

Modern Physics

Lecture 14

Quantum Mechanics

“I think that I can safely say that nobody understands quantum mechanics.”—Richard Feynman (Nobel Prize, 1965)

Wave function ψ

Physical significance

$|\psi|^2 \rightarrow$ Probability of finding a particle

Characteristics

Complex function

$$|\psi|^2 = \psi^* \psi$$

If $\psi = A + iB$

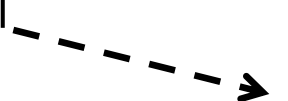
Then $\psi^* = A - iB$

Which means

$$|\psi|^2 = \psi^* \psi = (A - iB)(A + iB) = A^2 + B^2$$

Normalization of Wave function ψ

Total probability density equal to 1

$$\int_{-\infty}^{\infty} |\psi|^2 dV = 1$$


(Probability density)

Alternatively one can write

$$\int_{-\infty}^{\infty} P dV = 1$$

$$\int_{-\infty}^{\infty} |\psi|^2 dV = 0 \rightarrow \text{This means the particle does not exist}$$

$$\int_{x_1}^{x_2} P dx \rightarrow \text{It defines the probability of finding a particle in a certain region}$$

A particle limited to the x -axis has the wave function $\psi=ax$ between $x = 0$ and $x = 1$; $\Psi=0$ everywhere else. Find the probability of finding the particle between $x = 0.45$ and $x = 0.55$

We use the following
relation to find the probability

$$\int_{x_1}^{x_2} P dx$$

Here,

$$x_1 = 0.45; x_2 = 0.55; P = \psi^* \psi$$

Therefore,

$$\int_{x_1}^{x_2} P dx = \int_{x_1}^{x_2} |\psi|^2 dx$$

$$\int_{0.45}^{0.55} a^2 x^2 dx = a^2 \left[\frac{x^3}{3} \right]_{0.45}^{0.55} = 0.0251 a^2$$

ψ Must be well behaved

- Must be continuous and single valued everywhere
- First derivative must be continuous and single valued everywhere
- Must be normalizable meaning ψ must go to 0 as $x \rightarrow \infty$

This means that ψ over all space should be finite constant

Schrödinger Equation

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

Can you derive Schrodinger's equation

“Where did we get that from? It's not possible to derive it from anything you know. It came out of the mind of Schrödinger.”—Richard Feynman

However Schrödinger's equation can be think of as a quantum mechanical statement of the conservation of energy, and is probably the most important equation of quantum mechanics.

Schrodinger Equation and Energy Conservation

... The Schrodinger Wave Equation !

$$E = K + V$$

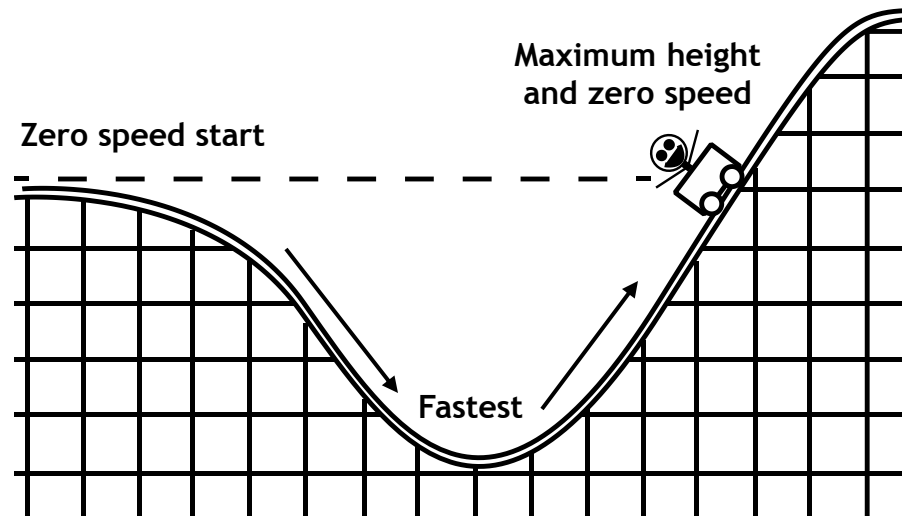


$$-j\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi$$

Total E term

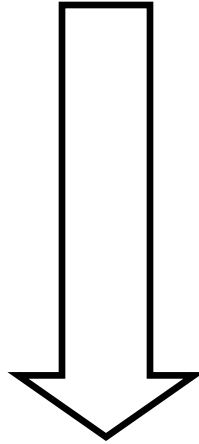
K.E. term

P.E. term



Schrodinger: A Wave Equation for Electrons

For free electrons



$$-j\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \quad (\text{free-particle})$$

..The Free-Particle Schrodinger Wave Equation !



