Quantum Mechanics Part 1

Ch 39/24/40

Outline

- wave functions and uncertainty (ch 39) (1,2)
  - Uncertainty
  - Photons – particles
  - electrons – waves (psi and prob)
- Sch eqn (ch 40) (2)
  - Particle in box (3)
  - finite boxes/forbidden regions (3)
  - SHO (3)
  - Bonds (4)
  - Tunneling and decay (4)
- examples/survey (Ken-5)

Waves or Particles?

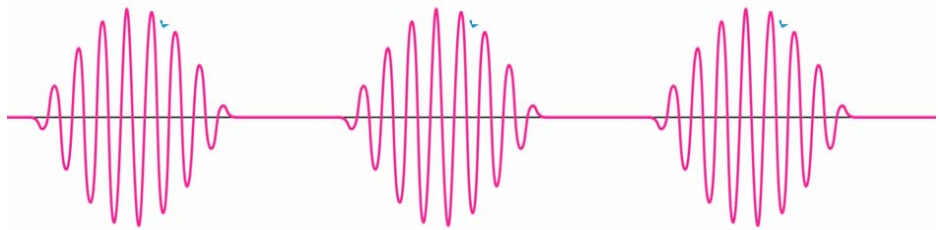
- We found out
  - electrons are particles
  - light is waves
- Later we found out
  - light is particles
  - electrons are waves
- What gives?
  - Neither?
  - Both?

Lets think about the description

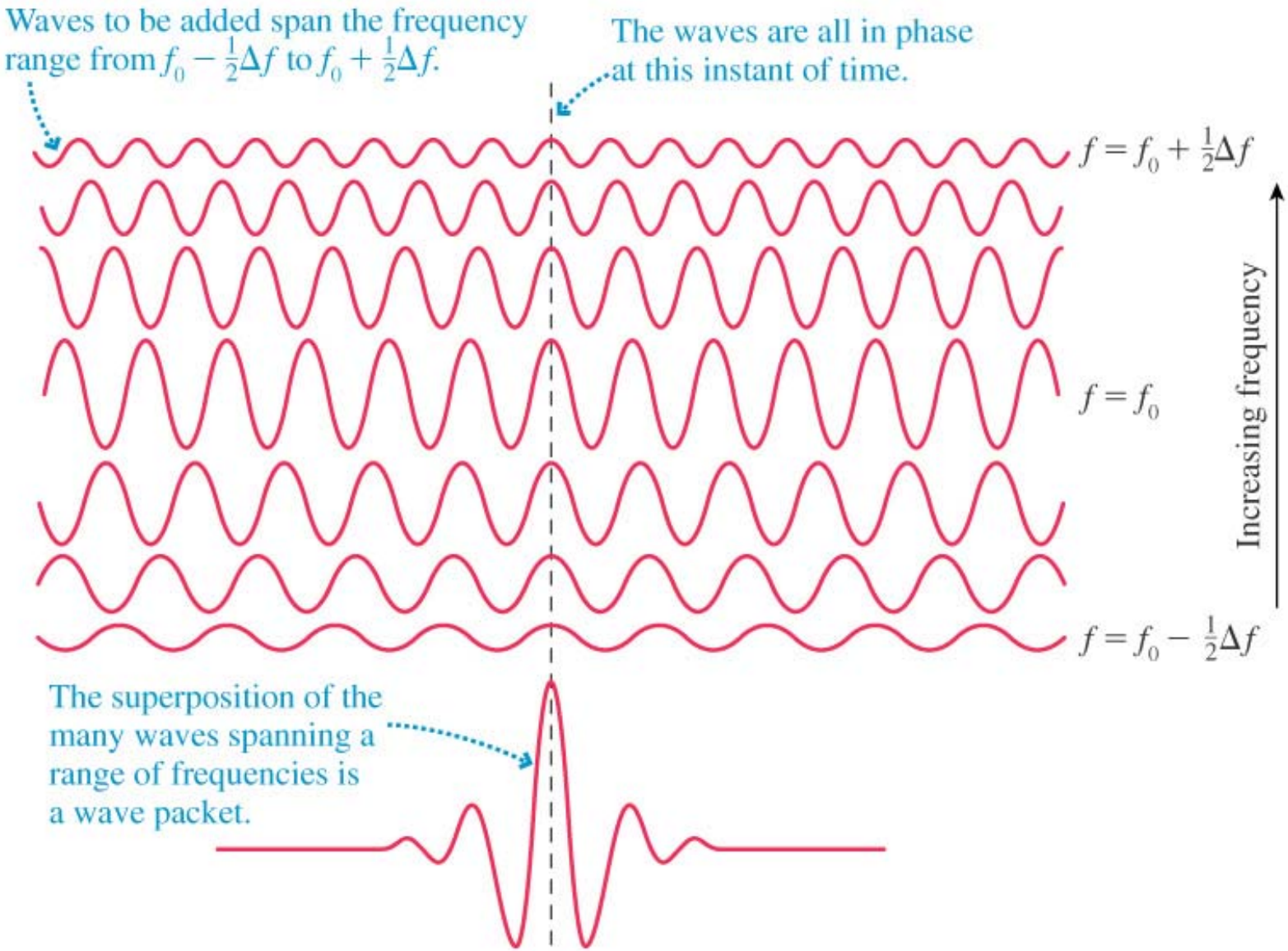
- Particles
  - position (x), velocity (v), energy (E), etc
- Light
  - Electric field (E), and magnetic field (B)
- Strategy
  - Let's First see if we can make Light look like a particle (sort of)
    - Light has to be like a ball (a small packet)
  - Then see if we can make electrons like waves
    - Make a "matter field" thing analogous to the Electric field $E(x) \sim A\sin(kx-\omega t)$
      - remember $k=2\pi/\lambda$ and $\omega=2\pi f$

Light as particles

- How can we make a wave pulse?
  - Drum beat
  - turn light on and off; ie make it blink

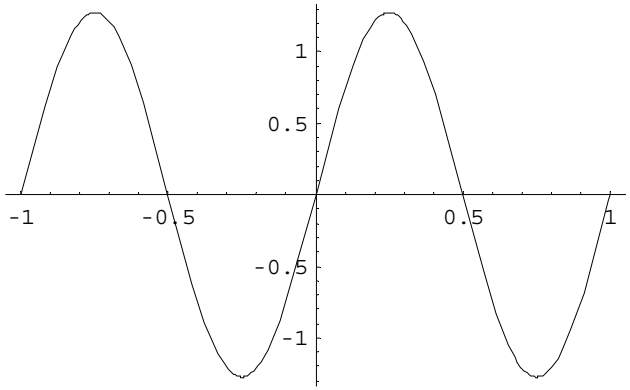


- beats!
  - Can we add up some waves of different frequency to get little light “particles”?
  - http://www.phy.ntnu.edu.tw/ntnujava/viewtopic.php?t=35 (50,54)
  - In fact, we can get any shape we want by adding enough waves
  - http://www.phy.ntnu.edu.tw/ntnujava/viewtopic.php?t=33

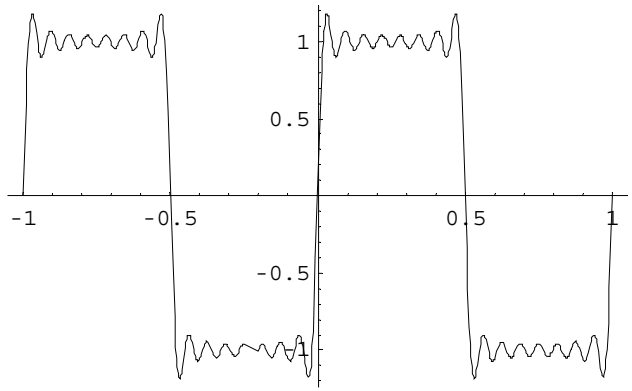

Waves to be added span the frequency range from $f_0 - \frac{1}{2}\Delta f$ to $f_0 + \frac{1}{2}\Delta f$.
The waves are all in phase at this instant of time.
$f = f_0 + \frac{1}{2}\Delta f$
$f = f_0$
$f = f_0 - \frac{1}{2}\Delta f$
Increasing frequency
The superposition of the many waves spanning a range of frequencies is a wave packet.

How many frequencies to make a nice square pulse?

