Quantum Mechanics (P304H)
Part 2 – Lecture 10

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Erwin with his psi can do
Calculations quite a few.
But one thing has not been seen:
Just what does psi really mean?

Erich Hückel, translated by Felix Bloch

Contents and Outline for Part 2

Applications of the Schrödinger Equation:

- Solution of the 1-dimensional Time Independent Schrödinger Equation (TISE) for the potential step and potential barrier.
- Interpret the solutions: the tunneling process.
- Solve the TISE for potential square wells of finite and infinite depth.
- Discuss the resulting quantised and continuous energy levels, eigenvalues and quantum numbers.
- Show that the TISE for the (1d) simple harmonic oscillator results in Hermite's equation, with solutions which are Hermite functions.
- Show that the boundary conditions result in the quantization of its energy levels.
- Use the optical spectroscopy of quantum wells in semiconductors and alpha particle decay as examples.

Contents and Outline for Part 2

Angular Momentum:

- Review "Classical" angular momentum.
- Motivate the angular momentum operators in quantum mechanics and derive their commutation relations.
- Solve the angular part of the TISE for a central potential and define spherical harmonics and Legendre polynomials in terms of eigenfunctions of angular momentum.
- Provide an elementary treatment of the addition of angular momenta by analogy to vectors.

Text books:

1. B.H. Bransden and C.J. Joachain, *Quantum Mechanics* (2nd edition), Pearson Education Ltd., 2000.
2. Alastair I M Rae, *Quantum Mechanics*, 3rd edition, IoP Publishing (1998)
3. Eisberg and Resnick, *Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particles*, (Wiley)

1. Introduction

- Summary of concepts already encountered:
  - In Quantum Mechanics, all information about a particle is contained in its wave function: $\Psi(x,t)$
  - Probability of finding particle in region x to x+dx is

$$P(x,t)dx = \Psi^*(x,t)\Psi(x,t)dx = \left|\Psi(x,t)\right|^2 dx$$

  - The particle must be somewhere in space (normalization condition):

$$\int_{-\infty}^{\infty} \left|\Psi(x,t)\right|^2 dx = 1$$

  - The behaviour of a particle is described by the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}\Psi(x,t)$$

where $\hat{H}$ is the Hamiltonian operator:

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

1. Introduction

- Operators:
  - In QM, dynamical variables are replaced by *operators*: $\hat{O}$

    (I will adopt the convention that an operator has a hat ^ on top)
  - Operator acting on an eigenfunction is the eigenvalue times the eigenfunction: $\hat{O}\Psi(x,t) = O_n\Psi(x,t)$

Quantity	Operator	Representation
Momentum	$\hat{p}_x$	$-i\hbar\dfrac{\partial}{\partial x}$
Position	$\hat{x}$	x
Kinetic energy	$\hat{T} = \dfrac{\hat{p}_x^{\,2}}{2m}$	$\dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}$
Potential energy	$\hat{V}$	$V(x)$
Total energy (Hamiltonian)	$\hat{H} = \hat{T} + \hat{V}$	$\dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2} + V(x)$

2. 1D Schrödinger Equation

To solve the Schrödinger equation, we need to perform separation of variables. Assume that:

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

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

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

Divide both sides by $\psi(x)T(t)$:

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

Hence both sides have to be equal to a constant *E* (with units of energy!).

The time part of the equation:

$$i\hbar\frac{1}{T(t)}\frac{dT(t)}{dt} = E \Rightarrow$$

$$i\hbar\frac{dT(t)}{dt} - ET(t) = 0 \Rightarrow T(t) = Ae^{-i\frac{Et}{\hbar}} = Ae^{-i\omega t} \quad \text{where} \quad \omega = \frac{E}{\hbar}$$

2. 1D Schrödinger Equation

- 1D Time-independent Schrödinger equation:
  - The spatial part of the Schrödinger equation is called the Time-Independent Schrödinger Equation TISE (in 1D):

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

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

This is an eigenvalue problem: $\hat{H}\psi(x)=E\psi(x)$
with $\hat{H}=\hat{T}+\hat{V}$ the Hamiltonian

We will solve the 1D time-independent Schrödinger equation for different assumptions of V(x)

2. 1D Schrödinger Equation

- Free particles: assume V(x)=0

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - E\psi(x) = 0 \Rightarrow \psi(x) = Ae^{ikx} + Be^{-ikx} \text{ with } k = \sqrt{\frac{2mE}{\hbar^2}}$$

  - Proof:

$$\frac{d^2\psi(x)}{dx^2} = -k^2\left(Ae^{ikx} + Be^{-ikx}\right) \quad \Rightarrow \quad k^2 - \frac{2mE}{\hbar^2} = 0 \quad \Rightarrow \quad k = \pm\sqrt{\frac{2mE}{\hbar^2}}$$

  - Total wave function:

$$\Psi(x,t) = \left(Ae^{ikx} + Be^{-ikx}\right)e^{-i\omega t} \qquad \text{where} \qquad \omega = \frac{E}{\hbar}$$

This solution is simply the sum of two **plane waves**, the solution to the wave equation, and E is interpreted as the total energy of the system.

