Quantum Mechanics I
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Primary textbook: “Quantum Mechanics” by Amit Goswami

Please read Chapter 1, Sections 4-9

Outline

I. What you should recall from previous courses
II. Motivation for the Schroedinger Equation
III. The relationship between wavefunction ψ and probability
IV. Normalization
V. Expectation values
VI. Phases in the wavefunction

I. 10 facts to recall from previous courses

1. Fundamental particles (for example electrons, quarks, and photons) have all the usual classical properties (for example mass and charge) + a new one: probability of location.
2. Because their location is never definite, we assign fundamental particles a wavelength.
   - Peak of wave – most probable location
   - length of wave – amount of indefiniteness of location
3. Wavelength λ is related to the object's momentum p

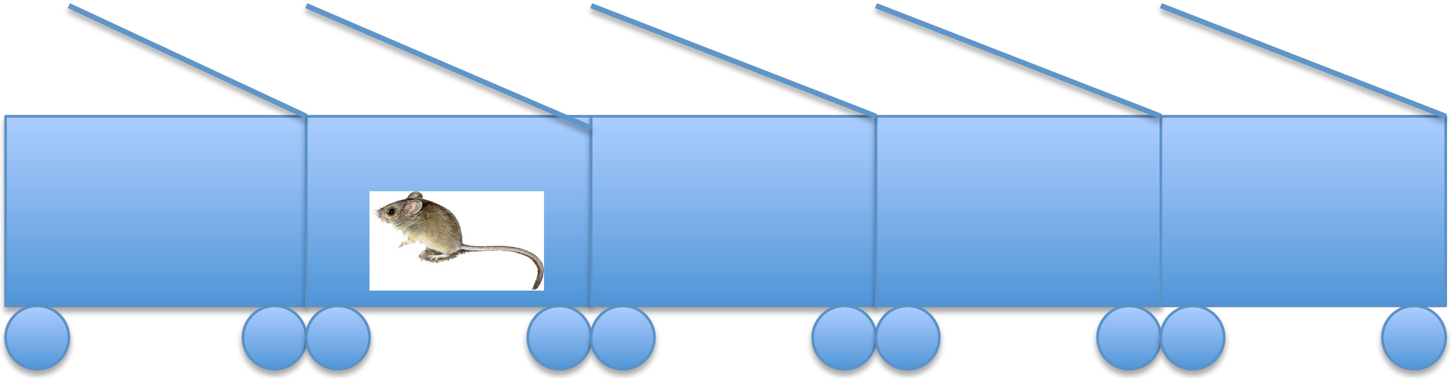
$$\lambda = \frac{h}{p}$$

Planck's constant
4.13×10^{-15} eV-sec

4. The object itself is not "wavy"...it does not oscillate as it travels. What is wavy is its probability of location.

Example of an object with wavy location probability distribution

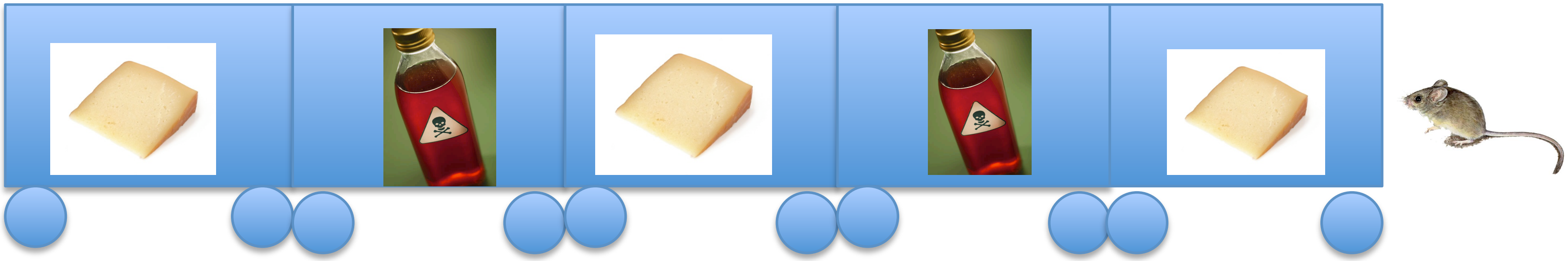
Consider a set of 5 large toy train cars joined end to end. Each car has a lid and a door leading to the next car.



Put a mouse into one box and close the lid. The mouse is free to wander among boxes. At any time one could lift a lid and have a 20% chance to find the mouse in that particular car.

Now equip Boxes 2 and 4 with mouse repellent
Equip Boxes 1, 3, and 5 with cheese

A diagram on the outside of the boxes shows how likely it is that the mouse is in any of the boxes. Now the probability of finding the mouse is not uniform in space: maxima are near the cheese, minima are near the poison.



Conclude:

- the mouse does not look like a wave---it looks like a mouse
- the mouse does not oscillate like a wave---it moves like a mouse
- but the map of probable locations for the mouse is shaped like a wave

The situation for the electron or photon is almost the same, except

- for the mouse example, Probability = Amplitude
- for the electron (or any quantum mechanical object,

Probability = (Amplitude)*(Amplitude)

5. As with all waves, wavelength λ is related to frequency υ:

$$\lambda \bullet \upsilon \quad = \text{velocity of wave}$$

6. QM says that the λ (or υ) is also related to the energy:

$$E = h\upsilon$$

7. Special relativity says that total E and momentum p are also related by

$$E = \sqrt{p^2c^2 + m_0^2c^4}$$

c = 3 x 10^8 m/s

rest mass of the object

8. QM says that every object in the universe is associated with a mathematical expression that encodes in it every property that it is possible to know about the object.

its charge, mass, location, energy...

This math expression is called the object's wavefunction ψ.

9. As the object moves through space and time, some of its properties (for example location and energy) change to respond to its external environment.

So ψ has to track these
Conclude: ψ has to include information about the environment of the particle (for example location x, time t, sources of potential V)

10. So if you know the ψ of the object, you can find out everything possible about it.

The goal of all QM problems is: given an object (mass m, charge Q, etc.) in a particular environment (potential V), find its ψ. The way to do this (in 1-dimension) is to solve the equation

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

The Schroedinger Equation

II. Motivation for the Schroedinger Equation

We can develop the Schroedinger Equation by combining 6 facts:

FACT 1: The λ and p of the ψ produced by this equation must satisfy λ=h/p.
FACT 2: The E and υ of the ψ must satisfy E=hυ.
FACT 3: Total energy = kinetic energy + potential energy

$E_{tota\ l}$= KE + PE

Restricting ourselves to non-relativistic problems, we can rewrite this as

$E_{total} = p^2/2m + V.$

(For relativistic problems, we would need $E = \sqrt{p^2c^2 + m_0^2c^4} + V$).

FACT 4: Because a particle's energy, velocity, etc, depend on any force F it experiences, the equation must involve F. Insert this as a V-dependence through

$$F = \frac{-\partial V}{\partial x}$$

To simplify initially, consider only cases where V = constant = V_0. Later we will generalize to V=V(x,y,z,t).

FACT 5: The only kind of wave that is present in the region of a constant potential is an infinite wave train of constant λ everywhere.

Example:

- An ocean wave over the flat ocean floor extends in all directions with constant amplitude and λ.
- When the wave reaches a change in floor level (i.e. a beach) then its structure changes.
- Conclude: if V = constant, $\psi \propto \cos[k(x-vt)]$ or $\sin[k(x-vt)]$

cos or sin indicate the wave shape.

k has units 1/length to make the argument of the cos dimensionless

Recall that the definition of a wave is an oscillation that maintains its shape as it propagates. For constant velocity v, "x-vt" ensures that as t increases, x must increase to maintain the arg=(x-vt)= constant. This is a rightward-traveling wave.

Again $\psi \propto \cos[k(x - vt)]$ or $\sin[k(x - vt)]$

Rewrite this as $\psi \propto \cos[kx - kvt]$

units are $\dfrac{1}{length} \cdot \dfrac{length}{time} = \dfrac{1}{time}$, a frequency.

So call kv = ω.

