PH 112: Quantum Physics and Applications

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Week 03, Lecture 2 : Schrodinger Equation

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Matter Waves: Recap

- The wave character of light and the photon character of light are both but different manifestations of the same thing.
- de Broglie: If waves can mimic particles, then particles can mimic waves

$$\lambda = \frac{h}{m\,v} = \frac{h}{p}$$

- de Broglie expression is only qualitative and does not help us to make precise *quantitative* predictions!

- The idea of a perfectly predictable universe cannot be true!

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

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

Matter Waves: Recap

- The idea of a perfectly predictable universe cannot be true!

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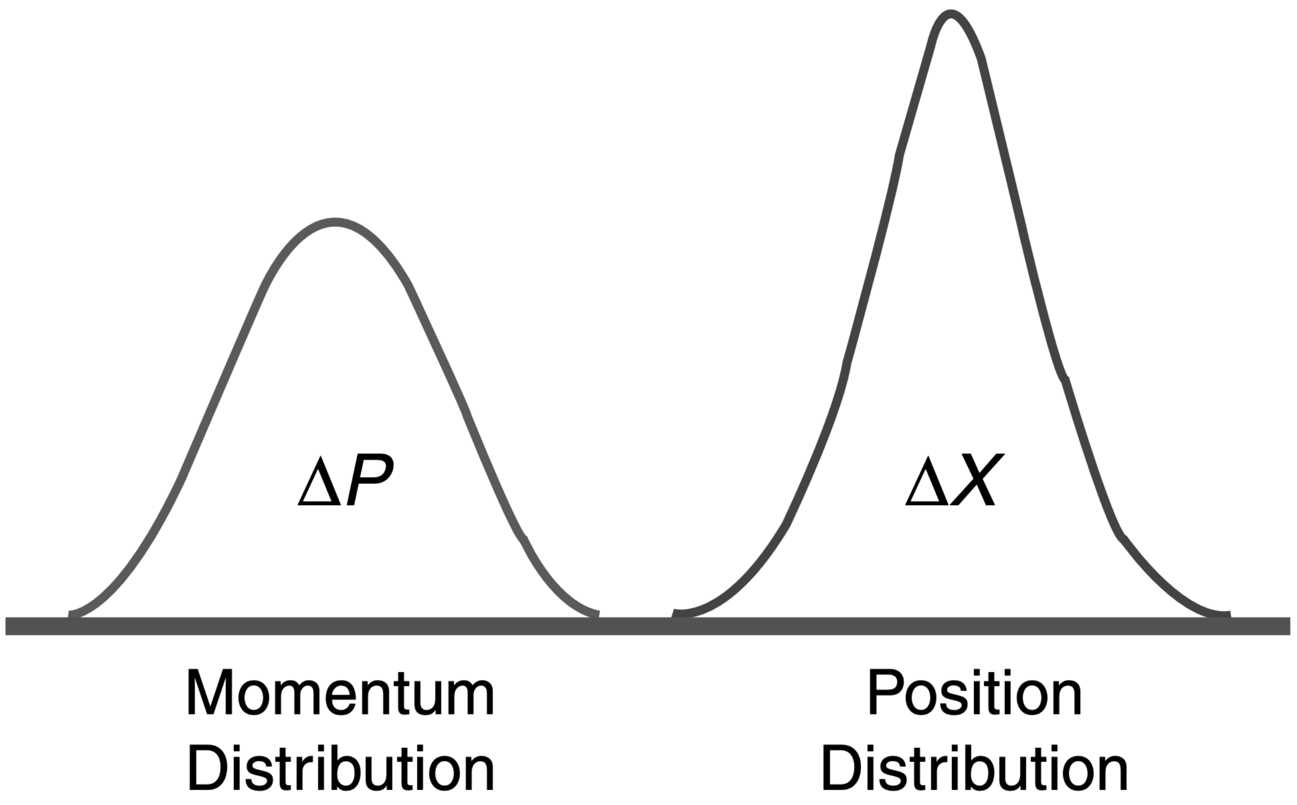
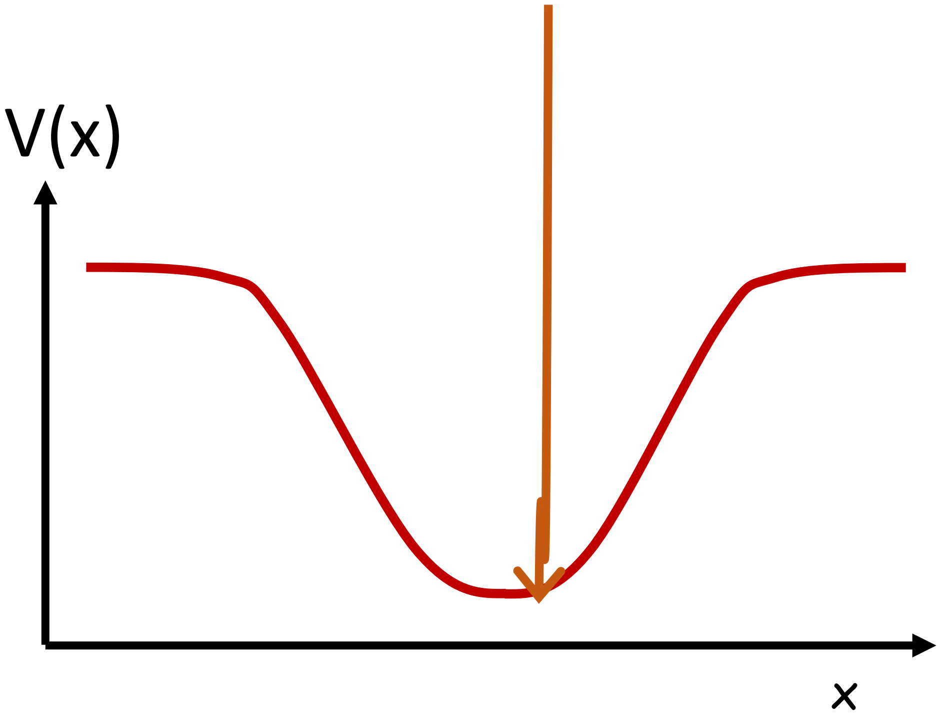