- wave $f(x)=\sin \omega_n x \quad \omega_n \sim n \quad n=1, 3, 5\ldots$



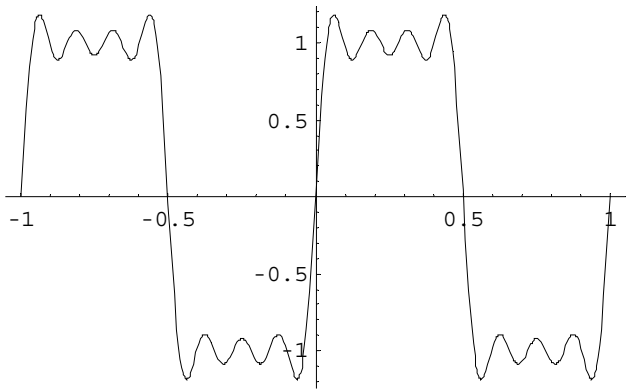
1 frequency



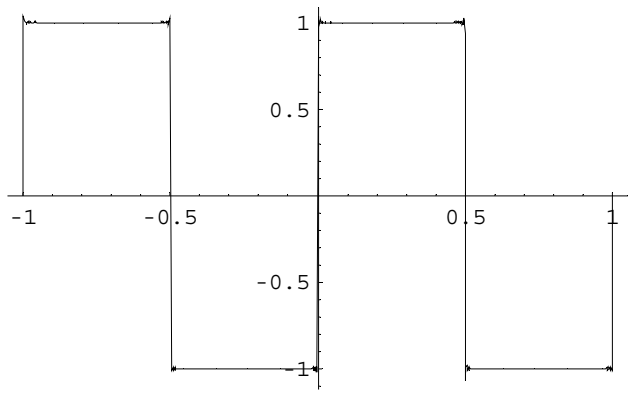
8 frequencies

More square

More frequencies



4 frequencies



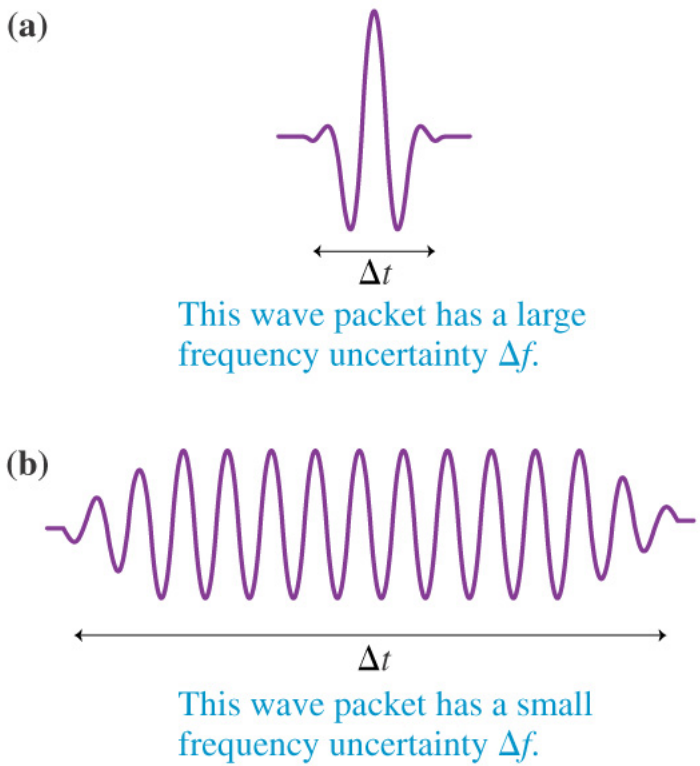
1000 frequencies

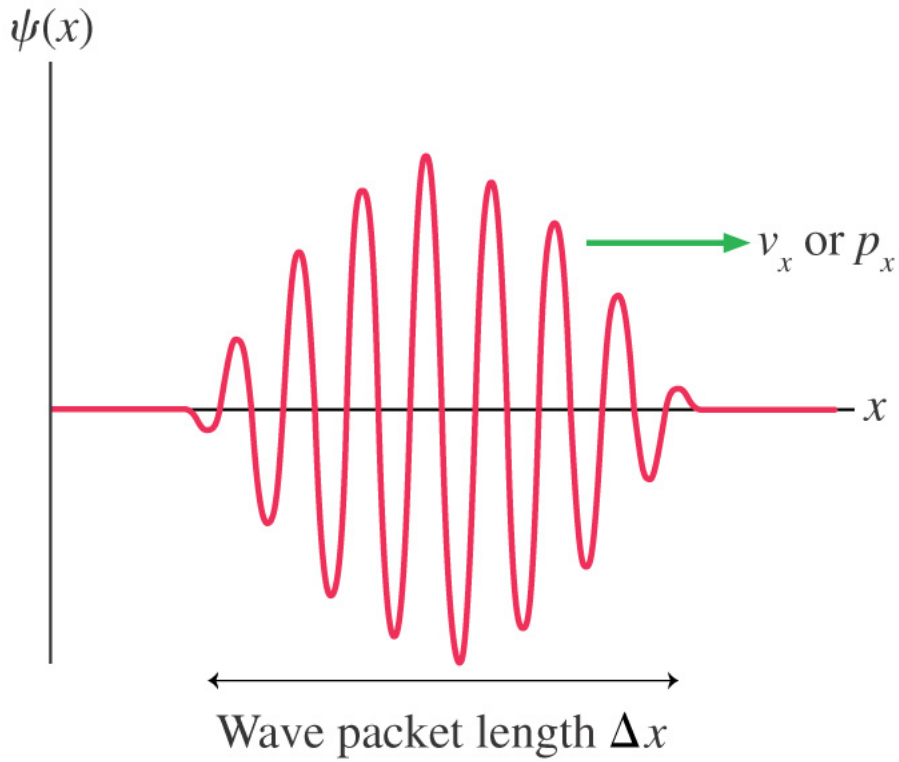
Heisenberg Uncertainty Principle

- So a wave packet or particle is a sum over lots of waves of different frequency
  - But since E=hf
    - what is its energy????
- heisenberg uncertainty principle….
  - better (more square) position ~smaller Δx

    ➔ worse $\Delta p = \Delta E/c = h\Delta f/c$
  - HEISENBERG: $\Delta x \Delta p \geq h/2$
    - it will turn out this affects EVERYTHING
    - Problem with signal transmission

for instance





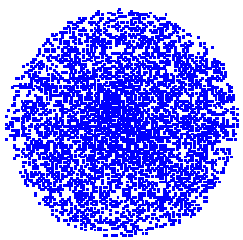
So is this a problem in life?

- SO
  - if we know how fast we are going, we have no idea where we are
  - If we know where we are, we don't know how fast we are moving
  - Real life
    - Car at the corner of Chicago and University and 100±1 MPH=44.7 ±0.447 m/s. Car weighs 2000 kg
      - Δp=2000 kg .447 m/s~1000 kg-m/s
      - $\Delta x \geq h/2/\Delta p$=6.625 x 10^{-34}/2/1000= 3 x10^{-37} m
      - Good enough to say you are at Chicago and University and not on the freeway – you get a ticket (a big one)

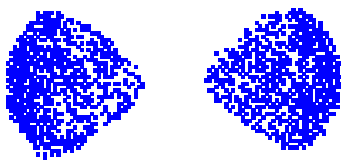
$$\Delta x \Delta p \geq h/2$$

What about for an atom?

