LECTURE 13-: Properties of the Schrodinger Equation and its solutions

Goals of the lecture: discuss general properties of the Schrodinger equation and its solutions in order to acquire the background knowledge necessary to solve simple problems

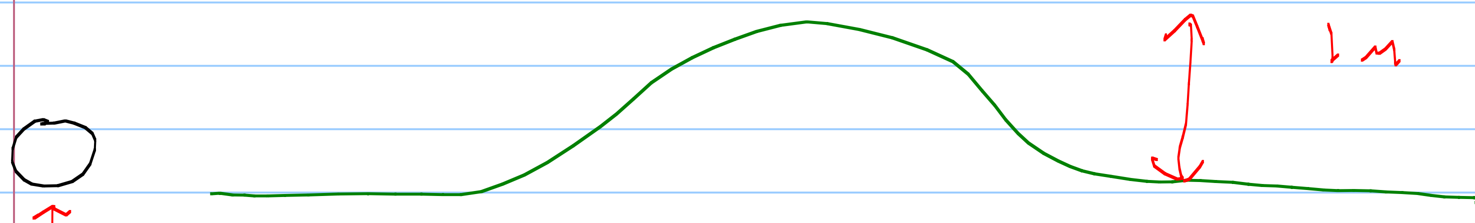
What I expect you to learn:

- -why we need continuity conditions
- - the conservation of probablility and the probability current density
- -What are expectation values and how to calculate them

(Roughly corresponds to sections 3.1 to 3.4 of textbook)

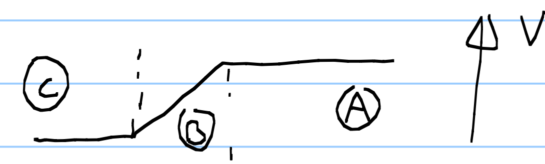
(Reminder: Problem set 2 due Friday the 13th)

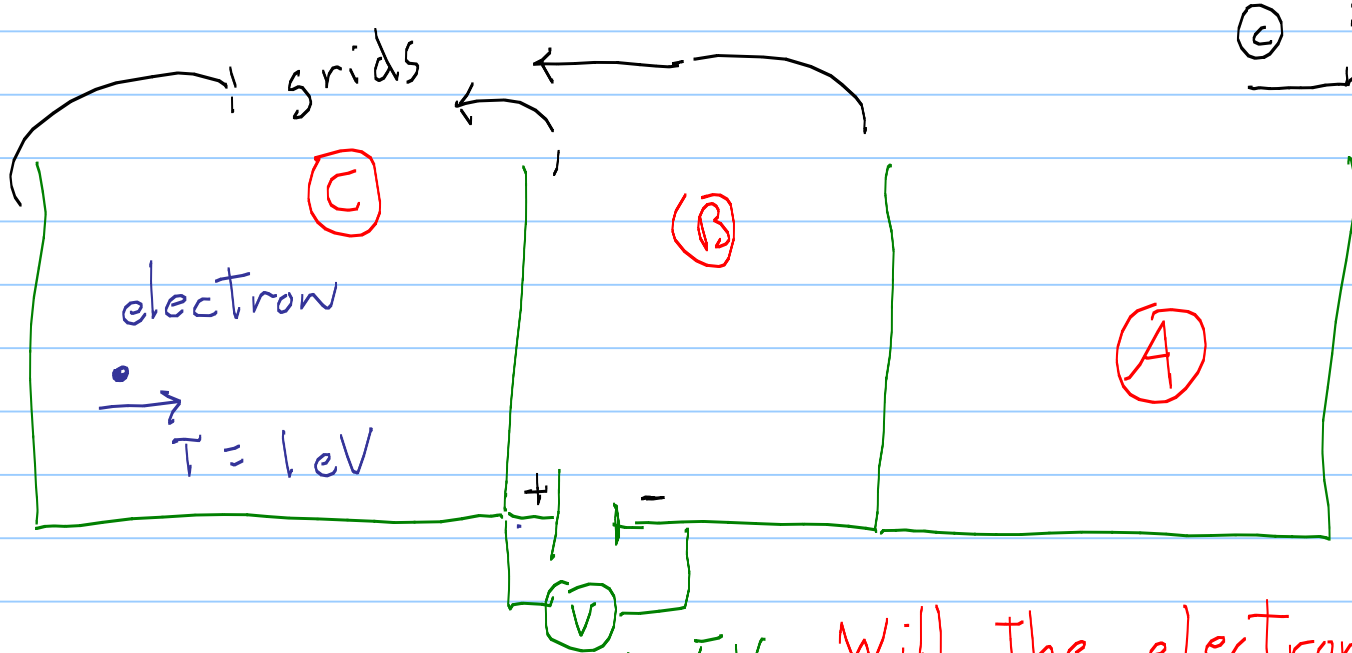
Consider the Following problems:



BALL WITH KINETIC ENERGY OF 1 JOULE (mass = 2 Kg, velocity 1 m/s)

WILL THE BALL GO OVER THE HILL?