What equation matter waves satisfy?

Classically, a particle in the lowest energy state would sit right at the bottom of the well.



- Free particles: $E = \hbar\omega \quad p = \hbar\, k$

- Consider a particle in a 1-D potential $\mathrm{V}(x)$

$$E = \frac{p^2}{2\,m} + V(x)$$

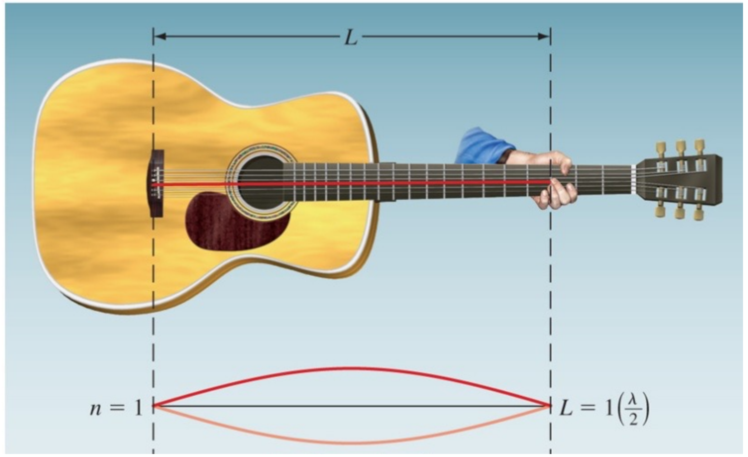
- Questions we need answers:
  1. How do we describe waves for such a particle?
  2. What happens to the particle in lowest energy state?