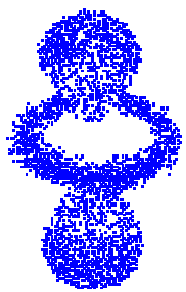
- Take E=-13.6 eV $\Delta E=1$ eV $\Delta x \Delta p \geq h/2$
  - $\Delta E/E = 1/13.6 \sim .1$
  - $E=p^2/2m$ so $\Delta p/p = \frac{1}{2}\Delta E/E$ so $\Delta p/p=.05$
  - $p=\sqrt{2mE}= \sqrt{2(9\times10^{-31})(13.6)(1.602\times10^{-19})}=2\times10^{-24}$
  - $\Delta p=.05\ p=5\times10^{-2}\ 2\times10^{-24}= 6\times10^{-25}$
  - $\Delta x \geq h/2/\Delta p= 6.625 \times 10^{-34}/2/10^{-25} \sim 3\times10^{-9}$m
  - size of atom 10^{-10}m
    - no idea where it is. So its spread out



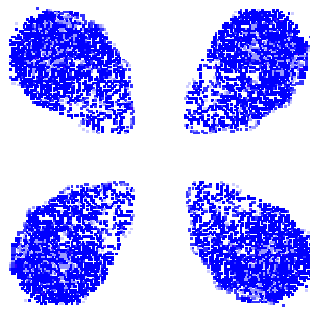
s orbital



p orbital



d orbitals



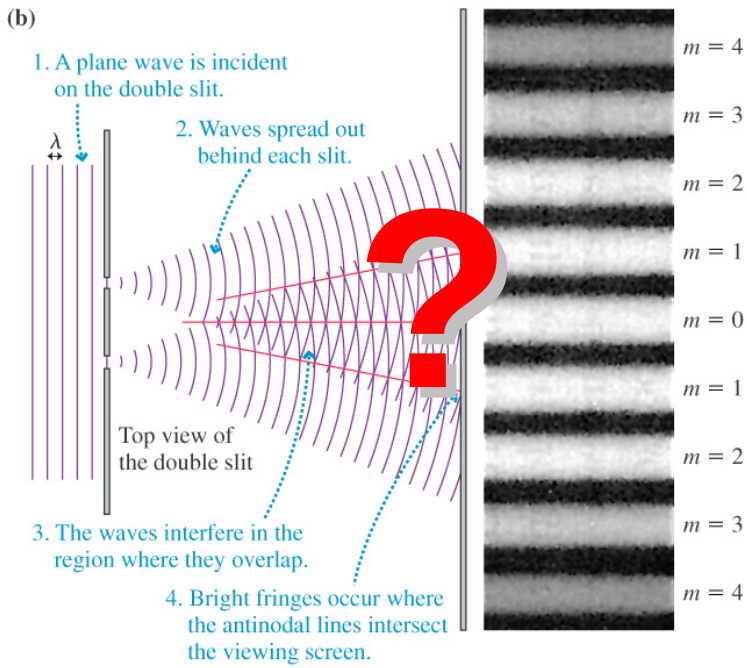
Now Electrons as waves?

- Maybe just like light. A nice localized electron is a mixture of many energies
- A nice energy electron is in a beam. We don't know exactly where it is.
- First lets take a slow motion view

  http://www.colorado.edu/physics/2000/schroedinger/two-slit2.html
- PROBABILITIES?? Electrons similar?

http://www.colorado.edu/physics/2000/schroedinger/two-slit3.html

applet run 2 slits



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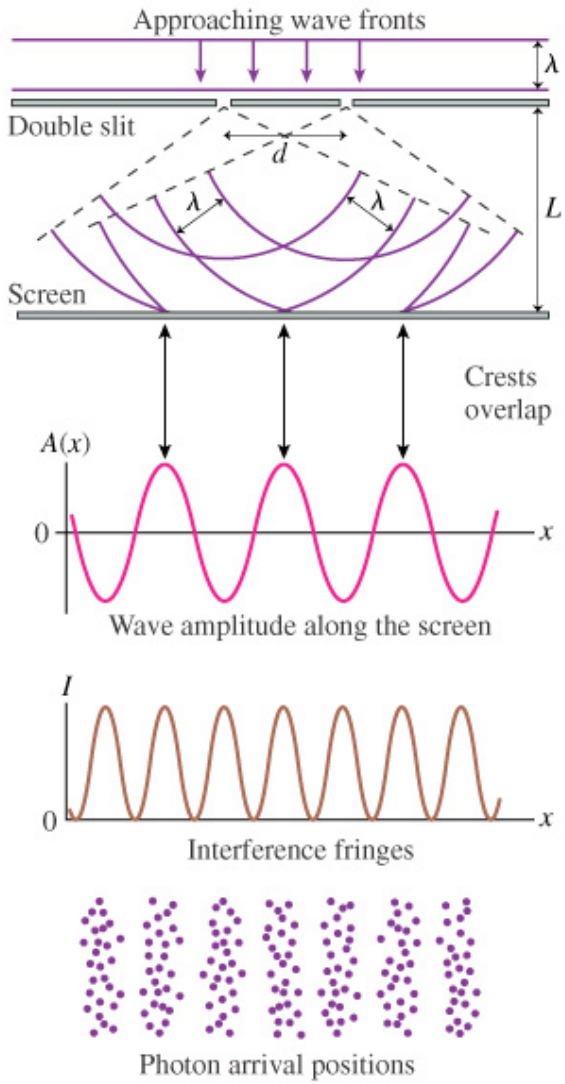
So this is what "really happens



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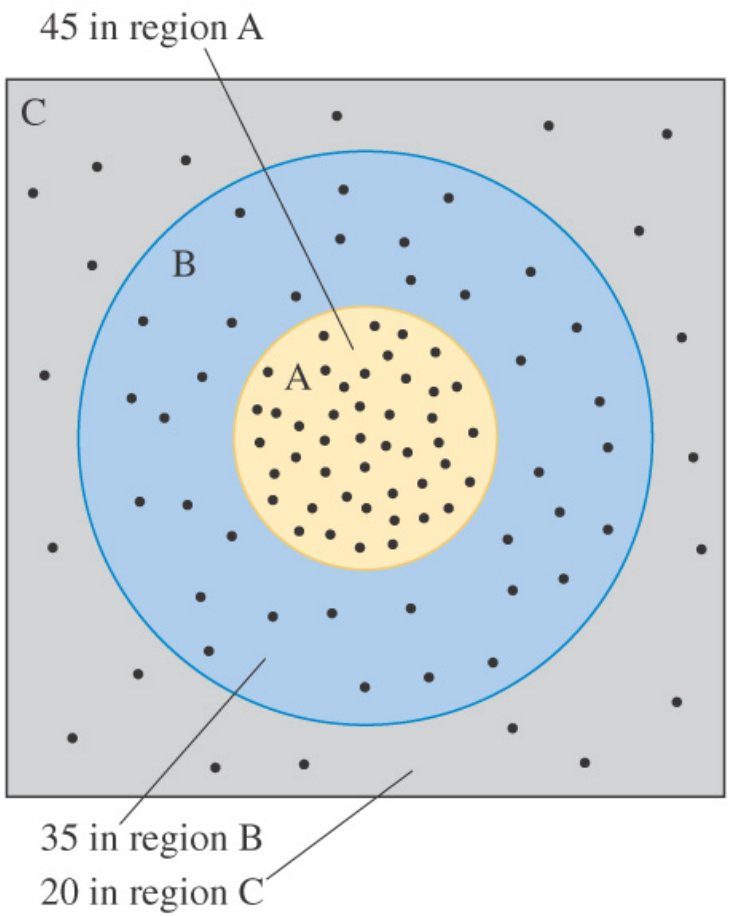
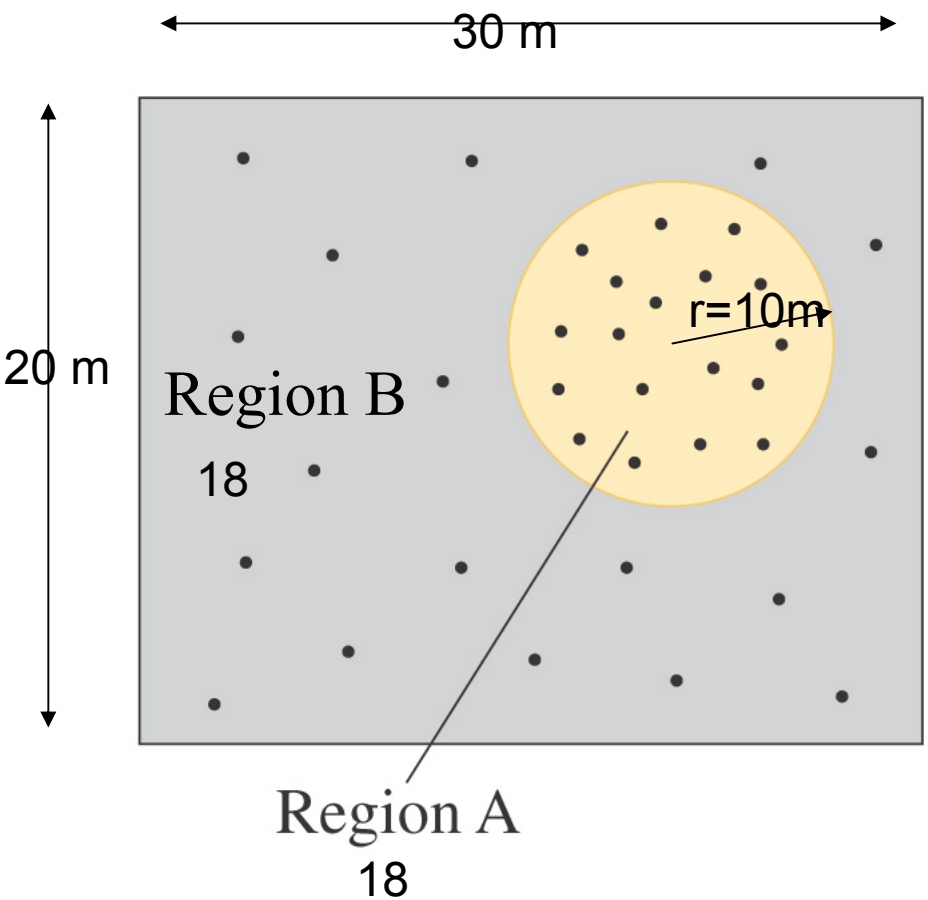
An exercise Target practice for a bomber – Probability and probability density



