

# Free Study Material from All Lab Experiments



Quantum Mechanics & Applications  
Chapter - 2  
Time Independent Schrodinger Equation

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## Time Independent Schrodinger Equation

**Syllabus:** Hamiltonian, stationary states and energy eigen-values; expansion of an arbitrary wave function as a linear combination of energy eigen functions; General solution of the time dependent Schrodinger equation in terms of linear combinations of stationary states; Application to spread of Gaussian wave-packet for a free particle in one dimension; wave packets, Fourier transforms and momentum space wave function; Position-momentum uncertainty principle.

**Q 1. Derive the time independent Schrodinger wave equation from time dependent wave equation.**

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**Ans.** The wavefunction of a particle has two parts- space and time.

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

If we substitute this trial solution into the schrodinger wave equation, and make use of the meaning of partial derivatives, we get:

$$\begin{aligned} &-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} e^{-iEt/\hbar} + V(x)\psi(x)e^{-iEt/\hbar} \\ &= i\hbar - iE/\hbar e^{-iEt/\hbar} \psi(x) = E\psi(x)e^{-iEt/\hbar} \end{aligned} \quad (6.10)$$

We now see that the factor  $\exp[-iEt/\hbar]$  cancels from both sides of the equation, giving us

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (6.11)$$

If we rearrange the terms, we end up with

$$\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + (E - V(x))\psi(x) = 0 \quad (6.12)$$

Which is the time independent schrodinger equation. We note here that the quantity E, which we have identified as the energy of the particle, is a free parameter in this equation.

**Q 2. What is a Hamiltonian operator? Find the energy eigen values of a wave function?**

**Ans.** In quantum mechanics, a Hamiltonian is an operator corresponding to the total energy of the system in most of the cases.

$$\begin{aligned}\hat{H} &= \hat{T} + \hat{V} \\ &= \frac{\hat{P} \cdot \hat{P}}{2m} + \hat{V}(r, t) \\ &= -\frac{\hbar^2}{2m} \nabla^2 + \hat{V}(r, t)\end{aligned}$$

A stationary state is a quantum state with all observables independent of time. It is an eigenvector of the Hamiltonian. In the time independent Schrodinger equation, the operation may produce specific values for the energy called energy eigenvalues. This situation can be shown in the form

$$H_{op}\psi_i = E_i\psi_i$$

Where the specific values of energy are called energy eigenvalues and the  $\psi_i$  functions are called eigenfunction.

In addition to its role in determining system energies, the Hamiltonian operator generates the time evolution of the wavefunction in the form

$$H\psi = i\hbar \frac{\partial}{\partial t} \psi$$

**Q 3. Write a general solution to time dependent Schrödinger wave equation.**

**Ans.** In his time-dependent equation

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

Suppose that, instead of proposing the solution  $\Psi(r)$  we propose  $\Psi(r, t) = \Psi(r) \exp(-iEt/\hbar)$

$$\begin{aligned}& -\frac{\hbar^2}{2m} \nabla^2 \Psi(r, t) + V(r) \Psi(r, t) \\ &= -\frac{\hbar^2}{2m} \nabla^2 \Psi(r) \exp(-iEt/\hbar) + V(r) \Psi(r) \exp(-iEt/\hbar) \\ &= \left[ -\frac{\hbar^2}{2m} \nabla^2 \Psi(r) + V(r) \Psi(r) \right] \exp(-iEt/\hbar) = E \Psi(r) \exp(-iEt/\hbar) \\ &= E \Psi(r, t)\end{aligned}$$

so  $\Psi(r,t) = \psi(r)\exp(-iEt/\hbar)$  solves the time-independent schrodinger equation

**Q 4. How to expand a wavefunction as a linear combination of energy eigen functions?**

**Ans.** A wavefunction that is not an eigenfunctions can be expanded as a linear combination of eigenfunctions

$$\psi(x) = c_1\psi_1(x) + c_2\psi_2(x)$$

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Verify that if  $\psi_1(x)$  and  $\psi_2(x)$  are normalized. then the normalized wavefunction is

$$\psi(x) = \frac{1}{\sqrt{c_1^2 + c_2^2}} c_1\psi_1(x) + c_2\psi_2(x)$$

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A generalization of the above statement is the superposition principle.

**Q.5. Write down the Gaussian wave packet for a free particle in one dimension.**

**Ans. Initial construction of the gaussian packet.** To express the circumstance that "x-measurement (performed at time t=0 with an instrument of imperfect resolution) has shown the particle to reside in the vicinity of the point x=a"

$P(x,0) \equiv |\psi(x,0)|^2$  = some properly positioned and shaped distribution function and notice that such a statement supplies only limited information about the structure of  $\psi(x,0)$  itself:

$$\psi(x,0) = \sqrt{p(x,0)} e^{ia(x,0)} : \text{phase factor remains at present arbitrary.}$$

The phase factor has entered with simple innocence upon the stage, but is destined to play a leading role as the drama unfolds.