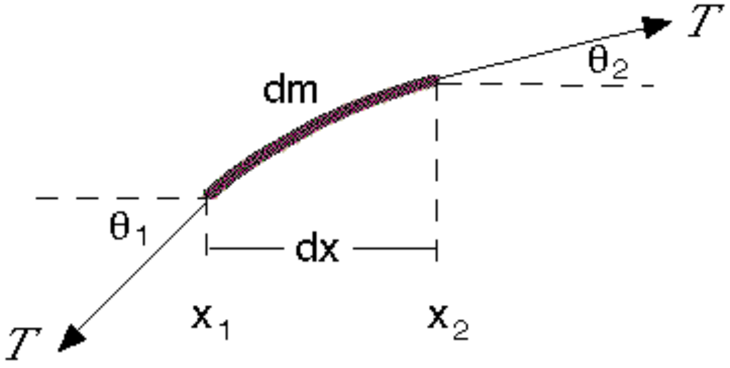
Examples:

1. Electron in hydrogen atom
2. Electron in a solid crystal
3. Electron in a nanostructure ‘quantum dot’
4. Proton in the nuclear potential inside the nucleus

Classical Wave equation

Wave equation for a string





Short section of a stretched string stretched.

- Consider a string with uniform mass per length (μ) that supports oscillations:

$$y(x,t) = A\sin(k[x - vt])$$

- We can derive the equation of motion of a string from Newton's laws of motion.

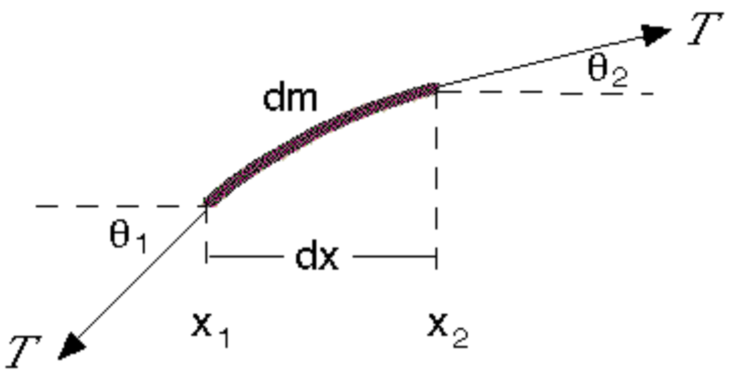
- String stretched by tension (T), Newton's law along y-axis

$$\mathrm{F_y} = \mathrm{ma_y}$$

- The sum of forces in the y-direction is

$$\mathrm{F_y} = T\sin\theta_2 - T\sin\theta_1$$

Wave equation for a string



section of the stretched string

- We now use small angle approximation,

$$\sin\theta \cong \tan\theta = \partial y/\partial x$$

- We have: $$F_y = T\left(\frac{\partial y}{\partial x}\right)_2 - T\left(\frac{\partial y}{\partial x}\right)_1$$

- Total force depends on the difference in slope between the two ends. For straight string, two forces add up to zero.

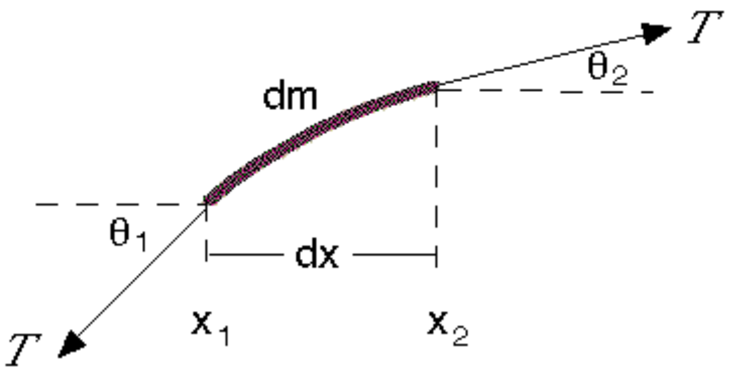
- For length dx, $\mathrm{dm} = \mu \mathrm{dx}$