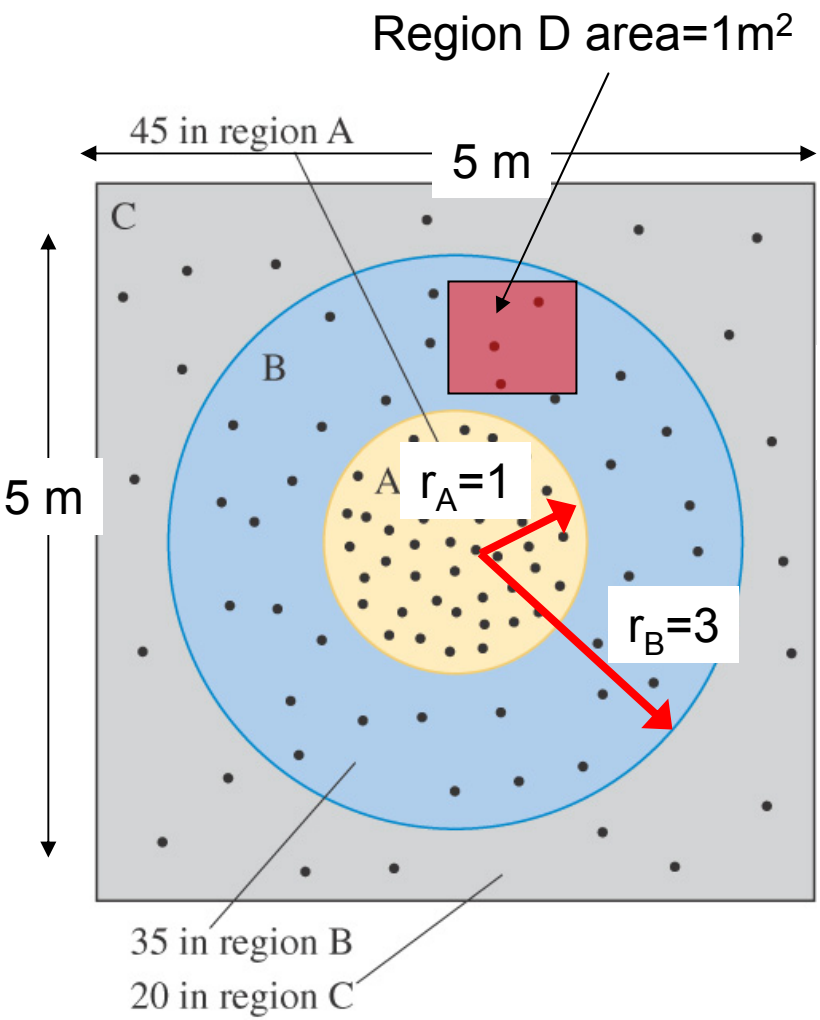
- total number
  - =45+35+20=100
  - normalization
- Prob A=45/100=.45
- Prob B=35/100=.35
- Prob C=20/100=.20
- Where would you rather stand, region A, B or C?

An exercise Target practice for a bomber – Probability and probability density



- Normaliztion=36
  - Prob A=18/36=0.5
  - Prob B=18/36=0.5
- Where would you rather stand??? Region A or B?
- Prob density =Prob/"area"
  - area A=310m^2
  - area B=600 m^2
  - Prob density A
    - P_A=0.5/310m^2=0.0016/m^2
    - P_B=0.5/600m^2=0.0008/m^2
    - Now its clear where you would stand

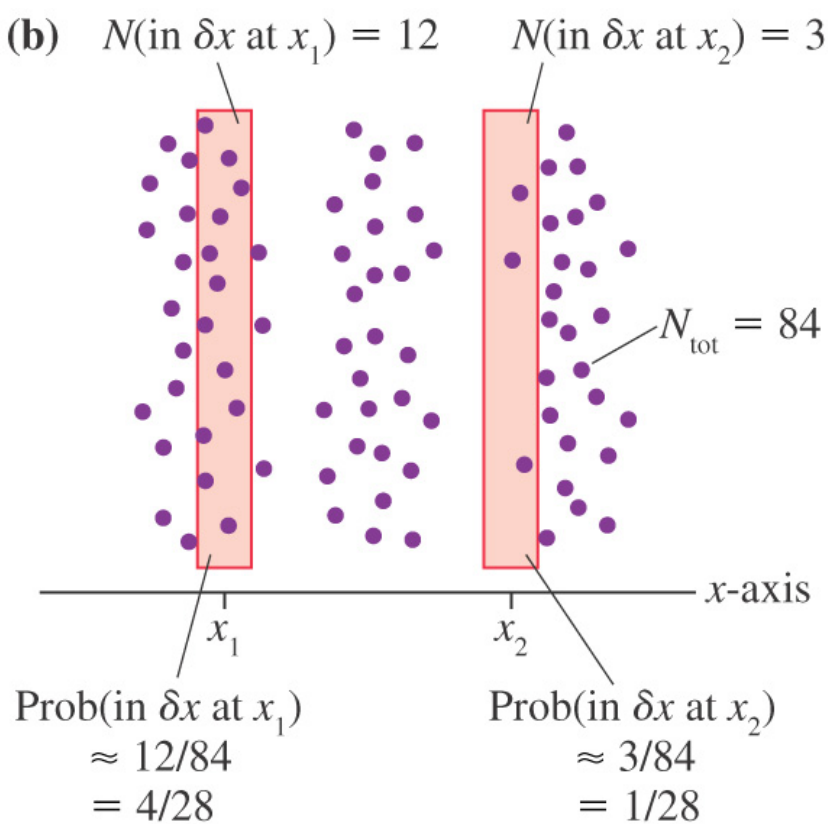
An exercise Target practice for a bomber – Probability and probability density

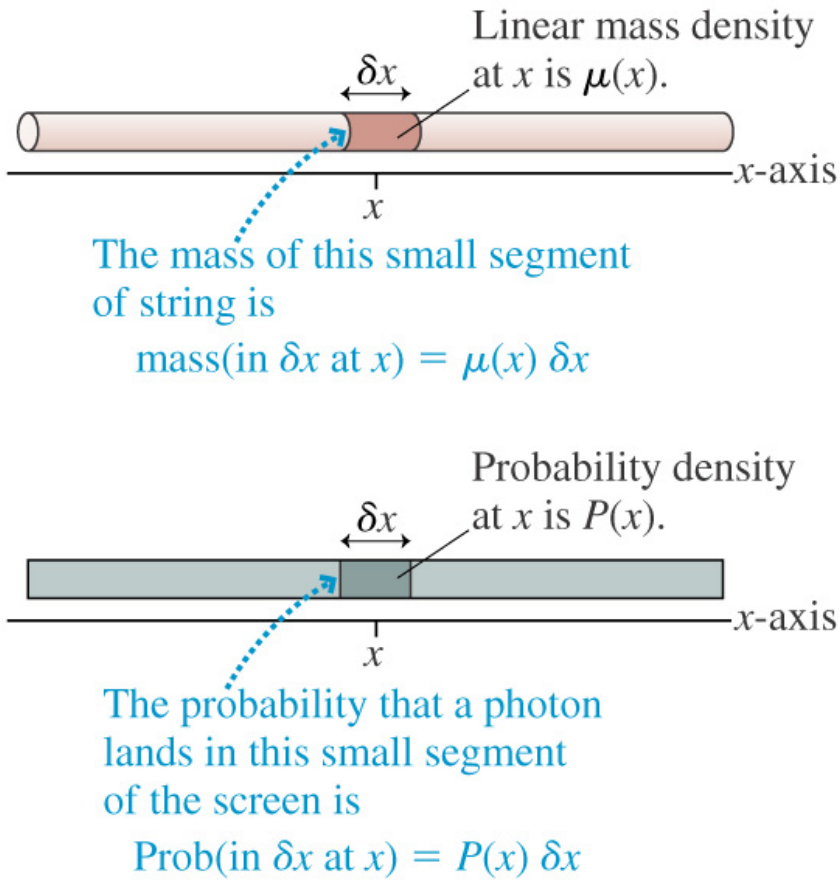


- Prob=Prob density *Area
- Prob A=.45
  - P_A=.45/3.1m²=.145/m²
  - Prob= P_AArea$_A$ =.145/m²3.1m²=.45
- Prob B=.35
  - P_B=.35/28.3m²=.0124/m²
  - Prob$_B$= P_BArea$_B$ =.0124/m²28.1m²=.35
  - Prob$_D$= P_BArea$_D$ =.0124/m² 1m²=.0124