Then $\psi \propto \cos(kx - \omega t)$ or $\sin(kx - \omega t)$

FACT 6: ψ represents a particle and wave simultaneously. Waves interfere. This means if we combine the amplitudes of 2 waves ($A(\psi_1)$ and $A(\psi_2)$), we get $A(\psi_{Total}) = A(\psi_1) + A(\psi_2)$.

That is...add the first powers of the ψ1 and ψ2 amplitudes, not functions that are more complicated.

Conclude: if we want the Schroedinger Equation to produce a wavelike ψ, then it too must include only first powers of ψ...that is, ψ, dψ/dx, dψ/dt, etc., but NOT, for example, ψ^2.

Now use all 6 facts to construct the Schroedinger Equation:

Start with FACT 5 : $\frac{p^2}{2m} + V = E$

Plug in FACT 1 for p : $\frac{h^2}{2m\lambda^2} + V = E$

Plug in FACT 2 for E : $\frac{h^2}{2m\lambda^2} + V = h\nu .$

Define $k = \frac{2\pi}{\lambda}$, $\omega = 2\pi\nu$, and $\hbar = \frac{h}{2\pi}$.

Then $\frac{\hbar^2 k^2}{2m} + V = \hbar\omega$ "Eq. 1"

Notice we are already using FACT 4 (i.e. V is included. Consider the simplified case V = constant = V0. This implies $F = \frac{\partial V}{\partial x} = 0.$

Recall this produces an infinite, single-λ wave.

The most general infinite single - υ wave would be $\psi = \delta\cos(kx - \omega t) + \gamma\sin(kx - \omega t)$.

Later we will need its derivatives, so calculate them here:

$$\frac{\partial\psi}{\partial x} = -\delta k\sin(kx - \omega t) + \gamma k\cos(kx - \omega t)$$

$$\frac{\partial^2\psi}{\partial x^2} = -k^2[\delta\cos(kx - \omega t) + \gamma\sin(kx - \omega t)]$$

$\frac{\partial\psi}{\partial t} = -\omega[\gamma\cos(kx - \omega t) - \delta\sin(kx - \omega t)]$. This is close to $-\omega\psi$ but not exactly, so we say

$$\frac{\partial\psi}{\partial t} \sim -\omega\psi.$$

Notice $\frac{\partial^2\psi}{\partial x^2} = -k^2\psi \rightarrow k^2 = -\frac{\frac{\partial^2\psi}{\partial x^2}}{\psi}$.

and $\frac{\partial\psi}{\partial t} \sim -\omega\psi \rightarrow \omega \sim -\frac{\frac{\partial\psi}{\partial t}}{\psi}$. Exchange the proportionality for an unknown constant β.

Then $\omega = \frac{+\beta\frac{\partial\psi}{\partial t}}{\psi}$.

Plug into $\dfrac{\hbar^2k^2}{2m}+V_0=\hbar\omega$:

$$\frac{\hbar^2}{2m}\left[\frac{-\dfrac{\partial^2\psi}{\partial x^2}}{\psi}\right]+V_0=\hbar\left[\frac{\beta\dfrac{\partial\psi}{\partial t}}{\psi}\right].$$ Multiply by ψ:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V_0\psi=\beta\hbar\frac{\partial\psi}{\partial t}. \qquad \text{"Eq. 2"}$$

Plug in ψ, take derivatives:

$$\frac{-\hbar^2}{2m}\cdot\left(-k^2\right)\delta\cos(kx-\omega t)-\frac{\hbar^2}{2m}\cdot(-k^2)\gamma\sin(kx-\omega t)+V_0\delta\cos(kx-\omega t)+V_0\gamma\sin(kx-\omega t)$$

$$=\beta\hbar\cdot(-\omega)\gamma\cos(kx-\omega t)+\beta\hbar\omega\delta\sin(kx-\omega t)$$

Collect sine and cosine terms separately:

$$\left[\frac{\hbar^2k^2}{2m}\delta+V_0\delta+\hbar\beta\omega\gamma\right]\cos(kx-\omega t)+\left[\frac{\hbar^2k^2}{2m}\gamma+V_0\gamma-\hbar\beta\omega\delta\right]\sin(kx-\omega t)=0.$$

This can only be solved if the coefficients of cosine and sine vanish separately:

cosine terms: $\frac{\hbar^2 k^2}{2m} + V_0 = \frac{-\hbar\beta\omega\gamma}{\delta}$ "Eq. 3"

sine terms: $\frac{\hbar^2 k^2}{2m} + V_0 = \frac{\hbar\beta\omega\delta}{\gamma}$ "Eq. 4"

This leaves 3 equations (Eq. 1, Eq. 3, and Eq. 4) and 3 unknowns (γ, δ, β).

Solve simultaneously to get $\beta = \pm i$.

Two roots indicate that the Schroedinger waves travel in $\pm\hat{\mathrm{x}}$. Plug $\beta = +i$ in Eq. 2:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V_0\psi = +i\hbar\frac{\partial\psi}{\partial t}$$

All of the assumptions that went into this were general except $\mathrm{V} = \mathrm{V}_0$ (free particle).

Guess that the equation also holds true for non-constant $V = V(x,t)$:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi = +i\hbar\frac{\partial\psi}{\partial t}$$ The Schroedinger Equation.

III. The connection between ψ and probability

Max Born proposed (1926) that the probability of finding a particle at a specific location x at time t,

$$\text{Prob}(x,t) = \psi^*\psi.$$

Justification:

If the particle that ψ describes is assumed to last forever [this must later be revised by Quantum Field Theory] then the probability associated with finding it somewhere must always be 1. So probability must have an associated continuity equation like the one that applies to electric charge.

In electricity and magnetism:

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

electric current density

electric charge density

We need an analogous expression to describe

- probability density ρ_{Prob} and
- probability current J_{Prob} which can flow in space but remain conserved.

Assume ρ_{Prob} and J_{prob} involve ψ somehow, but in an unspecified function.

Plan:

1. Use the only equation we have for ψ: the Schroedinger Equation
2. Manipulate it to get the form

$$\frac{\partial(\text{something})}{\partial t} + \vec{\nabla}\cdot(\text{something else}) = 0.$$

$$\text{Convert 1} - \text{d Schroedinger Eq to 3-d}: \quad \frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$\text{Form } [\psi^* \cdot (\text{Sch Eq})] - [\psi \cdot (\text{Sch Eq})^*] \Rightarrow$$

$$\psi^*\left(\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi - i\hbar\frac{\partial\psi}{\partial t}\right) - \psi\left(\frac{-\hbar^2}{2m}\nabla^2\psi^* + V^*\psi^* + i\hbar\frac{\partial\psi^*}{\partial t}\right) = 0$$

÷ by $i\hbar$ and collect terms:

$$\underbrace{\psi^*\frac{\partial\psi}{\partial t}+\psi\frac{\partial\psi^*}{\partial t}}_{\substack{\downarrow\\ \displaystyle\frac{\partial}{\partial t}(\psi^*\psi)}}+\frac{\hbar}{2mi}\underbrace{\left(\psi^*\nabla^2\psi-\psi\nabla^2\psi^*\right)}_{\substack{\downarrow\\ \displaystyle\frac{\hbar}{2mi}(\vec{\nabla}\cdot[\psi^*\vec{\nabla}\psi-\psi\vec{\nabla}\psi^*])}}+\underbrace{\left(\frac{V^*-V}{i\hbar}\right)}_{\substack{\downarrow\\ \text{(0 if V is real)}}}=0$$

Rewrite :

$$\frac{\partial}{\partial \mathrm{t}}\underbrace{\left(\psi^*\psi\right)}_{\substack{\downarrow\\ \displaystyle\rho_{\text{Prob}}}}+\vec{\nabla}\cdot\underbrace{\left[\frac{\hbar}{2mi}\left\{\psi^*\left(\vec{\nabla}\psi\right)-\left(\vec{\nabla}\psi^*\right)\psi\right\}\right]}_{\substack{\downarrow\\ \displaystyle\vec{J}_{\text{Prob}}}}=0$$

IV. Normalizing a wavefunction

Recall that when we were deriving the Schroedinger Eq. for a free particle, we got to this step:

1. We guessed $\psi=\delta\cos(kx-\omega t)+\gamma\sin(kx-\omega t)$
2. We found that $\gamma=\pm i\delta$

   So $\psi = \delta\cos(kx-\omega t) \pm i\delta\sin(kx-\omega t)$

   $=\delta[\cos(kx-\omega t) \pm i\sin(kx-\omega t)]$

2 options correspond to waves traveling right and left. We can choose either one.