2. 1D Schrödinger Equation

Note:

The normalization of plane waves is problematic, since:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{\infty} \left| \left(Ae^{ikx} + Be^{-ikx} \right) e^{-i\omega t} \right|^2 dx$$

$$= \int_{-\infty}^{\infty} \left(A^* e^{-ikx} + B^* e^{+ikx} \right) e^{+i\omega t} \left(Ae^{ikx} + Be^{-ikx} \right) e^{-i\omega t} dx$$

$$= \int_{-\infty}^{\infty} \left(A^* A + B^* B + B^* A e^{+i2kx} + A^* B e^{-i2kx} \right) dx$$

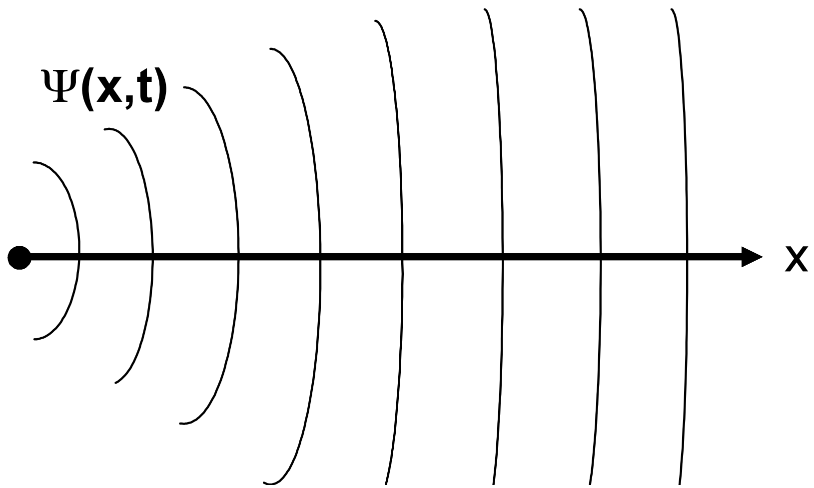
$$= \int_{-\infty}^{\infty} \left(|A|^2 + |B|^2 + B^* A e^{+i2kx} + A^* B e^{-i2kx} \right) dx = 1 \Rightarrow A = B = 0!!!$$

2. 1D Schrödinger Equation

A way around it:

1. Assume particles are moving in positive *x*-direction => *B=0*
2. Assume plane waves confined in space of dimension *L*, (justified, assuming that average separation between particles is *L*).

$$\int_0^L \left|\Psi(x,t)\right|^2 dx = \int_0^L \left|A\right|^2 dx = 1 \Rightarrow A = (L)^{-1/2} \Rightarrow \Psi(x,t) = \frac{1}{\sqrt{L}} e^{i(kx-\omega t)}$$



The particles propagate as wave fronts of constant phase (plane waves), since there are no potentials to distort the passage of the particles.

2. 1D Schrödinger Equation

- Momentum ($B=0$):

$$\bar{p}_x = \int \Psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\Psi(x,t)\right)dx$$

$$= \int A^* e^{-i(kx-\omega t)}\left(-i\hbar\frac{\partial}{\partial x}\right)Ae^{i(kx-\omega t)}dx$$

$$= \int A^* e^{-ikx} k\hbar A e^{ikx} dx = \hbar k$$

since $\int A^* A dx = 1$

Independent of x and t ($\Delta p_x=0$, therefore $\Delta x=\infty$)

2. 1D Schrödinger Equation

- Probability density (*B=0*):

$$P(x,t) = |\Psi(x,t)|^2 = \left|Ae^{i(kx-\omega t)}\right|^2 = |A|^2$$

Independent of x and t ($\Delta p_x=0$, therefore $\Delta x=\infty$)

Probability current density (see first part of lectures):

$$\mathbf{J}(x,t) = \frac{\hbar}{i2m}\left[\Psi^*(x,t)\left(\nabla\Psi(x,t)\right) - \left(\nabla\Psi^*(x,t)\right)\Psi(x,t)\right]$$

$$= \frac{1}{2}\left[\Psi^*(x,t)\left(\frac{\hbar}{im}\nabla\Psi(x,t)\right) + \left(\frac{\hbar}{im}\nabla\Psi(x,t)\right)^*\Psi(x,t)\right]$$

$$= \mathrm{Re}\left[\Psi^*(x,t)\left(\frac{\hbar}{im}\nabla\Psi(x,t)\right)\right] \Rightarrow$$

$$p = \hbar k = mv$$

$$J(x,t) = \mathrm{Re}\left[A^* e^{-i(kx-\omega t)}\frac{\hbar}{im}Aike^{i(kx-\omega t)}\right] = \frac{\hbar k}{m}|A|^2 = v|A|^2$$

2. 1D Schrödinger Equation

Probability current density is related to velocity and probability density

$$J(x,t) = vP(x,t)$$

(positive since moving from left to right, i.e. positive x):

Remember the continuity equation:

$$\frac{\partial P(x,t)}{\partial t} + \frac{\partial J(x,t)}{\partial x} = 0$$

Probability conservation: the rate of change of the probability of finding the particle in a given volume equals the probability current density escaping the volume.

2. 1D Schrödinger Equation

- Comparison with case A=0:

Probability current density:

The probability current density is negative since the movement is from right to left

$$P(x,t) = |\Psi(x,t)|^2 = |B|^2$$

$$J(x,t) = -\frac{\hbar k}{m}|B|^2 = -v|B|^2 = -vP(x,t)$$

For the next few lectures, we will just consider the time-independent part of the Schrodinger equation and test for possible solutions under different assumptions about the 1 dimensional potential V(x).