Prob density

We can also do this for linear density -





Now for a quantum leap

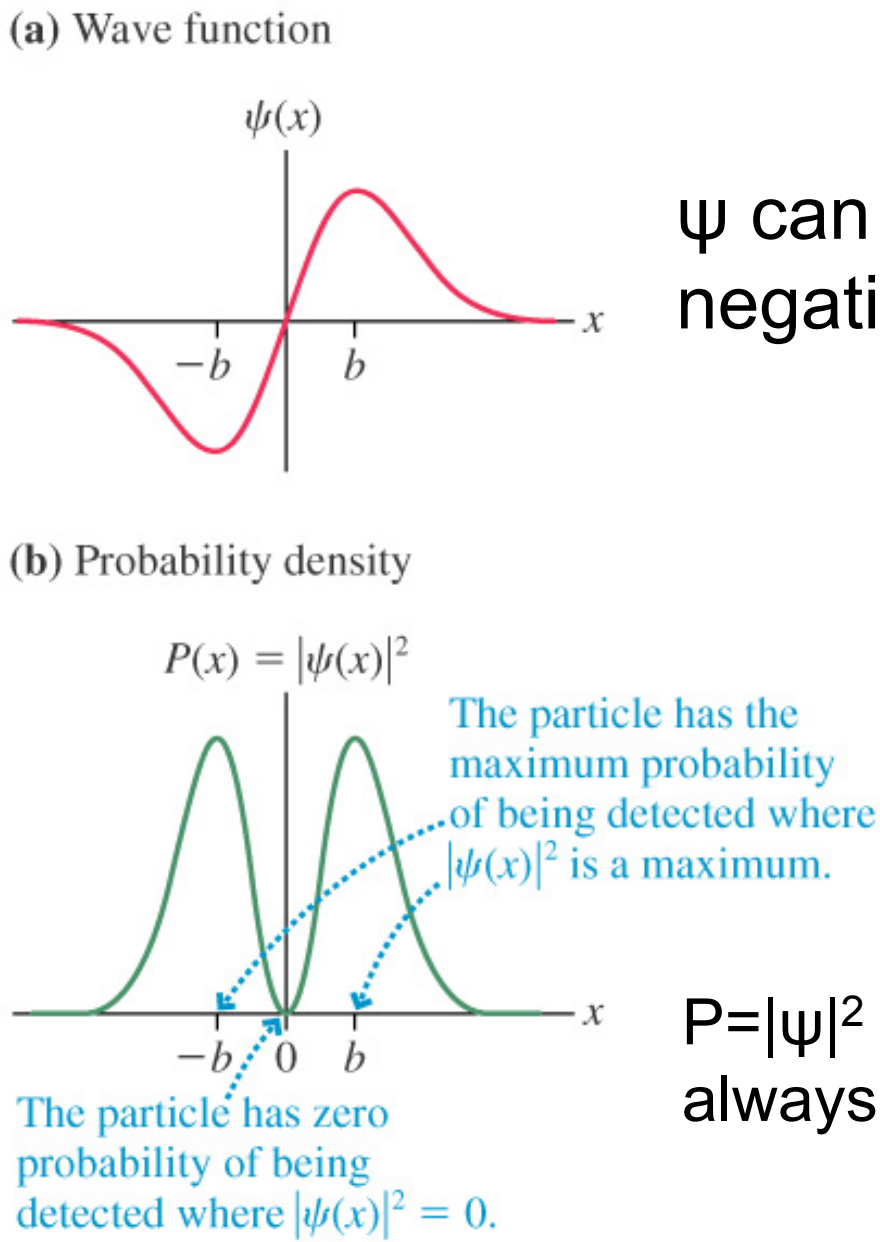
- Intensity for Light ~ (Electric Field)^2

$$I = \frac{Power}{Area} = S_{avg} = \frac{E_0^{\ 2}}{2c\mu_0}$$

- Intensity is like probability density
- DEFINE A MATTER FIELD $\psi(x)$
  - $P(x)=|\psi(x)|^2$

- This thing (a wave function) will tell us what matter is
- the square of it will give a probability density

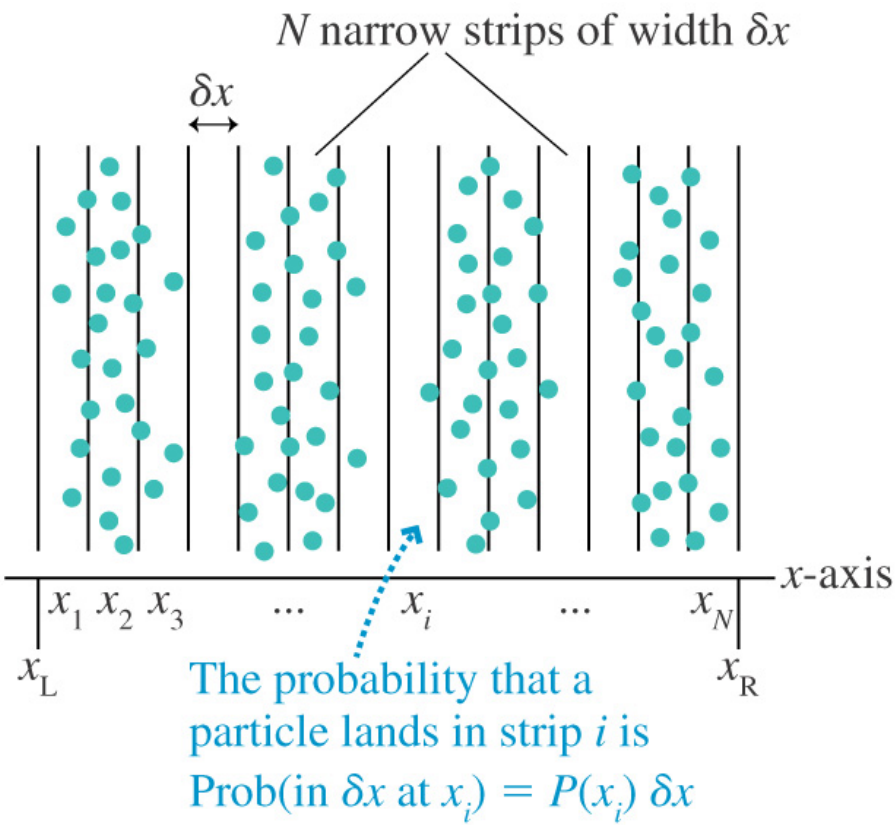
What do wave functions look like?