As-yet unspecified overall amplitude

Although this function corresponds to ψ_{free}, all ψ's have a "δ".

Next goal: find a general technique for obtaining δ. This is called *normalizing the wavefunction.*

To find δ, recall

1. P(x,t) = ψ*ψ
2. The sum of probabilities of all possible locations of the particle must be 1.

$$\int_{-\infty}^{+\infty} P(x,t)dx = 1$$

$$\int \psi^* \psi = 1$$

Example: suppose that for some choice of V(x,t), $\psi = \delta \mathrm{e}^{-\mathrm{k}^2 x^2} e^{-iEt}$ (where δ is real).

Compute $\int \psi^* \psi \mathrm{dx} = 1$

$$\int (\delta e^{-k^2x^2} e^{+iEt})(\delta e^{-k^2x^2} e^{-iEt})dx = 1$$

$$\delta^2 \int e^{-2k^2x^2} dx = 1$$

$$\delta^2 \frac{1}{k}\sqrt{\frac{\pi}{2}} = 1$$

$$\delta = \sqrt{k} \cdot \sqrt[4]{\frac{2}{\pi}}$$

V. Expectation values

Although particle is never in a definite location, it is more likely to be in one location than others, if any potential V is active.

Recall the definition of a weighted average position:

$$\bar{x} = \frac{\int_{-\infty}^{+\infty} xP(x)dx}{\int_{-\infty}^{+\infty} P(x)dx}$$

Use $P(x) = \psi^*(x)\psi(x):$

$$\boxed{x = \frac{\int_{-\infty}^{+\infty} \psi^* x\psi(x)dx}{\int_{-\infty}^{+\infty} \psi^*(x)\psi(x)dx}}$$

This is the "expectation value of x"

By convention, place x between ψ's

If ψ has been normalized, this denominator is 1.

We can find the expectation value of any function of x analogously as

$$\overline{f(x)} = \frac{\int \psi^* f(x) \psi dx}{\int \psi^* \psi dx}$$

Please read Goswami Chapter 2.

Outline

I. Normalizing a free particle wavefunction
II. Acceptable mathematical forms of ψ
III. The phase of the wavefunction
IV. The effect of a potential on a wave
V. Wave packets
VI. The Uncertainty Principle

Recall the free particle:

$$\psi = A[\cos(kx-\omega t) \pm i\sin(kx-\omega t) = Ae^{\pm i(kx-\omega t)}$$

Notice that $\int \psi^* \psi \, dx = A^2 \int_{-\infty}^{+\infty} e^{i(kx-\omega t)} e^{-i(kx-\omega t)} \, dx \to \infty.$

This reflects the fact that the wave spreads to infinity in a force-free (V=0) universe.

In the physical universe, V is nowhere constant as the Coulomb and gravitational forces have infinite range.

We can construct ψ_{bound} from Fourier superpositions of ψ_{free}.

So we need an (artificial) way to normalize ψ_{free} to achieve this.

Define the Dirac delta function

$$\delta(k-k') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dx e^{i(k-k')x} = \begin{cases} 0 \text{ if } k \neq k' \\ \infty \text{ if } k = k' \end{cases}$$

Apply Dirac δ to ψ_{free} :

Consider 2 free particles with different momenta, p=$\hbar k$ and p'=$\hbar k'$.

$$\psi_{\text{p}} = Ae^{i(kx-\omega t)}$$

$$\psi_{p'} = Ae^{i(k'x-\omega t)}$$

for A not yet normalized.

Construct $\int_{-\infty}^{+\infty} \psi_{p'}{}^* \psi_p \, dx = A^2 \int_{-\infty}^{+\infty} e^{-ik'x} e^{i\omega t} e^{ikx} e^{-i\omega t} \, dx = A^2 \int_{-\infty}^{+\infty} e^{i(k-k')x} \, dx = \begin{cases} A^2 2\pi & \text{if } k\text{=}k' \\ 0 & \text{if } k \neq k' \end{cases}$

With the use of the Dirac δ, we can draw 2 conclusions:

Conclusion #1: $A_{free} = \dfrac{1}{\sqrt{2\pi}}$, so $\psi^{\text{free}}_{\text{normalized}} = \dfrac{1}{\sqrt{2\pi}} e^{i(kx-\omega t)}$.

Conclusion #2: $\int \psi_{\text{p}'}{}^* \psi_p \, dx = 0$ if $p' \neq p$ $\rightarrow$ The ψ_{free}'s are orthonormal.

II Acceptable mathematical forms of wavefunctions

ψ must be normalizable, so $\int_{-\infty}^{+\infty} \psi^* \psi dx$ must be a convergent integral-

i.e., at minimum, require

$$\int_{-\infty}^{+\infty} \psi^* \psi dx < \infty$$

A ψ that satisfies this is called “square integrable.”

III The phase of the wavefunction

FACT 1: We cannot observe ψ itself; we only observe $\psi^*\psi$. So overall phase is physically irrelevant.

FACT 2: The relative phase of two ψ's in the same region affects the probability distribution, which is measurement, through superposition:

Suppose $\psi_1 = Ae^{i\alpha}$ and $\psi_2 = Be^{i\beta}$, where A and B are real.
$\psi_{tot} = Ae^{i\alpha} + Be^{i\beta} = e^{i\alpha}[A+Be^{i(\beta-\alpha)}]$, so
Prob$=\psi^*\psi=[A+Be^{i(\beta-\alpha)}][A+Be^{-i(\beta-\alpha)}]=A^2+B^2+AB[e^{i(\beta-\alpha)}+e^{-i(\beta-\alpha)}]= A^2 + B^2 + 2AB\cos(\beta-\alpha)$

FACT 3: The flow of probability depends on both the amplitude and the phase:
Consider $\psi=Ae^{i\alpha}$ where A can be complex.

$J_{\text{Prob}} = \frac{\hbar}{2mi}[\psi^* \nabla\psi - (\nabla\psi^*)\psi]$. Convert to 1-d for simplicity here:

$$= \frac{\hbar}{2mi}\left[\psi^* \frac{\partial\psi}{\partial x} - \left(\frac{\partial\psi^*}{\partial x}\right)\psi\right]$$

$$= \frac{\hbar}{2mi}\left[A^* e^{-i\alpha}\left(e^{i\alpha}\frac{\partial A}{\partial x} + Ai\frac{\partial\alpha}{\partial x}e^{i\alpha}\right) - \left(A^*(-i)\frac{\partial\alpha}{\partial x}e^{-i\alpha} + \frac{\partial A^*}{\partial x}e^{-i\alpha}\right)Ae^{i\alpha}\right]$$

$$= \frac{\hbar}{2mi}\left[A^*\frac{\partial A}{\partial x} + A^*Ai\frac{\partial\alpha}{\partial x} + A^*Ai\frac{\partial\alpha}{\partial x} - A\frac{\partial A^*}{\partial x}\right]$$