Erwin Schrödinger (1887–1961)

Image in the Public Domain

Time-Dependent Schrodinger Wave Equation

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



Total E term



K.E. term



P.E. term

Solution

$$\Psi(x, t) = e^{-iEt/\hbar} \psi(x)$$

Substituting in relation 1,

$$i\hbar \frac{-i}{\hbar} E \psi(x) e^{\cancel{\frac{-iEt}{\hbar}}}$$

$$= -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} e^{\cancel{\frac{-iEt}{\hbar}}} + V(x) \psi(x) e^{\cancel{\frac{-iEt}{\hbar}}}$$

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

Time-Independent Schrodinger Wave Equation

Schrödinger Equation

For a particle moving in +x direction

$$\psi(x, t) = Ae^{-i\omega(t-x/v)} \quad (1)$$

Now $\omega = 2\pi\nu$ and $v = \lambda\nu$

Replacing in relation 1

$$\psi(x, t) = Ae^{-i2\pi(\nu t - x/\lambda)} \quad (2)$$

Now, $E = h\nu = 2\pi\hbar\nu$ and $\lambda = \frac{h}{p} = \frac{2\pi\hbar}{p}$

Relation 2 can be written as,

$$\psi(x, t) = Ae^{-(i/\hbar)(Et - px)} \quad (3)$$

This describes a wave of energy E and momentum p moving in $+x$ direction

Differentiating relation (3) twice with respect to x ,

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2} \psi$$

Rearranging,

$$p^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} \quad (4)$$

Differentiating relation (3) once with respect to t ,

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar} \psi$$

Rearranging,

$$E \psi = -\frac{\hbar}{i} \frac{\partial \psi}{\partial t} \quad (5)$$

From conservation of energy,

$$E = E_{KE} + E_{PE}$$

$$E = \frac{p^2}{2m} + U(x, t) \quad (6)$$

Multiplying both sides by ψ in relation (6)

$$E\psi = \frac{p^2\psi}{2m} + U(x,t)\psi \quad (7)$$

Substituting $E\psi$ and $p\psi$ from relation 4 and 5 in relation 7

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

Schrödinger's equation in one dimension

Schrödinger's equation in three dimension

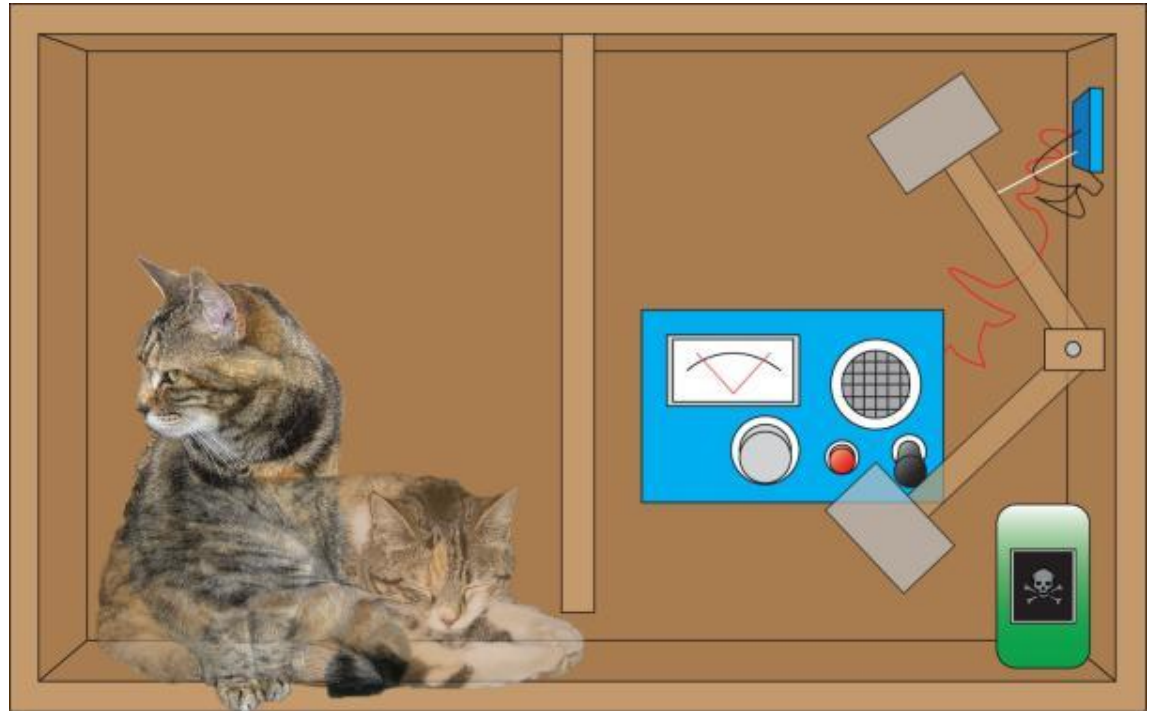
Copenhagen Interpretation of Quantum Mechanics