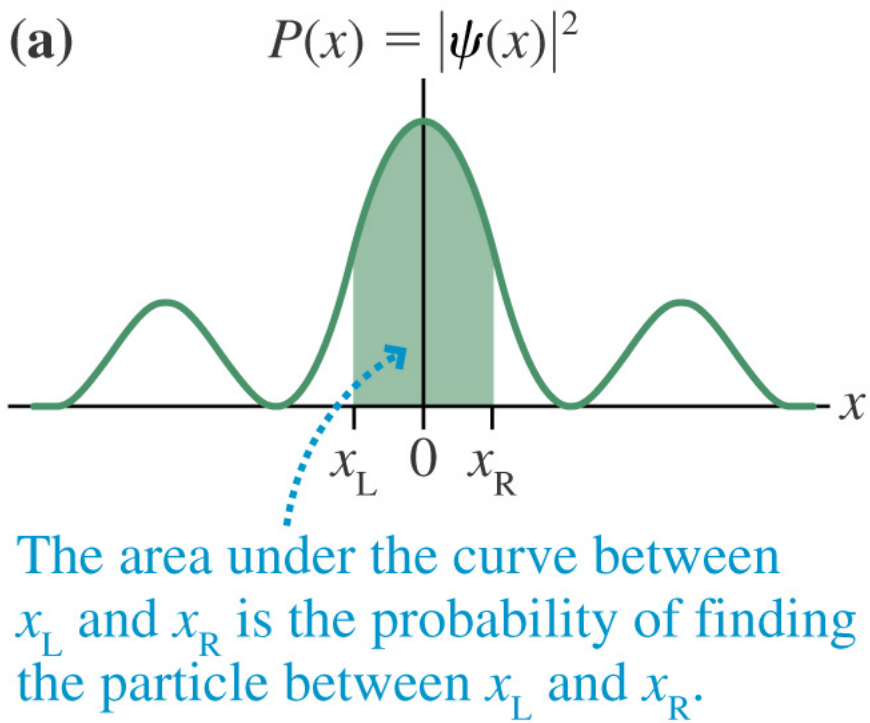


ψ can be negative

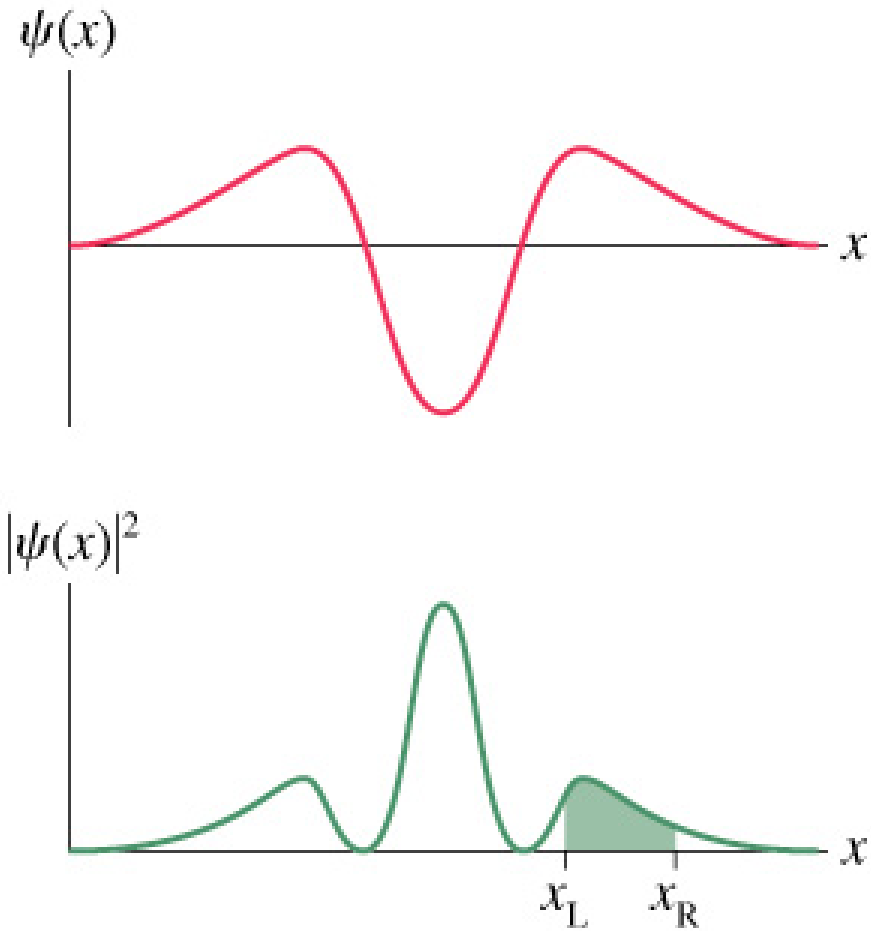
$P=|\psi|^2$ is always positive

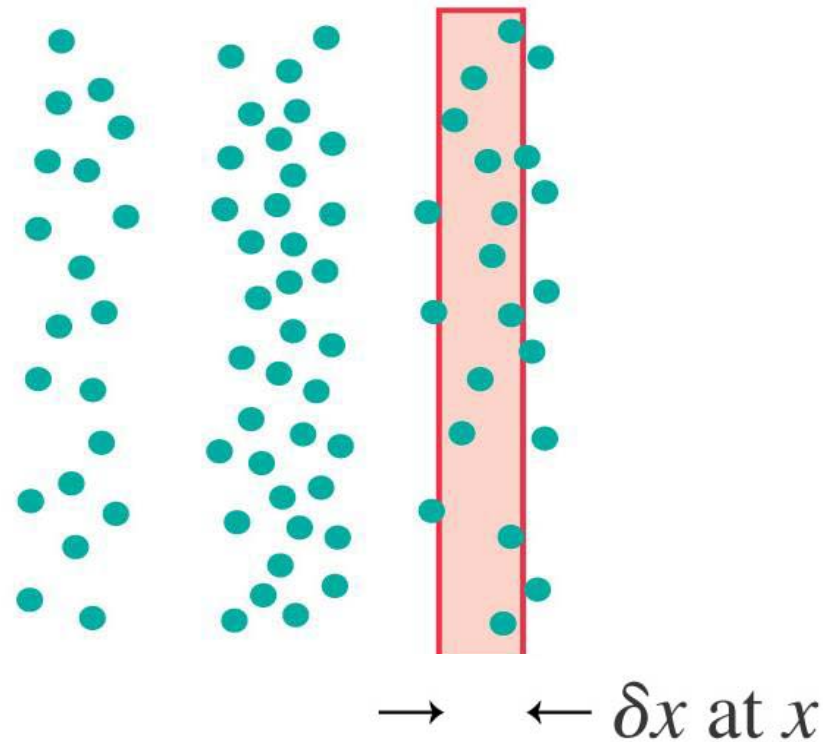
Double slit for electrons: the probability



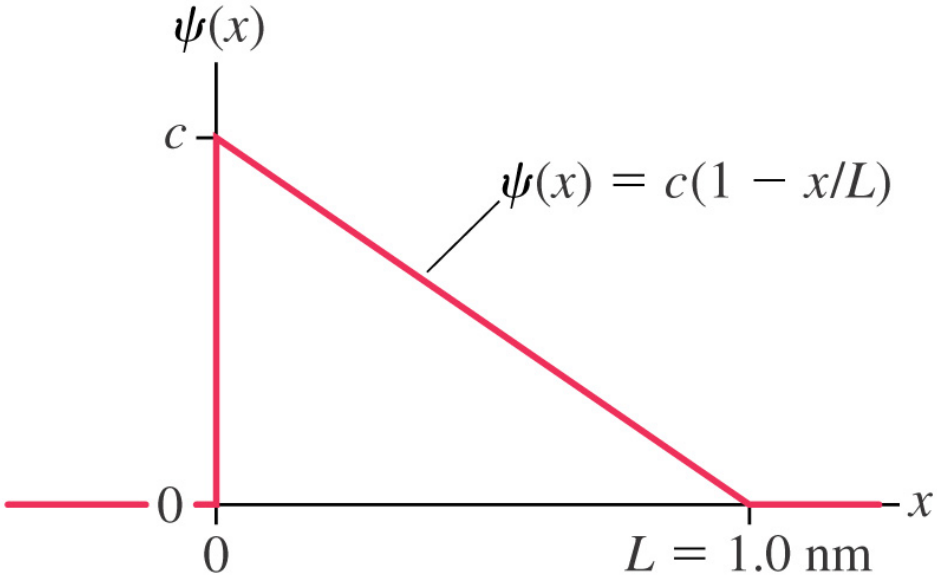


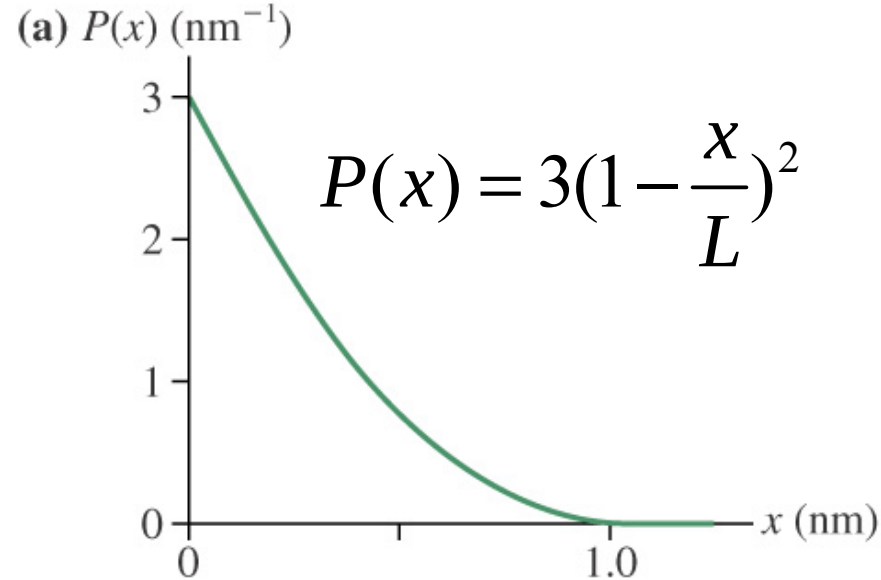
Double slit for electrons: the wave fuction