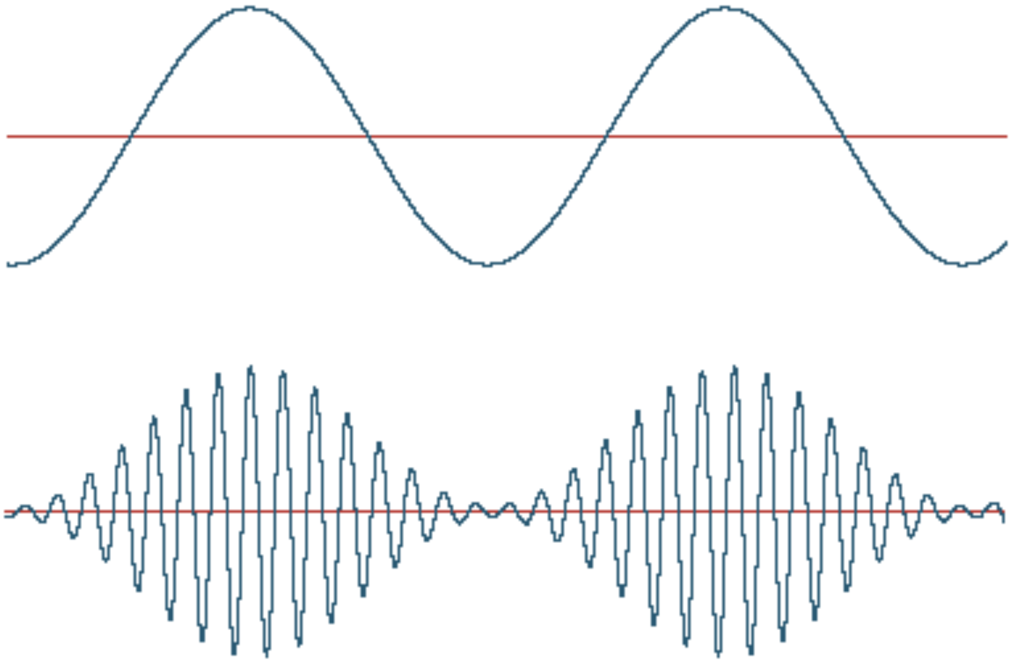
$$= \frac{\hbar A^* A}{m}\frac{\partial\alpha}{\partial x}$$

phase dependence

amplitude dependence

IV The effect of a potential upon a wave

If everywhere in the universe, V were constant, all particle/waves would be free and described by $\psi_{free}=e^{\, i(kx-\omega t)}$, an infinite train of constant wavelength λ.
If somewhere $V\neq$constant, then in that region ψ will be modulated.

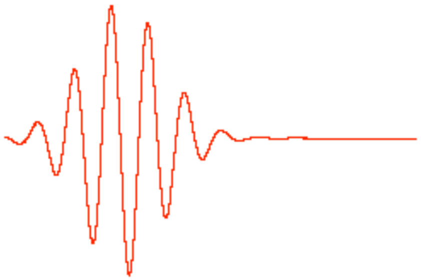


schematic
potential

schematic
wavefunction
response

A modulated wave is composed of multiple frequencies (i.e., Fourier components) that create beats or packets.

V. Wave packets



The more Fourier component frequencies there are constituting a wave packet, the more clearly separated the packet is from others. Specific requirements on a packet:

1. To achieve a semi-infinite gap on each side of the packet (i.e. a truly isolated packet/particle), we need an infinite number of waves of different frequencies.
2. Each component is a plane wave

$$\psi = Ae^{ikx}, \text{ where } k = \frac{2\pi}{\lambda},\ \lambda \propto \frac{1}{\upsilon},\ \text{so } k \propto \upsilon.$$

3. To center the packet at $x = x_0$, modify

$$e^{ikx} \rightarrow e^{ik(x-x_0)}$$

   so at $x \cong x_0$, all the k's (v's) superpose constructively.

4. To tune the shape of the packet, adjust the amplitude of each component separately---so $A \rightarrow A(k)$

Combine these 4 requirements to get :

$$\psi(x,x_0) = \int_{-\infty}^{+\infty} dkA(k)e^{ik(x-x_0)}.$$

A(k) is called the Fourier Transform of ψ(x)

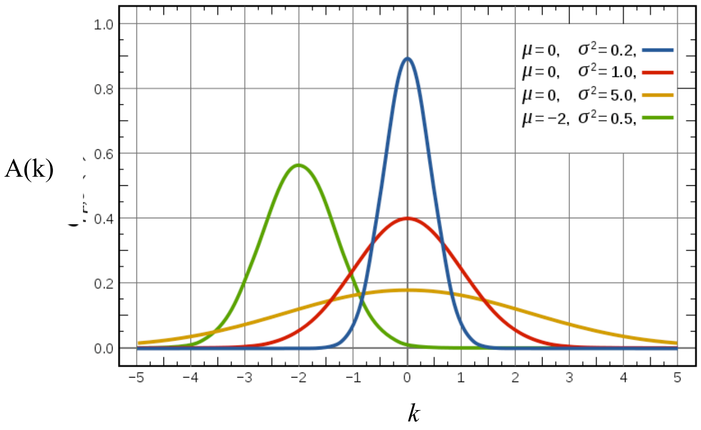
infinite number of ν's (k's)

This integral is a Fourier Integral Transformation.

VI. The Uncertainty Principle

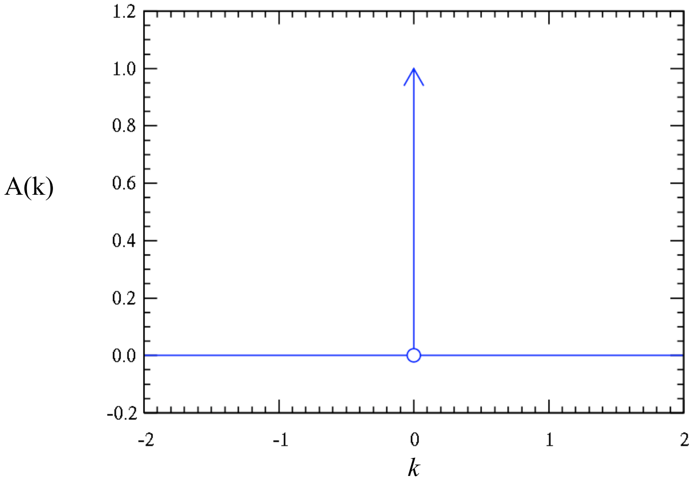
The shape of a packet depends upon the spectrum of amplitudes A(k) of its constituent Fourier components.

Examples of possible spectra:



$$A(k) = \exp\left[\frac{-(k-k_0)^2}{2(\Delta k)^2}\right]$$

Gaussian



$$A(k)=\delta(k-k_0)$$

Dirac delta

Note this is the A(k) not the $\psi(x)$.

Each A(k) spectrum produces a different wavepacket shape, for example

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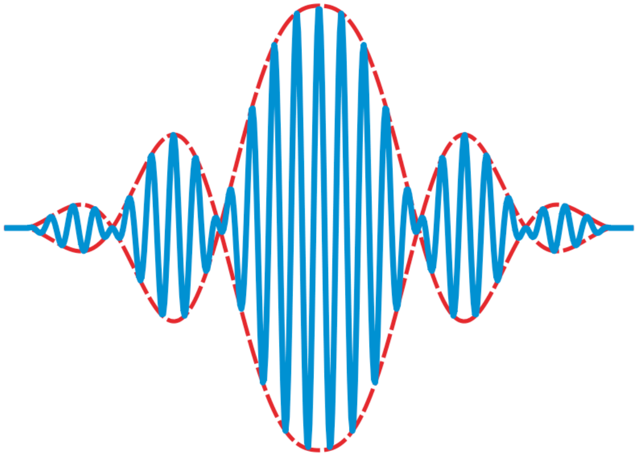
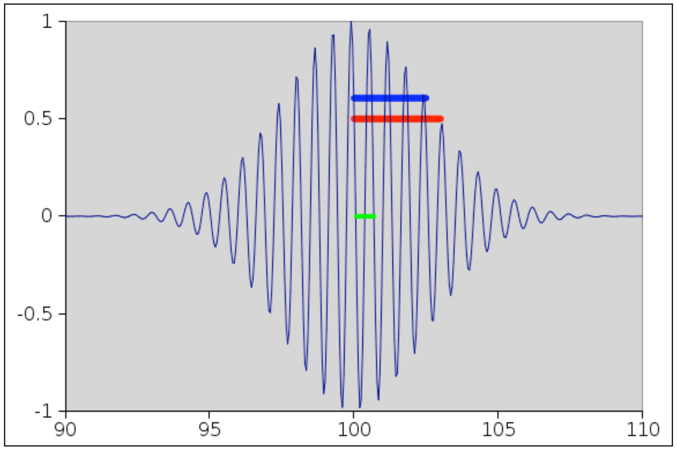


versus



Qualitatively it turns out that

•large number of constituent k's in the A spectrum (=large "Δk") produces a short packet (small "Δx").