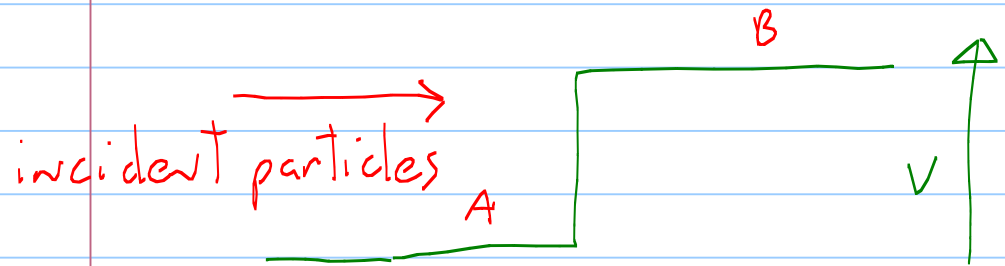


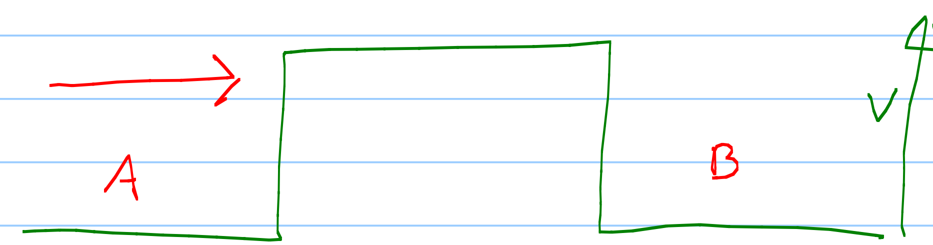
Will the electron get to A

A ROADMAP

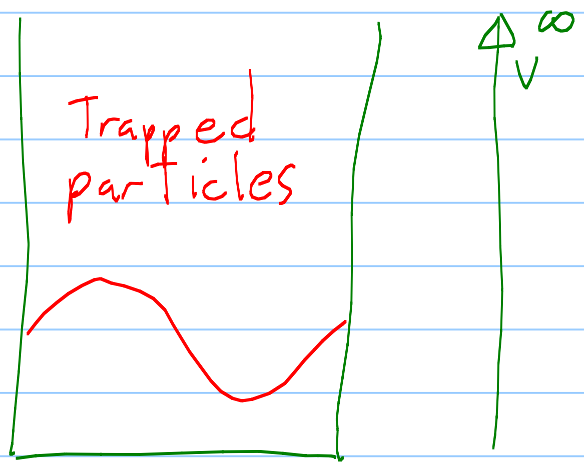
WHERE ARE WE GOING?

WE WANT TO BE ABLE TO SOLVE PROBLEMS LIKE THESE

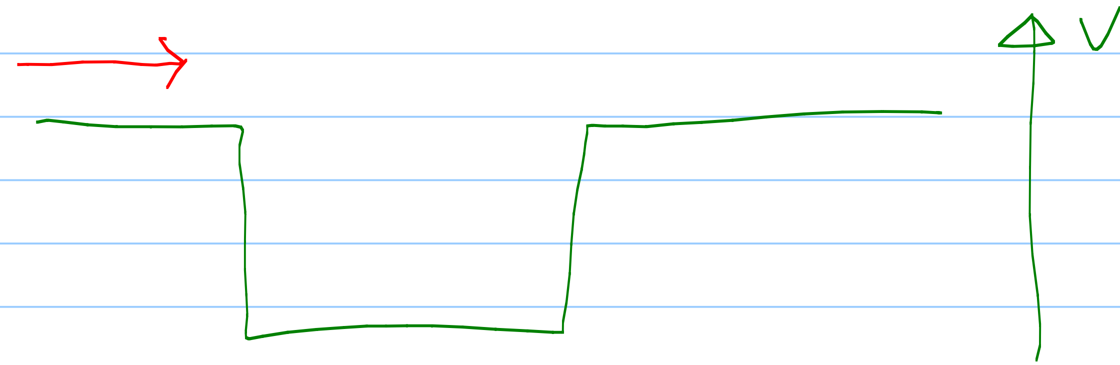




what fraction of particles reach region B?