- A system is completely described by a wave function ψ , representing an observer's subjective knowledge of the system.
- The description of nature is essentially **probabilistic**, with the probability of an event related to the **square of the amplitude** of the wave function related to it.
- It is not possible to know the value of all the properties of the system at the same time; those properties that are not known with precision must be described by probabilities. (**Heisenberg's uncertainty principle**)
- Matter exhibits a **wave–particle duality**. An experiment can show the particle-like properties of matter, or the wave-like properties; in some experiments both of these complementary viewpoints must be invoked to explain the results.
- Measuring devices are essentially classical devices, and measure only classical properties such as position and momentum.
- The quantum mechanical description of large systems will closely approximate the classical description (**correspondence principle**).

Schrödinger's cat experiment

“It is typical of these cases that an indeterminacy originally restricted to the atomic domain becomes transformed into macroscopic indeterminacy, which can then be resolved by direct observation. That prevents us from so naively accepting as valid a "blurred model" for representing reality. In itself, it would not embody anything unclear or contradictory. There is a difference between a shaky or out-of-focus photograph and a snapshot of clouds and fog banks.”

-Erwin Schrodinger, 1935



Linearity and Superposition

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

Schrödinger's equation is linear in Ψ . In other words, it has no terms independent of Ψ , and no terms involving higher powers of Ψ or its derivatives.

As a consequence of this linearity, if Ψ_1 and Ψ_2 are solutions to Schrödinger's equation, then so is the linear combination

$$\psi = a_1\psi_1 + a_2\psi_2$$

where a_1 and a_2 are constants.

A further consequence of this is that wave functions obey superposition and exhibit interference.

If a system is represented by a wave function $\Psi = a_1 \Psi_1 + a_2 \Psi_2$, how do we calculate the probability density for Ψ ?

Can probabilities be simply added!

You can't write $P = a_1 P_1 + a_2 P_2$,


where $P_1 = \Psi_1^* \Psi_1$ and $P_2 = \Psi_2^* \Psi_2$

Instead,

$$P = \psi^* \psi = (a_1 \psi_1 + a_2 \psi_2)^* (a_1 \psi_1 + a_2 \psi_2)$$

$$P = \psi^* \psi = (a_1^* \psi_1^* + a_2^* \psi_2^*)(a_1 \psi_1 + a_2 \psi_2)$$

$$P = (a_1^* \psi_1^*)(a_1 \psi_1) + (a_1^* \psi_1^*)(a_2 \psi_2) \\ + (a_2^* \psi_2^*)(a_1 \psi_1) + (a_2^* \psi_2^*)(a_2 \psi_2)$$