•So $\Delta k \propto \dfrac{1}{\Delta x}$

• Since $p = \hbar k$, this means $\Delta p \propto \dfrac{1}{\Delta x}$.

•So $\Delta p \Delta x$ cannot be arbitrarily small for any wave packet.

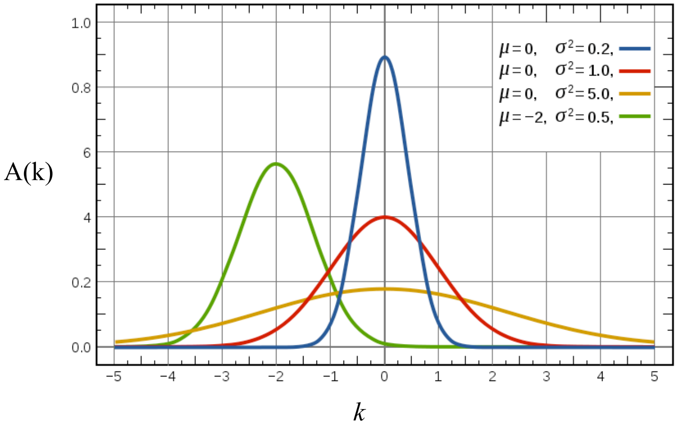
We begin to see that the Uncertainty Principle is a property of all waves, not just a Quantum Mechanical phenomenon.

The proportionality in $\Delta k \propto \dfrac{1}{\Delta x}$ is qualitative at this point.

To derive the Uncertainty Principle from this, we need to know:

1. a precise definition of Δp
2. a precise definition of Δx
3. what is the smallest combined choice of ΔpΔx (or ΔkΔx) that is geometrically possible for a wave.

To answer these, use the Gaussian wave packet in k-space to answer the questions above, in the reverse order.



The k-spectrum that produces the minimum product of $\Delta k \Delta x$ is the Gaussian. Find what this $\Delta k \Delta x$ is:

Recall $\psi = \int_{-\infty}^{+\infty} dk \; A(k) \; e^{ik(x-x_0)}$.

Find this amplitude by normalization later.

Plug in $A(k) = A'\exp\left[\frac{-(k-k_0)^2}{2(\Delta k)^2}\right]$

Then $\psi = \int_{-\infty}^{+\infty} A'\exp\left[\frac{-(k-k_0)^2}{2(\Delta k)^2} + ik(x-x_0)\right]dk$

Compute the integral and normalize (Goswami pp. 28-9) to find

$\psi = \frac{\sqrt{\Delta \mathrm{k}}}{\sqrt[4]{\pi}}\exp\left[ik_0(x-x_0) - \frac{1}{2}(x-x_0)^2(\Delta k)^2\right]$ for Gaussian A's

Answer to (2)--- “What is Δx?” :

For all A(k) spectra, the precise definition of Δx is

$$\Delta x \equiv \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

For simplicity, choose center of the packet at $x_0 = 0$. Then

$$\langle x \rangle = 0 \text{ and } e^{ik(x-x_0)} \rightarrow e^{ikx}$$

We need $\sqrt{\langle \mathrm{x}^2 \rangle}$

$$\langle x^2 \rangle = \frac{\int \psi^* x^2 \psi dx}{\int \psi^* \psi dx}$$

$$= \frac{\Delta k}{\sqrt{\pi}} \int e^{-ik_0 x} e^{-\frac{1}{2}x^2(\Delta k)^2} x^2 e^{+ik_0 x} e^{-\frac{1}{2}x^2(\Delta k)^2} dx$$

$$= \frac{1}{2(\Delta k)^2}$$

So $\Delta x = \dfrac{1}{\sqrt{2}\Delta k}$.

Now the answer to (1)---"what is Δp?"

Analogously to Δx, define $\Delta p \equiv \sqrt{\langle p^2\rangle - \langle p\rangle^2}$.

Assume packet is at the origin in momentum space, so $\langle p\rangle = 0$.

Then we need only $\langle p^2\rangle = \langle \hbar^2 k^2\rangle = \hbar^2 \langle k^2\rangle$.

Consider 2 ways to find $\langle k^2\rangle$:

WAY #1: $\langle k^2\rangle = \dfrac{\int \psi^*(x) k^2 \psi(x)\, dx}{\int \psi^*(x)\psi(x)\, dx}$.

This requires finding the functional dependence of k on x. We defer this to Chapter 3.

WAY #2: $\langle k^2\rangle = \dfrac{\int \psi^*(k) k^2 \psi(k)\, dk}{\int \psi^*(k)\psi(k)\, dk}$.

$\psi(k)$ is the form that ψ takes when it is represented in momentum space rather than position space.

To find $\psi(k)$, invert $\psi(x)=\int A(k)e^{+ikx}\, dk$ (Note Plancherel's Theorem.)

The inverted form is $A(k)=\int \psi(x)e^{-ikx}\, dx$.

So $A(k)$ IS $\psi(k)$, the k-dependent form of ψ.

So we need $$\left\langle k^2 \right\rangle = \frac{\int\limits_{-\infty}^{+\infty} A^*(k) k^2 A(k)\,dk}{\int\limits_{-\infty}^{+\infty} A^*(k) A(k)\,dk} = \frac{(\Delta k)^2}{2}$$

So $\left\langle p^2 \right\rangle = \hbar^2 \left\langle k^2 \right\rangle = \dfrac{\hbar^2 (\Delta k)^2}{2}$.

Then $\Delta p = \sqrt{\left\langle p^2 \right\rangle - \left\langle p \right\rangle^2} = \sqrt{\dfrac{\hbar^2 (\Delta k)^2}{2} - 0} = \dfrac{\hbar \Delta k}{\sqrt{2}}$.

Combine: $\Delta x \Delta p = \dfrac{1}{\sqrt{2}\Delta k} \cdot \dfrac{\hbar \Delta k}{\sqrt{2}} = \dfrac{\hbar}{2}$ for a Gaussian amplitude distribution.

For all other amplitude distributions, the value is $> \dfrac{\hbar}{2}$, so for ANY packet,

$\Delta x \Delta p \geq \dfrac{\hbar}{2}$.

We will cover the alternate uncertainty principle, $\Delta E \Delta t \geq \dfrac{\hbar}{2}$, after Chapter 6.

Please read Goswami Chapter 3.

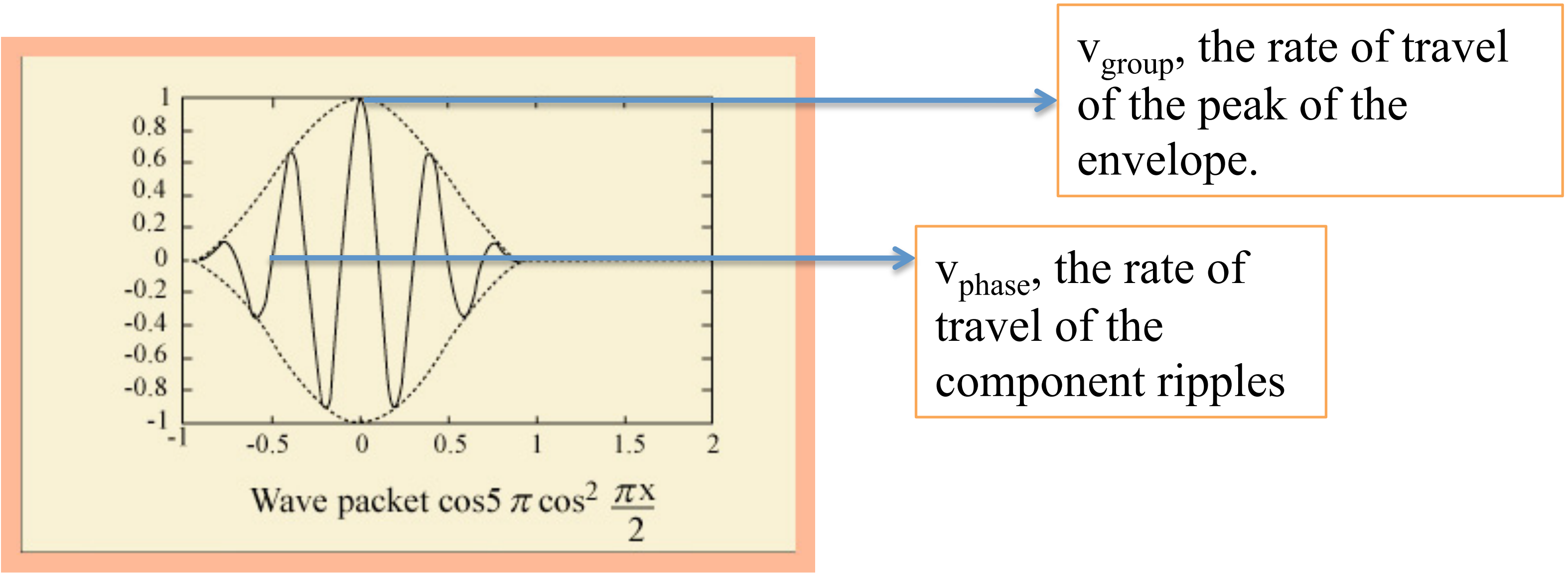
Outline

I. Phase velocity and group velocity
II. Wave packets spread in time
III. A longer look at Fourier transforms, momentum conservation, and packet dispersion.
IV. Operators
V. Commutators
VI. Probing the meaning of the Schroedinger Equation