WHAT ARE THE ALLOWED ENERGIES FOR PARTICLES IN THIS WELL?



what happens here??

ROADMAP (cont.)

To solve the previous problems, and eventually more complicated potential wells (e.g. the hydrogen atom), we'll need to investigate some properties of the Schrodinger equation and its solutions in more details.

So in this part (chapter 3 of book), we assemble the tools and knowledge we'll need to solve some simple problems

The mathematical space we are exploring is richer than what is dictated by physics. We need to determine some of the constraints. For starters, the wave function is constrained by:

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

It must be "square integrable"

Properties of Schrodinger's Equation (cont.)

We have also seen that the equation is linear:

if ψ_1 is a solution and ψ_2 is a solution

then $\psi_3 = a\psi_1 + b\psi_2$ is a solution

We have seen that the solution can be expressed as a sum of plane waves:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \varphi(k)\, e^{i(kx-\omega t)}\, dk \longrightarrow e^{\frac{i}{\hbar}(px - Et)}$$

We have seen that momentum and energy are represented by differential operators

$$\frac{\partial \psi}{\partial t} = \frac{-iE}{\hbar}\psi \rightarrow E = \frac{p^2}{2m}, \quad -\frac{i}{\hbar}\frac{p^2}{2m}\psi = \frac{\partial \psi}{\partial t}, \quad \boxed{i\hbar\frac{\partial}{\partial t}\psi = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi}$$

$$E_{op} = \frac{-\hbar}{i}\frac{\partial}{\partial t} = \boxed{i\hbar\frac{\partial}{\partial t}}, \quad p_{x\,op} = \boxed{-i\hbar\frac{\partial}{\partial x}}$$

Properties of Schrodinger's Equation (cont.)

So in 3 dimensions we can write: (with $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$)

$$p_{op}^2 = -\hbar^2 \nabla^2 \quad , \quad E_{op} \Psi = \frac{-\hbar^2 \nabla^2}{2m} \Psi$$

We can also write:

$$E = p^2/2m + V(r,t) \quad , \quad i\hbar \frac{\partial \Psi}{\partial t} = H \Psi$$

Where H is the Hamiltonian

classical version, QM version: $H = -\frac{\hbar^2}{2m}\nabla^2 + V$

$\hookrightarrow$ operator

We'll soon see:

$H\Psi = E\Psi$

$\longrightarrow$ eigenvalue of H (attend tutorial)

Properties of Schrodinger's Equation (cont.)

Continuity Relations:

ψ must be continuous wrt x, y, z or $\nabla\psi$ will diverge $\rightarrow$ momentum not physical

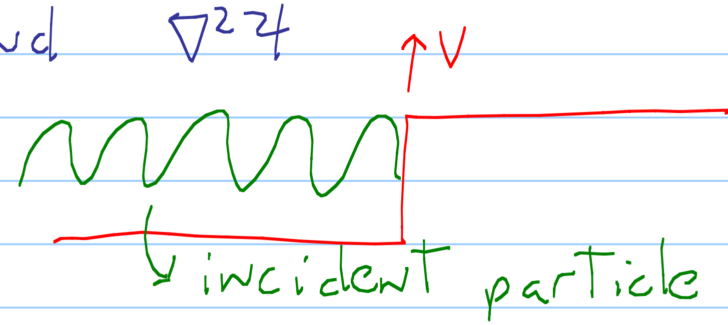
$\nabla\psi$ must be continuous or $\nabla^2\psi$ will diverge
$\rightarrow$ Energy not physical

Same argument regarding ψ wrt time

$\frac{\partial\psi}{\partial t}$ must not diverge

We will consider finite discontinuities
For $V(r,t)$ and $\nabla^2\psi$

e.g.



Properties of Schrodinger's Equation (cont.)