- Force along y-direction becomes $$F_y = \mu \mathrm{dx} \frac{\partial^2 y}{\partial t^2}$$

Wave equation for a string

- From the two equations, we get

$$T\left(\left(\frac{\partial y}{\partial x}\right)_2-\left(\frac{\partial y}{\partial x}\right)_1\right)=\mu dx\frac{\partial^2 y}{\partial t^2}$$



- Rewriting we get, $$\frac{\partial^2 y}{\partial t^2}=\frac{T}{\mu}\frac{\left(\frac{\partial y}{\partial x}\right)_2-\left(\frac{\partial y}{\partial x}\right)_1}{dx}$$

- RHS is the rate of change of first derivative w.r.t x:

$$\frac{\partial^2 y(x,t)}{\partial t^2}=v^2\frac{\partial^2 y(x,t)}{\partial x^2}\qquad v^2=\frac{T}{\mu}$$

Short section of string stretched along x-axis.

Solution to wave equation

- Wave equation is a partial differential equation $y(x, t)$.

- One technique is to choose a likely function, test to see if it is a solution and modify it!

- We know that sine waves can propagate in a one dimensional medium like a string!

$$y(x,t) = A sin(kx - \omega t)$$

- In taking the partial derivative with respect to t, we hold x constant and vice versa.

$$\frac{\partial y}{\partial t} = -\omega A \cos(kx - \omega t) \qquad \frac{\partial y}{\partial x} = kA \cos(kx - \omega t)$$

$$\frac{\partial^2 y}{\partial t^2} = -\omega^2 \ A \sin(kx - \omega t) \qquad \frac{\partial^2 y}{\partial x^2} = -k^2 \ A \sin(kx - \omega t)$$

Solution to wave equation

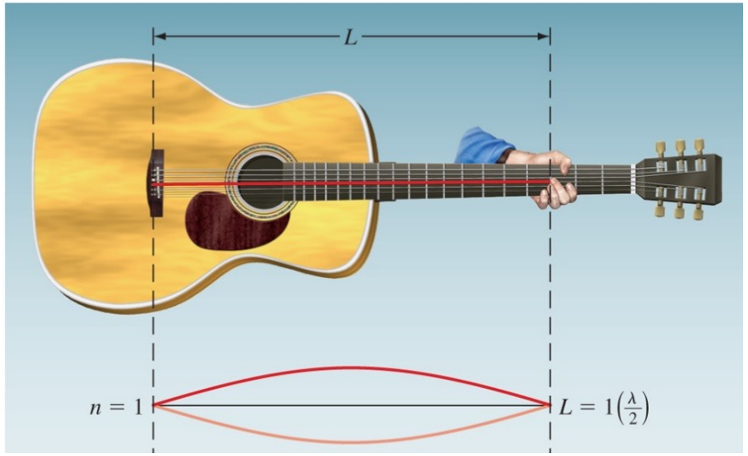
- $y(x,t) = A sin(kx - \omega t)$ is a solution of the wave equation if

$$\frac{T}{\mu} = \left(\frac{\omega}{k}\right)^2$$

$$\omega = 2\pi f; k = \frac{2\pi}{\lambda} \implies v = \sqrt{\frac{T}{\mu}} = f\lambda$$

- Not all frequencies are possible, only that satisfy condition $y_\omega(0) = 0 = y_\omega(L)$

- This leads to $\omega = \omega_n = v k_n = v \frac{\pi}{L} n$



- General solution:

$$y(x,t) = \sum_{n=1}^{\infty} A_n \sin(k_n x) e^{-i\omega_n t}$$

Relook at the classical wave equation and solution

Structure of the wave equation has ensured that the expected wave function is indeed a solution

$$y(x,t) = A\cos(kx - \omega t) \implies \frac{\partial^2 y(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y(x,t)}{\partial t^2}$$

$$\frac{\partial^2 y(x,t)}{\partial x^2} \longrightarrow k^2$$

$$\frac{\partial^2 y(x,t)}{\partial t^2} \longrightarrow \omega^2$$

$$\implies v^2 = \frac{\omega^2}{k^2} \implies v = f\lambda$$

Matter wave equation

Matter wave equation

- Schroedinger was interested in obtaining relationship between wave function and wave equation.