I. Phase velocity and group velocity

A classical particle has an unambigous velocity $\Delta x/\Delta t$ or dx/dt because its “x” is always perfectly well known.

A wave packet has several kinds of velocity:



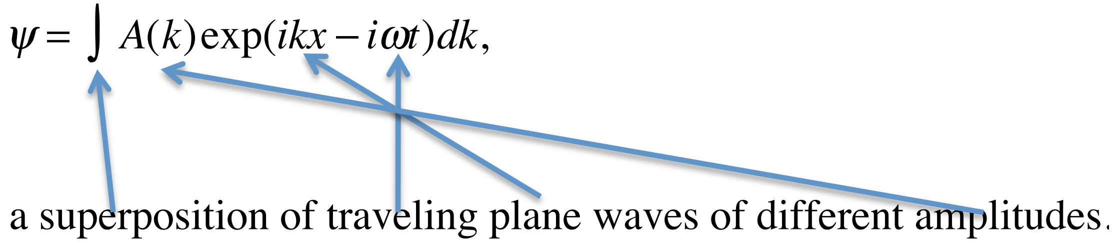
Wave packet $\cos 5\pi \cos^2 \frac{\pi x}{2}$

v_{group}, the rate of travel of the peak of the envelope.

v_{phase}, the rate of travel of the component ripples

In general $v_{phase} \neq v_{group}$. Which velocity is related to the velocity of the particle that this wave represents?

Recall a traveling wave packet is described by



$$\psi = \int A(k)\exp(ikx - i\omega t)dk,$$

a superposition of traveling plane waves of different amplitudes.

Bear in mind the definitions

- k = 2π/λ “inverse wavelength” and
- ω = 2πυ “angular frequency”

Recall ω = ω(k).

- If the packet changes shape as it travels, the function may be complicated.
- If the packet changes shape rapidly and drastically, the notion of a packet with well-defined velocity becomes vague.

For clarity, consider only those packets that do not change shape “much” as they travel. For them, ω(k)=constant + small terms proportional to some function of k. Taylor expand ω about some k=k_0.

$$\omega = \underbrace{\omega_0 + (k-k_0)\left.\frac{d\omega}{dk}\right|_{k=0}}_{\Downarrow} + \ldots$$

Plug this into ψ:

$$\psi = \int A(k)\exp\left\{ikx - i\left[\omega_0 + (k-k_0)\frac{d\omega}{dk} + \dots\right]t\right\}dk$$

Compare $\psi(t=0)$ and $\psi(t \neq 0)$:

At $t=0$, $\psi(x,0) = \int A(k)e^{ikx}dk$.

At t later, $\psi(x,t) = \underbrace{e^{i\left(-\omega_0 + k_0 \left.\frac{d\omega}{dk}\right|_{k_0}\right)t}}\,\underbrace{\int A(k)e^{ik\left(x - \left.\frac{d\omega}{dk}\right|_{k_0} t\right)}dk}$.

This is an overall phase which has no meaning in ψ*ψ, so forget it.

This is identical to ψ(x,0) except the position of the packet is shifted by $\left.\frac{d\omega}{dk}\right|_{k_0} t$, so that must be the velocity of the packet:

$$\left.\frac{d\omega}{dk}\right|_{k_0} = \text{the group velocity.}$$

Show that this is the same as the particle's velocity v:

Recall:

$$E = \hbar\omega$$

$$E = \frac{p^2}{2m} \text{ when } V = 0$$

$$p = \hbar k$$

So $$\frac{d\omega}{dk} = \frac{d\omega}{dE}\frac{dE}{dp}\frac{dp}{dk}$$

$$= \frac{1}{\hbar}\frac{2p}{2m}\hbar$$

$$= \frac{p}{m} = v.$$

Conclude: $v_{group} = d\omega/dk$ is the velocity of the packet envelope AND of the associated particle.

$v_{phase} = \omega/k$ is usually different from $d\omega/dk$.

Notice $$v_{phase} = \frac{\omega}{k} = \frac{E/\hbar}{p/\hbar} = \frac{E}{p} = \frac{p^2/2m}{p} = \frac{p}{2m} = \frac{v_{group}}{2}.$$

II. Wave packets spread in time

The lecture plan:

1. Recall $\psi_{General\ A's}(x,t=0)$
2. Specialize to $\psi_{Gaussian\ A's}(x,t=0)$
3. Extrapolate from x to $x\text{-}vt$, so $e^{ikx} \rightarrow e^{i(kx-\omega t)}$
4. Find $P(x,t)=\psi^*(x,t)\psi(x,t)$.

We will find that $|\psi(x,t)|^2$ is proportional to $exp(-x^2/(stuff)^2)$.
Since the width of ψ is defined as the distance in x over which ψ decreases by e, this "stuff" is the width.
We will see that the "stuff" is a function of time.

Carry out the plan...

(1) $\psi_{General\ A's}(x,t=0)=\int\limits_{-\infty}^{+\infty} dkA(k)e^{ikx}$

(2) $A_{Gaussian}=\frac{1}{\sqrt[4]{2\pi}}\frac{1}{\sqrt{\Delta k}}e^{-\left[\frac{(k-k_0)^2}{2(\Delta k)^2}\right]}$

So $\psi_{Gaussian\ A's}(x,t=0)=\frac{1}{\sqrt[4]{2\pi}}\frac{1}{\sqrt{\Delta k}}\int\limits_{-\infty}^{+\infty} dke^{-\left[\frac{(k-k_0)^2}{2(\Delta k)^2}+ikx\right]}$

(3) Extend this to $\mathrm{t}\neq 0$:

$$\psi_{Gaussian\ A's}(x,t=0)=\frac{1}{\sqrt[4]{2\pi}}\frac{1}{\sqrt{\Delta k}}\int\limits_{-\infty}^{+\infty} dke^{-\left[\frac{(k-k_0)^2}{2(\Delta k)^2}+i(kx-\omega t)\right]}$$

Recall $\frac{\omega}{k}=\frac{p}{2m}$. But $p=\hbar k$, so $\omega=\frac{\hbar k^2}{2m}$, so

$\psi_{Gaussian\ A's}(x,t=0)=\frac{1}{\sqrt[4]{2\pi}}\frac{1}{\sqrt{\Delta k}}\int\limits_{-\infty}^{+\infty} dke^{-\left[\frac{(k-k_0)^2}{2(\Delta k)^2}+ik\left(x-\frac{\hbar kt}{2m}\right)\right]}$. Integrate to get:

$$\psi(\mathrm{x,t})\propto\exp\left[\frac{-\left(\mathrm{x}-\frac{\hbar \mathrm{k}_0 t}{m}\right)^2}{2\left(\frac{1}{(\Delta k)^2}+\frac{i\hbar t}{m}\right)}\right]\exp\left[ik_0\left(x-\frac{\hbar k_0 t}{2m}\right)\right]$$

$$(4)\ \psi^*\psi \propto \exp\left[\frac{-\left(x\text{-}\frac{\hbar k_0 t}{m}\right)^2}{2\left(\frac{1}{(\Delta k)^2}+\frac{i\hbar t}{m}\right)}\right]\exp\left[\frac{-\left(x\text{-}\frac{\hbar k_0 t}{m}\right)^2}{2\left(\frac{1}{(\Delta k)^2}-\frac{i\hbar t}{m}\right)}\right]$$

$$\propto \exp\left\{\frac{-1}{(\Delta k)^2}\left[\frac{\left(x-\frac{\hbar k_0 t}{m}\right)}{\frac{1}{(\Delta k)^4}+\frac{\hbar^2 t^2}{m^2}}\right]\right\}.$$