another example with a formula





$$P(x) = 3(1 - \frac{x}{L})^2$$

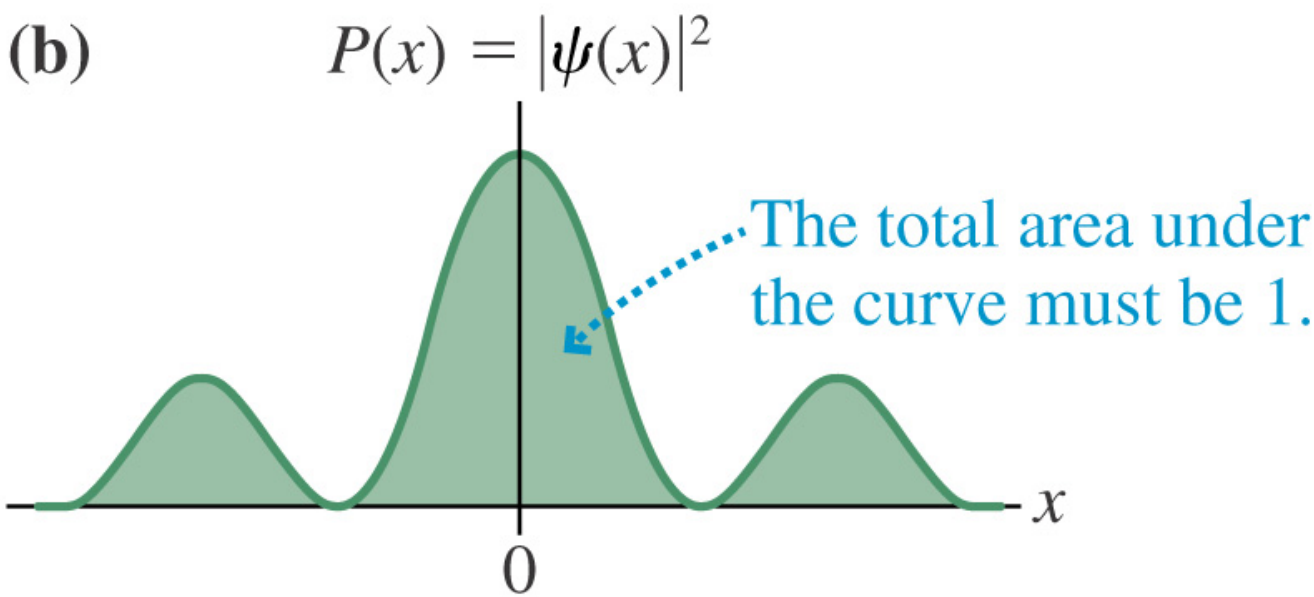
$L = 1$ nm

and it will turn out c= $\sqrt{\frac{3}{L}}$

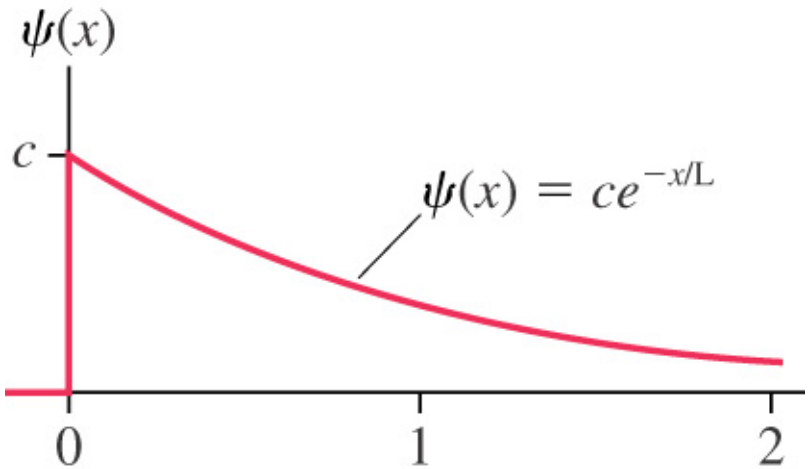
Normalization

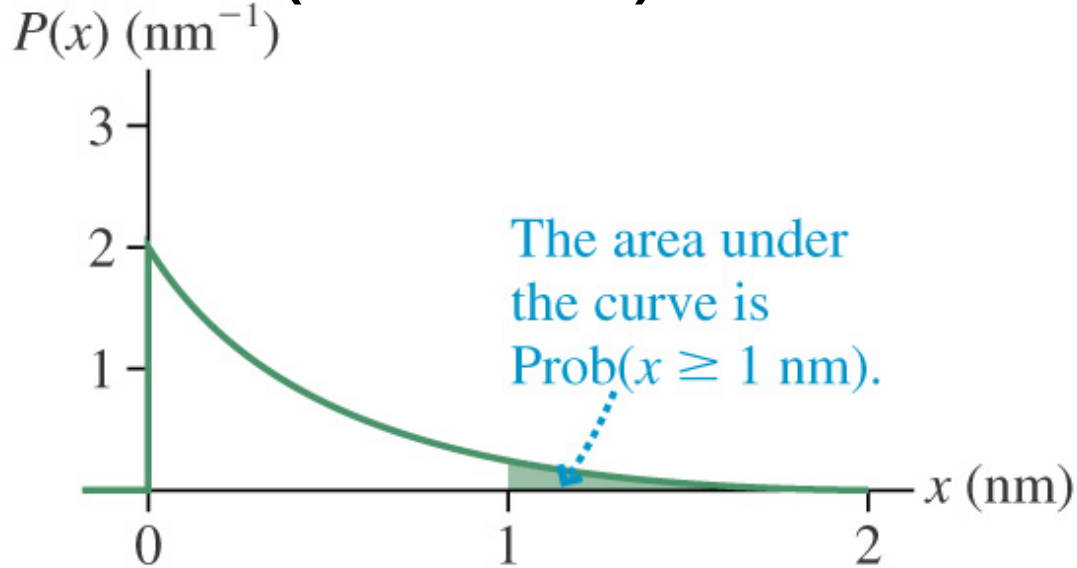
- Now if we have 1 particle (say), it had better be somewhere.
- So P(x) has to normalize to 1

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



set L=1nm find Prob(x>1nm)





$$\psi(x) = \sqrt{2}e^{-x/L}$$

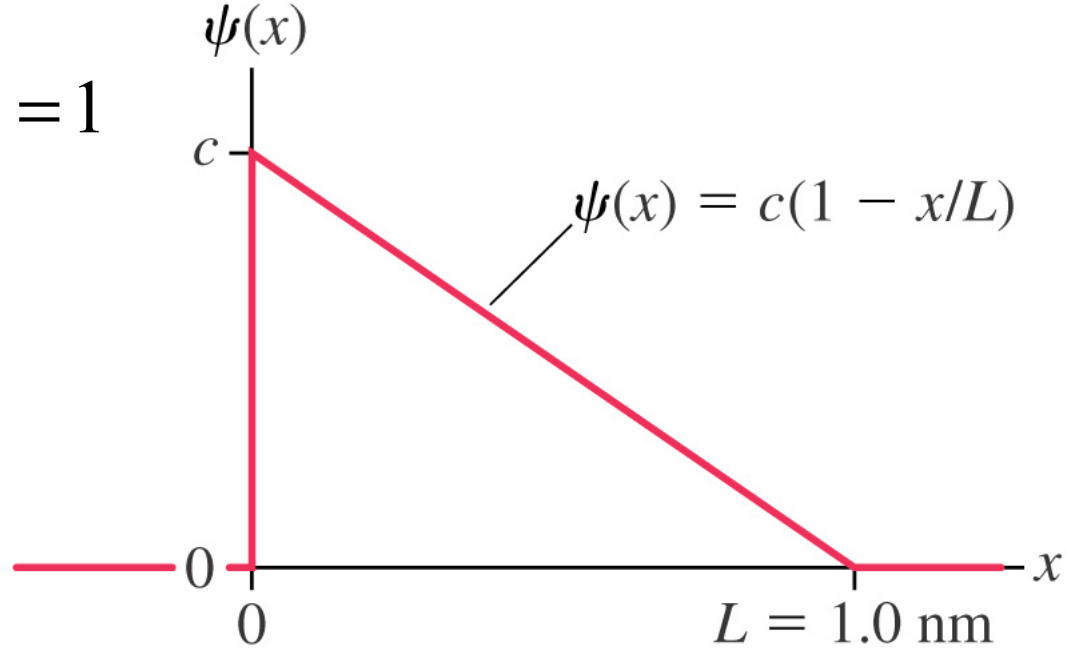
$$P(x) = 2e^{-2x}$$

$$\text{Prob(x>1nm)} = \int_1^\infty P(x)dx = \int_1^\infty |\psi(x)|^2\, dx = 2\int_1^\infty e^{-2x}dx =$$