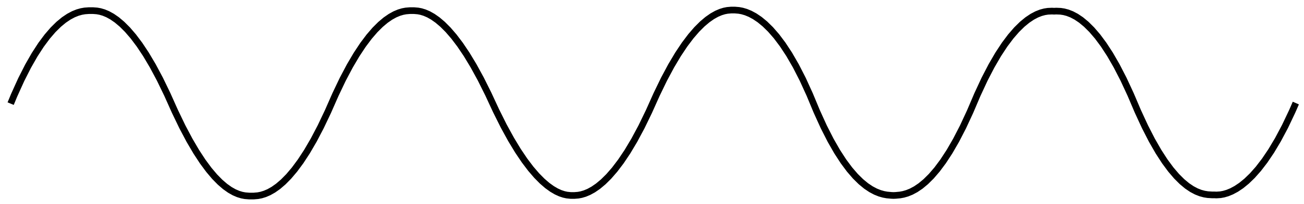
- if de broglie was correct, particles behave like waves then these de Broglie wave functions should be solutions to a wave equation.

Questions:

1. What form should this wave equation take?
2. Will it have the same form as classical wave equation?
3. If not, why classical wave equation can not describe matter waves?

Constructing a quantum wave equation

- Consider a freely moving particle is to be described by an associated wave then a reasonable first guess would be to



$$\Psi(x,t) = A\cos(kx - \omega t)$$

- According to de Broglie and Einstein relation:

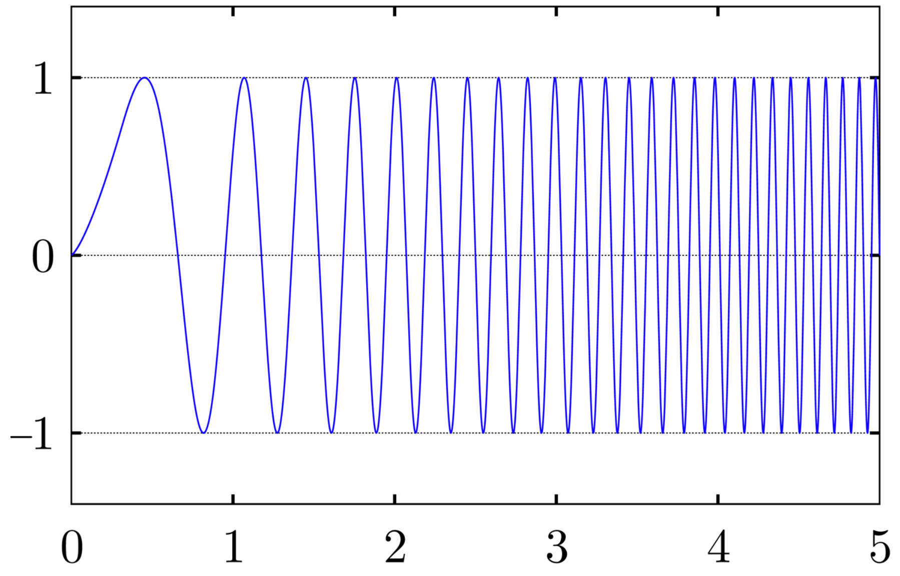
$$\text{Constant } p \longleftrightarrow \text{ Constant } \lambda \quad \text{Constant } E \longleftrightarrow \text{ Constant } f$$

- However, if a force acts on a particle

$$\text{Force} \overset{F=\frac{dp}{dt}}{\Longrightarrow} \text{ Change in } p \overset{\lambda=\frac{h}{p}}{\Longrightarrow} \text{ Change in } \lambda$$

Constructing a quantum wave equation

- If the wavelength changes rapidly, the concept of wavelength is not well defined.