Notice $\psi^*\psi$(t=0) decreases by1/e when x=1/$(\Delta k)^2$. Call this Δx(t=0). But $\psi^*\psi$(t $\neq$ 0) decreases by 1/e when the new "advanced in time x", $\text{x-}\frac{\hbar\text{kt}}{\text{m}}=\Delta\text{k}\left[\frac{1}{(\Delta\text{k})^4}+\frac{\hbar^2t^2}{m^2}\right]^{1/2}$. Call this Δx(t).

$$\text{Notice } \Delta x(t)=\frac{1}{\Delta k}\sqrt{1+\frac{t^2}{\left[\frac{m}{\hbar(\Delta k)^2}\right]^2}}.$$

call this T, the characteristic spreading time.

Notice this is Δx(t=0).

$$\text{So } \Delta x(t\neq 0)=\Delta x(t=0)\cdot\left[1+\left(\frac{t}{T}\right)^2\right]^{1/2}$$

Conclusions:

(1) The width Δx of the probability distribution increases with t, i.e., the packet spreads.

(2) This only works because the amplitudes A are time-independent, i.e., the A(k) found for ψ(t=0) can be used for ψ(all t). The A(k) distribution is a permanent characteristic of the wave.

(3) Notice the "new x": $$x - \frac{\hbar kt}{m} = x - \frac{pt}{m} = x - v_{group}t.$$

The group velocity naturally appears because this Δx describes a property of the packet as a whole.

(4) Recall the A(k) are not functions of t, so
Prob(k,t) = A*A does not have time-dependence, so Δp does not spread as Δx does.
This is momentum conservation.

III. A longer look at Fourier transforms, momentum conservation, and packet dispersion

Recall that ψ(x) and $A(k)$ are related by the Fourier transform equation

$$\psi(x)=\int_{-\infty}^{+\infty} dkA(k)e^{ikx}.$$

When $t \neq 0$,

$$\psi(x)=\int_{-\infty}^{+\infty} dkA(k)e^{i(kx-\omega t)}.$$

One can invert this by multiplying by $\frac{e^{-i(k'x-\omega t)}}{2\pi}dx$ and integrating:

$$\frac{1}{2\pi}\int dx\psi(x,t)e^{-i(k'x-\omega t)} = \frac{1}{2\pi}\int dx\int dkA(k)e^{i(kx-\omega t)}e^{-i(k'x-\omega t)}$$

$$=\int_{-\infty}^{+\infty} dkA(k)\underbrace{\frac{1}{2\pi}\int_{-\infty}^{+\infty} dxe^{i(k-k')x}}_{\substack{\downarrow \\ \delta(k\text{-}k')}}$$

$$=A(k')$$

Rewrite this $A(k')$, renaming k' as k:

$$A(k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dx\psi(x,t)e^{-i(kx-\omega t)}.$$

Notice the minus sign.

Notice that while $\psi = \psi(x,t)$, $A = A(k$ but not $t)$.

We can use this fact to determine $\psi(t \neq 0)$ given $\psi(t = 0)$.

For example, suppose $\psi(x,t=0) = Ce^{-\beta x^2}$. What is $\psi(x,t \neq 0)$?

We CANNOT assume that $\psi(x,t) = Ce^{-\beta x^2 - i\omega t}$ because ψ is a superposition (packet) of frequencies.

Each component wave in the packet could have its own $\omega(k)$.

Procedure to get ψ(x,t) from ψ(x,0):

Write $\psi(x',t)=\int dkA(k)e^{i(kx'-\omega t)}$. "Eq. 5"

In general $A(k)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} dx\psi(x,t)e^{-i(kx-\omega t)}$.

Because $A \neq A(t)$, this integral must be valid at any particular time t. Pick t=0:

$A(k)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} dx\psi(x,0)e^{-ikx}$. Plug this into Eq. 5:

$$\psi(x',t)=\frac{1}{2\pi}\int dk\int dx\psi(x,0)e^{-ikx}e^{i(kx'-\omega t)}.$$

These ω's are the frequencies of the Fourier components. The components are plane waves---the ψ's of free particles.

So their $\mathrm{E} = \frac{\mathrm{p}^2}{2\mathrm{m}}$ (all kinetic, no potential).

$$\text{So } \omega = \frac{\mathrm{E}}{\hbar} = \frac{p^2}{2m\hbar} = \frac{\hbar^2 k^2}{2m\hbar} = \frac{\hbar k^2}{2m}$$

Rewriting, $\psi(x',t)=\frac{1}{2\pi}\int dk\int dx\psi(x,0)e^{-ikx}e^{i(kx'-\omega t)}$. Plug in $\psi(x,0)$ and integrate.

IV. Operators

Recall earlier we wanted $\left\langle p^2 \right\rangle = \int \psi^*(x) p^2 \psi(x) dx$

but we needed to represent p as a function of x. How to find this representation:

Recall the wavefunction for a free particle is $\psi = e^{i(kx-\omega t)}$.
Notice

$$\frac{\partial \psi}{\partial x} = ik\psi.$$

But $p = \hbar k$, so

$$\frac{\partial \psi}{\partial x} = \frac{ip}{\hbar}\psi.$$

Rewrite :

$$p\psi = \frac{\hbar}{i}\frac{\partial \psi}{\partial x} = -i\hbar\frac{\partial \psi}{\partial x}.$$

This says: if ψ represents a free particle, any time we have “pψ”, we can replace it with

$$-i\hbar\frac{\partial \psi}{\partial x}.$$

Q. What if ψ is NOT a free particle?...what if ψ is influenced by a potential V so is a packet?

Ans. The packet is a superposition of free particle states, so the replacement is still valid.

Use a similar method to find the operator for energy E:
Begin with is $\psi_{\text{free}} = e^{i(kx-\omega t)}$.
Notice

$$\frac{\partial\psi}{\partial t} = -i\omega\psi = \frac{-iE}{\hbar}\psi.$$

So $E\psi = +i\hbar\dfrac{\partial\psi}{\partial t}$.

We will use a similar procedure later to get operators for other qualities such as angular momentum $\vec{L}$.

Facts about this procedure:

1. The order of the symbols is important here: so far this applies to “pψ” not “ψp”.
2. when a mathematical expression (like p or E) precedes a function (like ψ) and has the possibility of changing the function (for example multiplying it, taking its derivative), call the expression an *operator*.
   So p is an operator applied to ψ.
3. Operators can be expressed in coordinate space or momentum space:

Operator	Coordinate Space Representation	Momentum Space Representation
p	$-i\hbar\frac{\partial}{\partial x}$	p

4. Pick the representation that matches the space in which the function is expressed.
   ex.—is p acting on ψ(x) or on A(k)?
5. Any measureable attribute of a particle has an associated operator Examples....

Attribute / operator	**in x - space**	**in k - space**
p	$- i\hbar \frac{\partial}{\partial x}$	p
x	x	$+ i\hbar \frac{\partial}{\partial p}$
p^2	$\left(-i\hbar \frac{\partial}{\partial x} \right)\left(-i\hbar \frac{\partial}{\partial x} \right) = -\hbar^2 \frac{\partial^2}{\partial x^2}$	p^2
x^2	x^2	$- \hbar^2 \frac{\partial^2}{\partial p^2}$
E	$+ i\hbar \frac{\partial}{\partial t}$	$+ i\hbar \frac{\partial}{\partial t}$

6. If you need to apply 2 or more operators successively to a function, the order in which you apply them affects the answer.

$$xp\psi = x\left(-i\hbar\frac{\partial}{\partial x}\right)e^{i(kx-\omega t)} = -i\hbar x\cdot ik\psi = \hbar kx\psi$$

$$px\psi = -i\hbar\frac{\partial}{\partial x}\left[xe^{i(kx-\omega t)}\right] = -i\hbar\left[xik\psi + \psi\right] = \hbar kx\psi - i\hbar\psi .$$

So $\underbrace{(xp\text{-}px)}_{\downarrow}\psi = i\hbar\psi$

This expression is called "the commutator of x and p" and is abbreviated as $[x,p]$.