Conservation of probablility:

we have: $|\Psi(r,t)|^2 = P(r,t)$

$$\int P(r,t)\,dr = 1 \Rightarrow \frac{d}{dt}\int P(r,t)\,dr = 0$$

Let's consider a finite volume:

$$\frac{\partial}{\partial t}\int_V P(r,t)\,dr = \int_V \frac{\partial}{\partial t}|\Psi(r,t)|^2\,dr = \int_V \frac{\partial}{\partial t}(\Psi^*\Psi)\,dr$$

$$= \int_V \left[\frac{\partial \Psi^*}{\partial t}\Psi + \Psi^*\frac{\partial \Psi}{\partial t}\right] dr$$

Properties of Schrodinger's Equation (cont.)

Conservation of probablility:

we have:
$$\frac{\partial}{\partial t}\int_V \rho(r,t)\,dr = \int_V \left[\frac{\partial \psi^*}{\partial t}\,\psi + \psi^*\frac{\partial \psi}{\partial t}\right] dr \qquad (1)$$

we also have:
$$-i\hbar\frac{\partial}{\partial t}\psi^* = \left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\psi^*$$

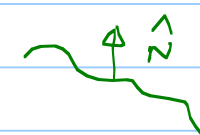
with V "real", we get (1) =
$$\frac{i\hbar}{2m}\int_V \left[\psi^*(\nabla^2\psi) - (\nabla^2\psi^*)\psi\right] dr$$

$$\boxed{\frac{1}{i} = -i}$$

$$= \frac{i\hbar}{2m}\int_V \nabla\cdot\left[\psi^*(\nabla\psi) - (\nabla\psi^*)\psi\right] dr$$

use $\vec{j} = \hbar/2mi\,[\psi^*\nabla\psi - \nabla\psi^*\psi]$

$$\frac{\partial}{\partial T}\int_V \rho(r,T)\,dr = \underbrace{-\int_V \vec{\nabla}\cdot\vec{j}\,d\vec{r} = -\int_S \vec{j}\cdot d\vec{S}}_{\text{Gauss theorem}}$$



$d\vec{S} = \hat{n}\cdot dS$

Conservation of probability cont.

we have

$$\frac{\partial}{\partial t}\int_V P(r,t)\,dr = -\int_S \vec{J}\,dS$$

At infinity, $\psi(r)$ must vanish $\Rightarrow$ surface integral will vanish

$\vec{J}$ can be interpreted as a "current probability density". we have

$$\frac{\partial P(r,t)}{\partial t} + \nabla\cdot\vec{J}(r,t) = 0$$

analogous to charge conservation in electrodynamics

$$\frac{\partial Q}{\partial t} + \nabla\cdot\vec{J} = 0$$

Properties of Schrodinger's Equation (cont.)

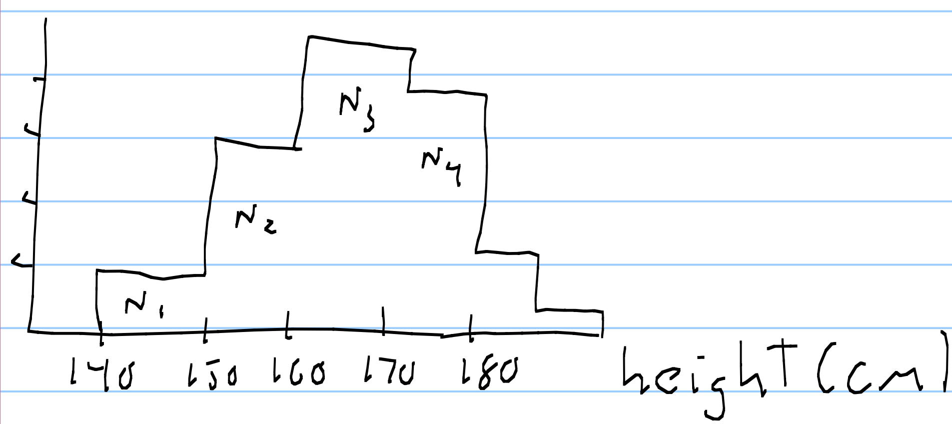
Probablility current density:

Note that the probablility current vanishes if the wave function is real. We'll deal with complex wave functions to describe non-vanishing currents

The probablility current and the probablility are continuous with respect to r and t given that the wave function and its derivatives are continuous.