- If matter wave changes rapidly, it's difficult to define variable wavelength, since separation between adjacent maxima is not equal to the separation between adjacent minima!

- If the linear momentum of a particle is not of constant magnitude, then more complicated functions than

$$\Psi(x,t) = A\cos(kx - \omega t)$$

We need a wave equation that determine $\Psi(x,t)$ for any physical situation.

Requirements of quantum wave equation

1. To be consistent with de Broglie-Einstein relations $E = \hbar\omega \qquad \lambda = \frac{h}{p}$

2. $\Psi(x,t)$ provide information about the force acting on the associated particle. Specifying Potential energy corresponding to the force.

3. To be consistent with Energy conservation $E = \frac{p^2}{2\,m} + V(x,t) \Longrightarrow F = -\frac{\partial V}{\partial x}$

4. Superposition principle of waves $\Psi(x,t)$ must be satisfied

5. For free particle $V(x) = 0$, solution should correspond to traveling wave

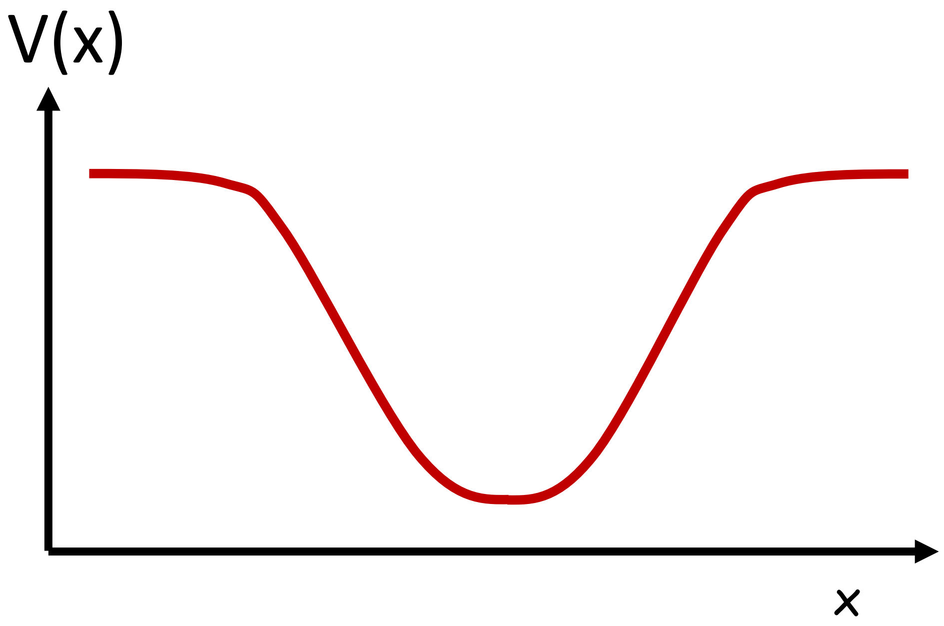
$$V(x,t) = 0 \;\Longrightarrow F = -\frac{\partial V}{\partial x} = 0 \Longrightarrow p, E = constant \Longrightarrow \;\lambda, f = constant$$

Matter Wave equation: Step I

Consider a particle in a 1-D potential $\mathrm{V}(x)$.

- Combining the first and third requirements, we have

$$E = \hbar\omega(k) = \frac{\hbar^2 k^2}{2m} + V(x)$$



- Fourth requirement implies quantum wave equation must be a linear differential equation (like classical wave equation)!