$$P = P_1 + P_2 + (a_1^* \psi_1^*)(a_2 \psi_2) + (a_2^* \psi_2^*)(a_1 \psi_1)$$


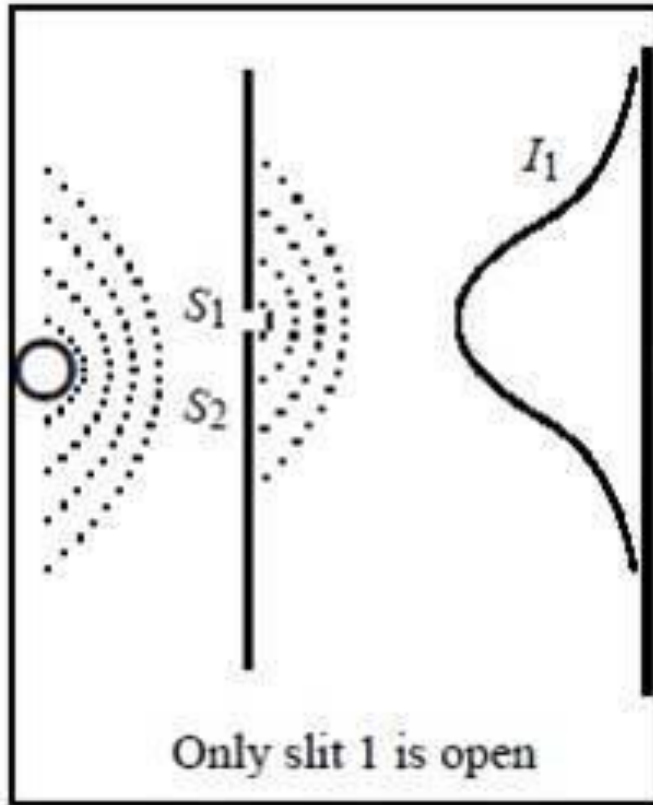
Interference terms!

Waves interfere!

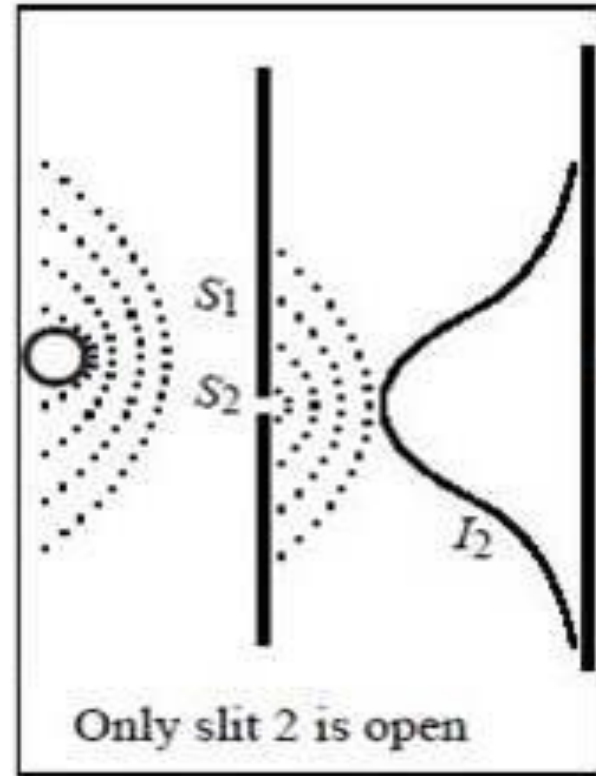
We will see why electrons “shot” through a double slit exhibit interference effects.

(unlike “pure particles” but like waves)

