wave function $\Psi(x,t)$ describes the behaviour of particle
- $\Psi(x,t)$ can be a **complex** quantity.

Analysis of the wave equation (W.E.)

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

1. The independent variables/quantities are position x and time t whereas the dependent variable is the wave function Ψ. Therefore, wave function is a function of position and time
$$\Psi(x,t)$$
2. W.E. is a **partial** differential equation.
    - A differential equation relates dependent variable y to the independent variable x. The relationship is given by derivatives $\frac{\mathrm{d}\,y}{\mathrm{d}\,x}, \frac{\mathrm{d}^2\,y}{\mathrm{d}\,x^2}, \ldots$
    - A partial differential equation relates dependent variable z to the independent variables x and y. The relationship is given by partial derivatives $\frac{\partial\,z}{\partial\,x}, \frac{\partial\,z}{\partial\,y}, \frac{\partial^2\,z}{\partial\,x^2}, \ldots$
3. W.E. is a **second order** differential equation.
    - A first order differential equation has only first order derivative.
    - A second order differential equation has upto second order derivatives.
4. The potential energy $V(x)$ is a parameter whereas $\hbar, m, j$ are constants.

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

- The goal is to find the solution $\Psi(x,t)$ for a given $V(x)$.
- We assume form of the solution as

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

where $\psi(x)$ is a function of the position only and $\phi(t)$ is a function of the time only.

- Upon substitution of above form, W.E. reduces to

$$-\frac{\hbar^2}{2m}\phi(t)\frac{\mathrm{d}^2\,\psi(x)}{\mathrm{d}x^2}+V(x)\,\psi(x)\,\phi(t)=j\hbar\,\psi(x)\frac{\mathrm{d}\,\phi(t)}{\mathrm{d}t}$$

W.E. $$-\frac{\hbar^2}{2m}\phi(t)\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + V(x)\psi(x)\phi(t) = j\hbar\,\psi(x)\frac{\mathrm{d}\,\phi(t)}{\mathrm{d}t}$$

W.F. $$\Psi(x,t) = \psi(x)\,\phi(t)$$

- Divide the above equation by total wave function so that

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + V(x) = j\hbar\frac{1}{\phi(t)}\frac{\mathrm{d}\,\phi(t)}{\mathrm{d}t}$$

- Since L.H.S. is a function of x only and R.H.S. is a function of t only, each side must be equal to constant. Let us call this the **separation constant** η.

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + V(x) = \eta, \qquad j\hbar\frac{1}{\phi(t)}\frac{\mathrm{d}\,\phi(t)}{\mathrm{d}t} = \eta$$

Solution: Time dependent part of W.F

$$j\hbar \frac{1}{\boxed{\phi(t)}} \frac{\mathrm{d}\,\boxed{\phi(t)}}{\mathrm{d}t} = \eta$$

- The time dependent side of W.E. is then given by

$$\frac{\mathrm{d}\,\boxed{\phi(t)}}{\mathrm{d}t} = -j\frac{\eta}{\hbar}\boxed{\phi(t)} \qquad \text{related to} \qquad \frac{\mathrm{d}\,y}{\mathrm{d}\,x} = cx$$

- The solution is a sinusoidal wave given by

$$\boxed{\phi(t)} = e^{-j\left(\frac{\eta}{\hbar}\right)t} \qquad \text{related to} \qquad y = e^{-j\omega t}$$

with angular frequency ω given by $[\nu = \frac{\omega}{2\pi}]$

$$\omega = \frac{\eta}{\hbar}, \quad \Rightarrow \eta = \hbar\omega = \frac{h}{2\pi}\cdot 2\pi\nu = h\nu$$

- From Planck's law, $E = h\nu$. Therefore,

$$\eta = E, \qquad \text{and} \qquad \boxed{\phi(t)} = e^{-j\left(\frac{E}{\hbar}\right)t} = e^{-j\omega t}$$

Solution: Time independent part of W.F

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}+V(x)=\eta$$

- The time independent portion can now be written as

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}+V(x)=E$$

  where the separation constant is replaced by the total energy E.
- Therefore, the time independent part of W.E. is

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}+\frac{2m}{\hbar^2}\left(E-V(x)\right)=0$$

- This is called the time independent Schrödinger wave equation. The aim is to solve for the time independent wave function $\psi(x)$ for a given potential $V(x)$.

Physical meaning of wave function

Probability density hypothesis

If the **wave function** of a particle is $\Psi(x,t)$, then the probability density function is given by

$$|\Psi(x,t)|^2$$

- Max Born in 1926 postulated the **interpretation** of wave function.
- Let us assume that we have solved for the time independent part of wave function. Thus,

$$\Psi(x,t) = \psi(x)e^{-j\omega t}$$

- Since $\Psi(x,t)$ is a complex function, it cannot represent physical quantity. Its modulus squared is the **probability density** of finding particle between x and $x + \mathrm{d}x$ and is given by

$$|\Psi(x,t)|^2 = \Psi(x,t) \cdot \Psi^*(x,t) = \psi(x)e^{-j\omega t} \cdot \psi^*(x)e^{+j\omega t} = |\psi(x)|^2$$

- The probability of finding particle between x and $x + \mathrm{d}x$ is then

$$|\psi(x)|^2 \cdot \mathrm{d}x$$

Boundary conditions

- Total probability is unity.

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

This condition is called **normality condition**.

- Continuity condition
  1. $\psi(x)$ must be finite, single-valued and continuous.
  2. $\frac{\partial \psi(x)}{\partial x}$ must be finite, single-valued and continuous.
- $\psi(x)$ must vanish at infinity.

$$\lim_{x \to \infty} \psi(x) = 0, \qquad \lim_{x \to -\infty} \psi(x) = 0$$

This condition is due to the **physicality condition**.

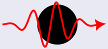
Problem

Normalization of wave function

1. *Consider the wave function* $\Psi(x, t) = A \cos\left(\frac{\pi x}{2}\right) e^{-j\omega t}$ *for* $-1 \leq x \leq +3$. *Determine* A *so that* $\int_{-1}^{+3} |\Psi(x, t)|^2 \, \mathrm{d}x = 1$.

Summary

Postulates of quantum mechanics



The work of Planck, de Broglie, Heisenberg, Born, and Schrödinger can be summarized as

1. The state of a particle is given by the wave function $\Psi(x, t)$.
2. The probability density of the particle is $|\Psi(x, t)|^2$. The probability of finding the particle in between x and $x + \mathrm{d}x$ is $|\Psi(x, t)|^2 \mathrm{d}x$.
3. If the uncertainty in position is Δx and uncertainty in position is Δp, then $\Delta x \, \Delta p \geq \frac{\hbar}{2}$.
4. The de Broglie wavelength of particle with momentum p is $\lambda = \frac{h}{p}$.
5. The energy E of the particle with frequency ν is $E = h\nu$.