Whether we proceed from some tentative sense of the operating characteristics of instruments of finite resolution or seek only to model such statements on a concrete but analytically tractable way, it becomes fairly natural to look to the special case

$$p(x,0) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left[\frac{x-a}{\sigma}\right]^2} \quad (1)$$

The Gaussian on the right defines the "normal distribution with

mean :  $\langle x \rangle = a$

variance  $\equiv$  uncertainty :  $\langle (x-a)^2 \rangle = \sigma^2$

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and the associated wave function reads

$$\psi(x,0) = \left[ \frac{1}{\sigma\sqrt{2\pi}} \right]^{\frac{1}{2}} e^{-\frac{1}{4} \left[ \frac{x-\sigma}{\sigma} \right]^2} \cdot e^{ia(x,0)}$$

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**Q 6. What is a wave packet? How Fourier transforms of momentum and space wave functions are related?**

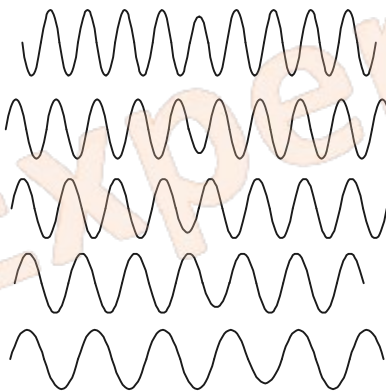
Since the traveling wave solution to the wave equation

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

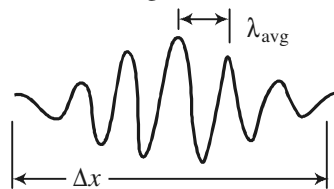
is valid for any values of the wave parameters, and since any superposition is also a solution, then one can construct a wave packet solution as a sum of traveling waves:

$$y(x,t) = \sum_i A_i \sin(k_i x - \omega_i t)$$

If discrete traveling wave solutions to the wave equation are combined, they can be used to create a wave packet which begins to localize the wave. This property of classical waves is mirrored in the quantum mechanical uncertainty principle.



Adding several waves of different wavelength together will produce an interference pattern which begins to localize the wave.



But that process spreads the wave number  $k$  values and makes it more uncertain. This is an inherent and inescapable increase in the uncertainty  $\Delta k$  when  $\Delta x$  is decreased.  $\Delta k \Delta x \approx 1$

We can represent a state with  $\psi(x)$  either or with  $\phi(p)$ . We can (Fourier) transform from one to the other.

We have the symmetric Fourier Transform.

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

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

When we change variable from K to P, we get the Fourier Transforms in terms of  $x$  and  $p$ .

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

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

Fourier transform of a gaussian is a gaussian. Let a Gaussian wave packet representing the position of a particle then its FT in momentum space is also a Gaussian. If the Gaussian Wave packet in position space is narrow then the wave packet in momentum space is broad and vice versa. This gives rise to the uncertainty principle.

**Q 7. Explain Position-Momentum Uncertainty Principle.**

**Ans.** The position and momentum of a particle cannot be simultaneously measured with arbitrarily high precision. There is a minimum for the product of the uncertainties of these two measurements.

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

Important steps on the way to understanding the uncertainty principle are wave-particle duality and the De Broglie hypothesis. As you proceed downward in size to atomic dimensions, it is no longer valid to consider a particle like a hard sphere, because the smaller the dimension, the more wave-like it becomes. It no longer makes sense to say that you have precisely determined both the position and momentum of such a particle. When you say that the electron acts as a wave, then the wave is the quantum mechanical wavefunction and it is therefore related to the probability of finding the electron at any point in space. A perfect sine wave for the electron wave spreads that probability throughout all of space, and the "position" of the electron is completely uncertain.



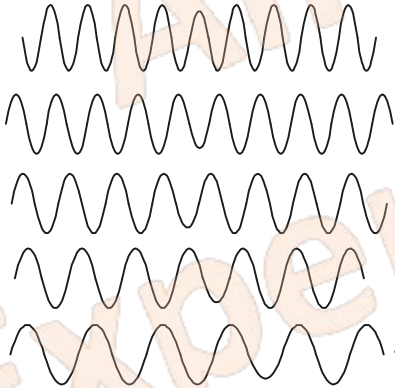
Precisely determined momentum



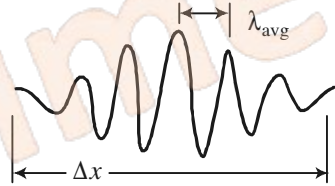
A sine wave of wavelength  $\lambda$  implies that the momentum is precisely known, But the wavefunction and the probability of finding the particle  $\Psi^* \Psi$  is spread over all of space!

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

$p$  precise  
 $x$  unknown



Adding several waves of different wavelength together will produce an interference pattern which begins to localize the wave.



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