Average height of people in the class:

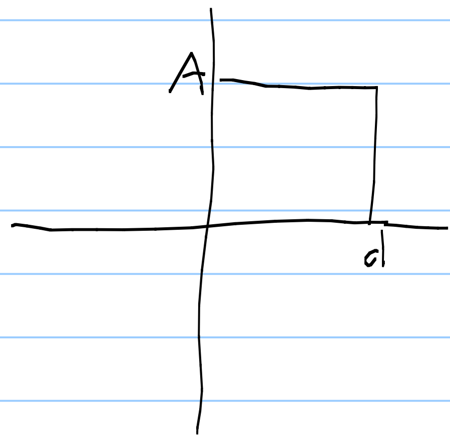
$$\langle h \rangle = \frac{\sum_{i=1}^{N_{bins}} N_i h_i}{\sum_{i=1}^{N_{bins}} N_i}$$



h_i : height for bin i
N_i : number of students in bin i

Average of a Function in "x"

$$f(x) = A \quad , \quad 0 < x < d$$
$$f(x) = 0 \quad \text{elsewhere}$$



$$\langle x \rangle = \frac{\int_0^d x \cdot A \, dx}{\int_0^d A \, dx} = \frac{\left.\frac{x^2}{2} A \right|_0^d}{\left. A x \right|_0^d} = \frac{d}{2}$$

Average Position of a particle:

$$\langle r \rangle = \frac{\int r \, P(r,t) \, dr}{\int P(r,t) \, dr} = \boxed{\int r \, P(r,t) \, dr}$$

$$1 = \int P(r,t) \, dr$$

$$= \int \Psi^*(r,t) \, r \, \Psi(r,t) \, dr \quad (2)$$

Properties of Schrodinger's Equation (cont.)

Expectation Values for momentum:

$$\langle p \rangle = \int_{-\infty}^{\infty} \varphi(p)^* \, p \, \varphi(p) \, dp$$

↳ analog in momentum space of (2)

What about $\langle p \rangle$ in "ordinary space"?

$$\rightarrow \langle p \rangle = m \frac{d}{dt} \langle x \rangle \qquad \left(p = mv = m \frac{dx}{dt} \right)$$

$$\rightarrow \langle p \rangle = m \frac{d}{dt} \int_{-\infty}^{\infty} dx \, \Psi^*(x,t) \, x \, \Psi(x,t)$$

does not depend on t!

depends on t

$$\langle p \rangle = m \int_{-\infty}^{\infty} dx \; \frac{\partial \Psi^*}{\partial t} \, x \, \Psi + \Psi^* \, x \, \frac{\partial \Psi}{\partial t} \qquad (3)$$

use Schrodinger's equation to replace $\frac{\partial \Psi}{\partial t}$

Expectation Values

from (3) we get

$$\langle p \rangle = \frac{\hbar}{2i}\int_{-\infty}^{\infty} dx \left(\frac{\partial^2\psi}{\partial x^2} x \psi - \psi^* x \frac{\partial^2\psi}{\partial x^2} \right) \quad (4)$$

$$= \frac{\partial}{\partial x}\left[\frac{\partial\psi^*}{\partial x} x \psi\right] - \frac{\partial\psi^*}{\partial x}\psi - \frac{\partial\psi^*}{\partial x} x \frac{\partial\psi}{\partial x}$$

$$= \frac{\partial}{\partial x}\left[\frac{\partial\psi^*}{\partial x} x \psi\right] - \frac{\partial}{\partial x}(\psi^*\psi) + \psi^*\frac{\partial\psi}{\partial x} - \frac{\partial}{\partial x}\left[\psi^* x \frac{\partial\psi}{\partial x}\right]$$

$$+ \psi^*\frac{\partial\psi}{\partial x} + \psi^* x \frac{\partial^2\psi}{\partial x}$$

— cancels

Integrand:

$$\underbrace{\frac{\partial}{\partial x}\left(\frac{\partial\psi^*}{\partial x} x\psi - \psi^* x \frac{\partial\psi}{\partial x} - \psi^*\psi\right)}_{} + 2\psi^*\frac{\partial\psi}{\partial x}$$

will vanish, why?

Expectation values

(4) becomes $\langle p \rangle = \int_{-\infty}^{\infty} dx\, \Psi^*(x,t) \boxed{\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)} \Psi(x,t)$

note that in momentum space:

$$\langle x \rangle = \int_{-\infty}^{\infty} dp\, \varphi^*(p)\, i\hbar \frac{\partial}{\partial p}\, \varphi(p)$$

momentum operator

Also note that:

$$\boxed{x\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \neq \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) x}$$

X and p operators do not commute!
(more on this later)

Example calculations on the blackboard...