$$2(-\frac{1}{2})e^{-2x}\,|_1^\infty = -0-(-e^{-2}) = e^{-2} = 0.135$$

Another normalization

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



$$1 = \int_0^L |c(1-\frac{x}{L})|^2 \, dx =$$

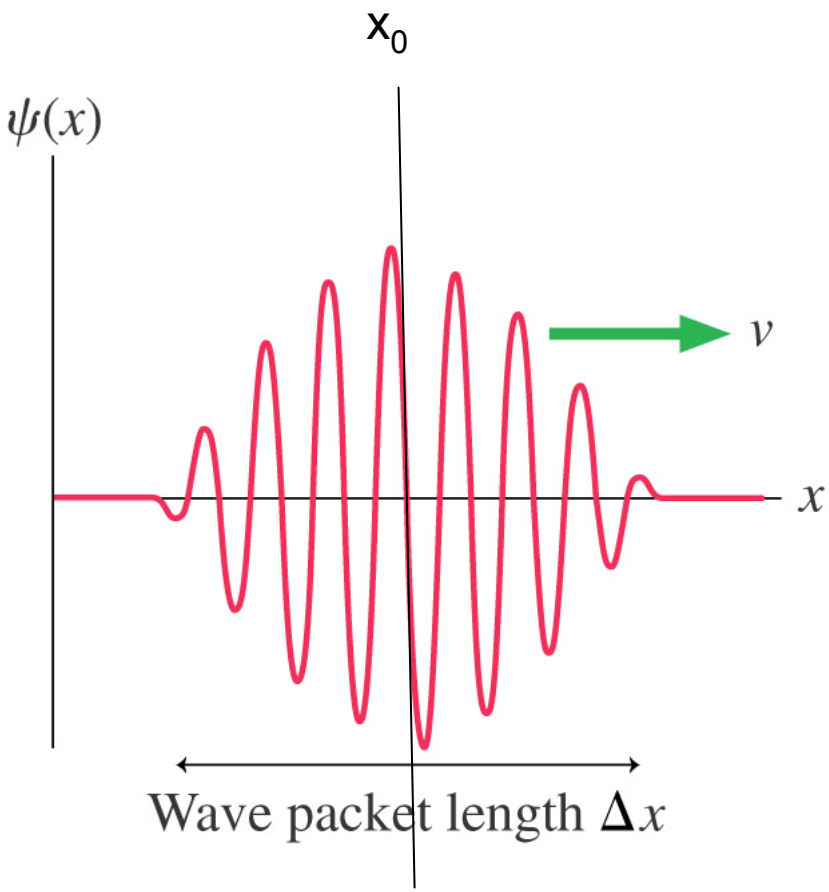
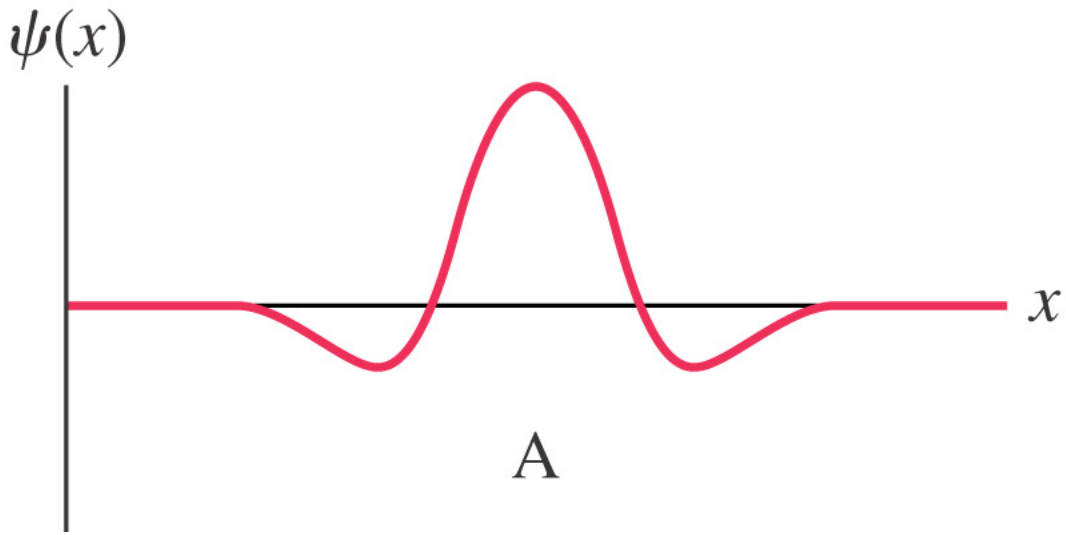
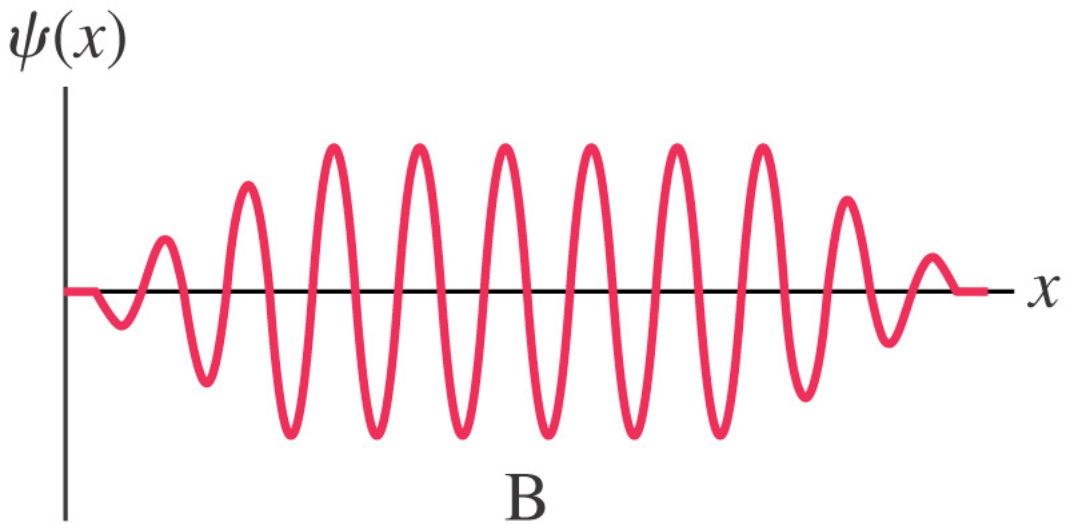
$$c^2 \int_0^L (\frac{x^2}{L^2} + 2\frac{x}{L} - 1)dx =$$

$$c^2 (\frac{x^3}{3L^2} + \frac{x^2}{L} - x)\Big|_0^L = c^2 (\frac{L^3}{3L^2} + \frac{L^2}{L} - L) =$$

$$c^2 (\frac{L}{3} + L - L) = c^2 \frac{L}{3} = 1 \qquad c = \sqrt{\frac{3}{L}} \qquad \psi(x) = \sqrt{\frac{3}{L}}(1 - \frac{x}{L})$$

So what is an electron?

- A matter wave packet
- Its mostly at position x_0
- It has a median velocity v
- However there is an smearing of both position and velocity no neither of these are exact



- Which of these can be located more precisely?