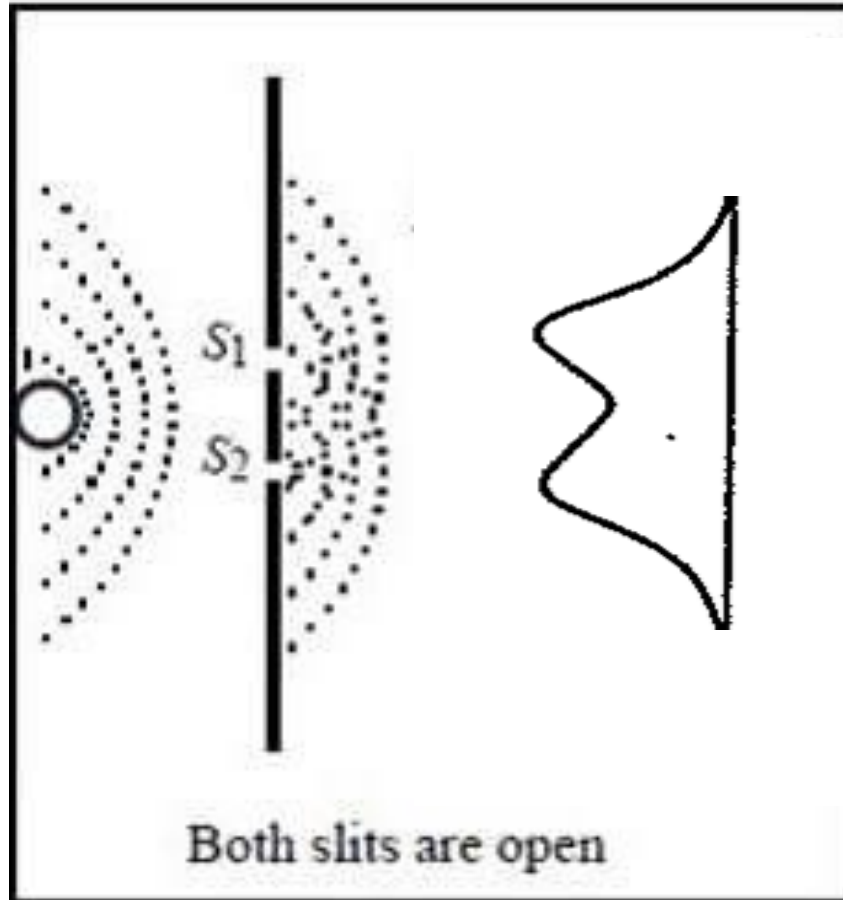
If first slit (S_1) is open only



If second slit (S_2) is open only



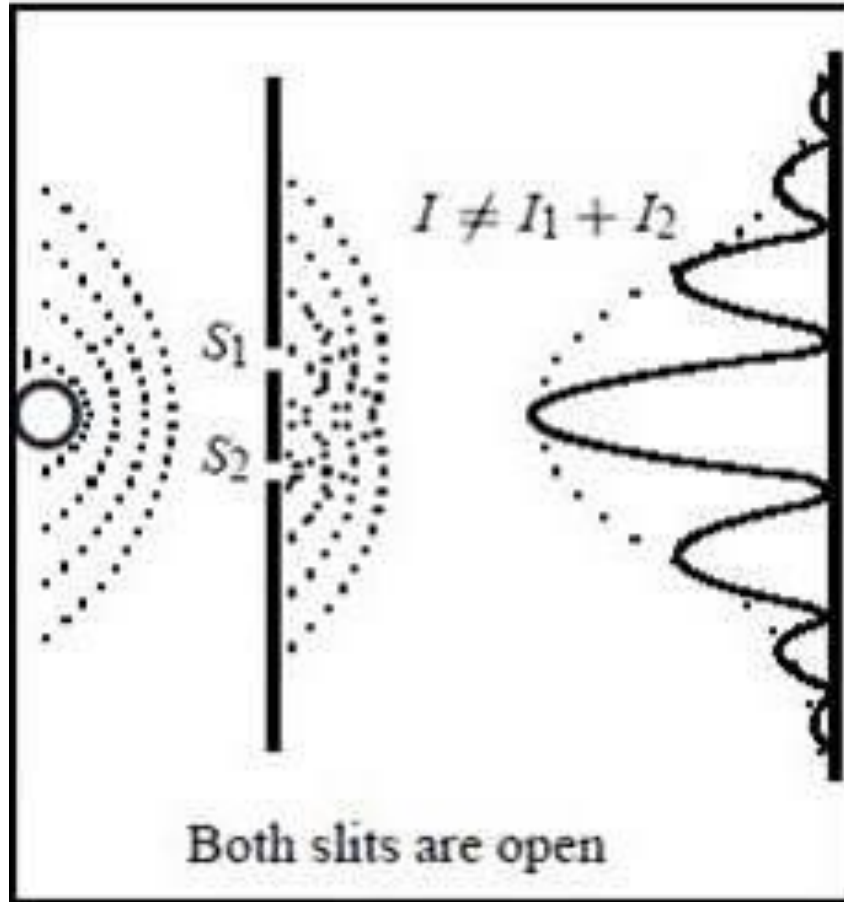
When both slits are open



If $I = I_1 + I_2$

But something else happens

When both slits are open



In reality we see interference patterns

$$I = I_1 + I_2 + (a_1^* \psi_1^*)(a_2 \psi_2) + (a_2^* \psi_2^*)(a_1 \psi_1)$$