Matter Wave equation: Step II

- Fifth requirement, implies the solutions must be of the form

$$\hbar\omega(k) = \frac{\hbar^2 k^2}{2m} \implies \Psi(x,t) = \sin(kx - \omega t) \quad \text{or} \quad e^{i(kx-\omega t)}$$

- Note that

$$\frac{\partial^2}{\partial x^2} \text{ leads to } k^2 \text{ factor}$$
$$\frac{\partial}{\partial t} \text{ leads to } \omega \text{ factor}$$

- Thus we might guess a wave equation to be

$$\alpha \frac{\partial \Psi(x,t)}{\partial t} = \beta \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t)$$

α, β are constants that are fixed such that wavefunction is consistent with de Broglie-Einstein relations.

Time-dependent Schrodinger Equation

- Constants α and β can be obtained using the exponential free particle solution.

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

- Erwin Schrodinger proposed this equation in 1926 to describe the time and position dependence of the matter waves.
- This is referred to as time-dependent Schrodinger equation.

Time-independent Schrodinger equation

Suppose the potential is independent of time
i.e. $V(x, t) = V(x)$ then TDSE is:

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

In this course:

1. We will ONLY focus on time-independent Schrodinger equation.
2. We will restrict ourselves to 1-D problems.
3. It is difficult to obtain solutions even for 1-D potentials!

Time-Dependent to time-independent Schrödinger equation

Suppose the potential is independent of time i.e. $V(x, t) = V(x)$ then TDSE is:

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

LHS involves variation of ψ with *t* while RHS involves variation of ψ with *x*. Hence look for a separated solution:

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

Leading to

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

Now divide by ψT:

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2\psi}{\partial x^2} + V(x) = i\hbar\frac{1}{T}\frac{\partial T}{\partial t}$$

LHS depends only upon *x*, RHS only on *t*. True for all *x* and *t* so both sides must equal a constant, *E* (*E* = separation constant). We then have

$$i\hbar\frac{1}{T}\frac{\partial T}{\partial t} = E$$

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

Time-independent Schrödinger equation

Solving T(t) equation, we have

$$i\hbar \frac{1}{T}\frac{dT}{dt} = E \quad \Rightarrow \quad \frac{dT}{T} = -\frac{iE}{\hbar}\,dt \quad \Rightarrow \quad T(t) = Ae^{-iEt/\hbar}$$

This is exactly like a wave $e^{-i\omega t}$ with $E = \hbar\omega$. Therefore $T(t)$ depends upon the energy E.

To find out what the energy actually is we must solve the space part of the problem....

The space equation becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = E\psi \quad \text{or} \quad \hat{H}\psi = E\psi$$

This is the **time independent Schrödinger equation (TISE)** .

The TISE can often be very difficult to solve – it depends on $V(x)$!

Classical wave solutions satisfy?

Solutions of Schrodinger Equation

Question: Whether the solutions of classical wave equation are also solutions to Schrodinger equation?

$$\Psi(x,t) = A\sin(kx - \omega t)$$

Answer: No

Proof:

$$\frac{\partial \Psi}{\partial t} = -\omega A\cos(kx - \omega t)$$

$$\frac{\partial \Psi}{\partial x} = kA\cos(kx - \omega t)$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A^2 \cos(kx - \omega t)$$

$$-i\hbar\omega A\cos(kx - \omega t) \neq \left(\frac{\hbar^2 k^2}{2m} + V\right) A\sin(kx - \omega t)$$

Solutions of Schrodinger Equation

Question: What about $\Psi(x,t) = A\exp\left(i[kx - \omega t]\right)$? Answer: Yes

$$\frac{\partial \Psi}{\partial t} = -i\omega A e^{i(kx-\omega t)}$$

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

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A e^{i(kx-\omega t)}$$

$$-i\hbar(i\omega) = \left(\frac{\hbar^2 k^2}{2m} + V\right)$$

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

The solution is complex!

$\Rightarrow$. $\Psi(x,t)$ *cannot* be a physical wave (e.g. electromagnetic waves).

How to relate $\Psi(x,t)$ to measurements on a system?

Summary

Time-dependent Schrodinger equation

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

Time-independent Schrodinger equation

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

Recommended Reading

Schrödinger equation sections 6.1, 6.2 and 6.3