The expression $[x,p]=i\hbar$ is called "the commutation relation of x and p."

Why do we care about commutators?

An operator represents a measurement.

A commutator's value indicates whether the order of doing 2 measurements matters.

It does not matter in all cases----this depends upon the particular pair of measurements.

If the order does matter, this means that the first measurement disrupts the system in a way that influences the result of the second.

This is the Uncertainty Principle.

7. In QM we care mostly about operators that represent measureable quantities.

"observables"

8. This kind of operator
   - always produces real, not complex, expectation values
   - is called "Hermitian."

V. How to calculate a commutator

(1) Act with it on a dummy wavefunction

Example: What is $\left[\mathrm{x},\frac{\partial}{\partial \mathrm{x}}\right]$?

Apply it to a free particle e^{ikx}

$$\left[x,\frac{\partial}{\partial x}\right]e^{ikx}=x\frac{\partial(e^{ikx})}{\partial x}-\frac{\partial}{\partial x}\left(xe^{ikx}\right)=-1\cdot e^{ikx}$$

Then remove the dummy wavefunction and see what is left over:

So $\left[\mathrm{x},\frac{\partial}{\partial \mathrm{x}}\right]=-1$.

(2) If the operators in the commutator are functions of simpler operators whose commutators you know, expand the commutator with the functions expressed explicitly and look for simpler commutators whose value you know.

Example: Find $[x,p^2]$.

$$\left[x,p^2\right]=xpp-ppx$$

$=(xp)p-p^2x$ Use $[\mathrm{x,p}]=\mathrm{xp}-\mathrm{px}=\mathrm{i}\hbar$, so $\mathrm{xp}=\mathrm{i}\hbar+\mathrm{px}$

$=(\mathrm{i}\hbar+\mathrm{px})\mathrm{p}-\mathrm{p}^2x$ Reassociate (px)p as p(xp)

$=\mathrm{i}\hbar\mathrm{p}+\mathrm{p}(\mathrm{xp})-\mathrm{p}^2\mathrm{x}$ Use again $\mathrm{xp}=\mathrm{i}\hbar+\mathrm{px}$

$=\mathrm{i}\hbar\mathrm{p}+\mathrm{p}(\mathrm{i}\hbar+\mathrm{px})-\mathrm{p}^2x$

$$=i\hbar p+pi\hbar+\underbrace{ppx-p^2x}_{0}$$

$$=2i\hbar p.$$

The student will show all of the following commutator identities in homework. Once they have been proven explicitly one time, they can afterward be used whenever convenient without re-proof:

- [A,B]=-[B,A]
- [A,B+C]=[A,B]+[A,C]
- [AB,C]=[A.C]B+A[B,C]
- [A,BC]=[A,B]C+B[A,C]

VI. A longer look at the Schroedinger Equation

Recall the equation

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

Notice this is $p_{operator}^2/2m$

Notice this is $E_{operator}$

These operator relationships were the basis of Schroedinger's thought when he discovered the equation. He thought:

- Assume ψ is built of plane waves $e^{i(kx-\omega t)}$
- Find the operators
- Guarantee non-relativistic energy conservation, $p^2/2m + V = E$.

The operator $\frac{p_{op}^2}{2m} + V$ represents the total energy and is also called the Hamilton operator H. Applying H to ψ evolves ψ in time. Time itself is not an operator.

Please read Goswami Chapter 4

Outline

I. How to solve the Schroedinger Equation
II. Why do we concentrate on ψ's that are separable?
III. Why E is real if $\psi=u(x)T(t)$

I. How to solve the Schroedinger Equation

Recall the equation:

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

Why we want to solve it:

Solving it gives us Ψ(x,t), which includes EVERYTHING that can be known about a particle, including its mass, energy, location, response to V, etc.

Once we have Ψ(x,t), we extract these properties by using Ψ to compute expectation values.

How to solve the Schroedinger Equation

- Consider the case where *V=V(x* only, not *t*). [Later we will consider more general *V*.
- GUESS that *Ψ(x,t)=u(x)T(t)* and plug this guess into the equation:

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left[u(x)T(t)\right]+V(x)u(x)T(t)=i\hbar\frac{\partial}{\partial t}\left[u(x)T(t)\right]$$

$$\frac{-\hbar^2}{2m}T(t)\frac{d^2}{dx^2}\left[u(x)\right]+V(x)u(x)T(t)=i\hbar u(x)\frac{d}{dt}\left[T(t)\right]$$

÷ both sides by $u(x)T(t)$:

$$\underbrace{\frac{\frac{-\hbar^2}{2m}T(t)\frac{d^2}{dx^2}\left[u(x)\right]}{u(x)T(t)}+\frac{V(x)u(x)T(t)}{u(x)T(t)}}_{\substack{\downarrow \\ \text{function of x only}}}=\underbrace{\frac{i\hbar u(x)\frac{d}{dt}\left[T(t)\right]}{u(x)T(t)}}_{\substack{\downarrow \\ \text{function of t only}}}$$

These 2 functions can be equal only if both actually equal something that is neither a f(x) nor a f(t). i.e., both = a constant "G". This leads to 2 ODE's:

$$\underbrace{i\hbar\frac{1}{T(t)}\frac{dT(t)}{dt}=G}_{\substack{\downarrow \\ T=e^{\frac{-iGt}{\hbar}}}}$$ "Eq 1" and $$\underbrace{\frac{1}{u(x)}\left\{\frac{-\hbar^2}{2m}\frac{d^2u(x)}{dx^2}+V(x)u(x)\right\}=G}_{\substack{\downarrow \\ \frac{-\hbar^2}{2m}\frac{d^2u(x)}{dx^2}+V(x)u(x)=Gu(x)}}$$ "Eq 2"

What is G? To answer this, examine the solution to Equation 1:

Recall that e - i(stuff) can be written as cos(stuff) – i sin(stuff), so

So $T = \cos\left(\frac{Gt}{\hbar}\right) - i\sin\left(\frac{Gt}{\hbar}\right)$, a sum of waves.

The argument of these trigonometric functions must be dimensionless, so

$\frac{G}{\hbar}$ must be an angular frequency "ω".

So $G = \hbar\omega$. But $\hbar\omega$ is the total energy of this quantum mechanical system.

So $G =$ Energy E.

Then $T(t) = e^{\frac{-iEt}{\hbar}}$

Return to Eq 2:

$$\frac{-\hbar^2}{2m}\frac{d^2u(x)}{dx^2}+V(x)u(x)=Gu(x)$$

Replace $G \to E$.

Rename $u(x) \to \psi(x)$.

Then $\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$ The Time-Independent Schroedinger Equation

Facts about the Time-independent Schroedinger Equation:

1. The ψ's are called the eigenfunctions of the Hamiltonian $\frac{-\hbar^2}{2m}\frac{d^2u(x)}{dx^2}+V(x)$
2. Sometimes, depending on the form of V, more than one value of ψ can solve it.

   For example: if V is the Coulomb potential of a nucleus, then each ψ includes information about the properties an electron would have in one of the energy shells around the nucleus.

3. Method: Plug in a V, solve for u(x) (which is ψ), then solve for E. [We will work examples of this.] Then insert u(x) into the full solution

$$\Psi = uT = ue^{-iEt/\hbar}$$

II. Why do we concentrate on Ψ's that are separable?

Note, some systems have $\Psi \neq u(x)T(t)$ so separable Ψ's are not the most general kind. Reasons why they are interesting:

1. The energy E associated with them is mathematically real; i.e. measureable in the lab. Note one can't take this for granted since Ψ itself is complex. The reality of E leads to

2. The probability density is not a function of time, so the states do not change their properties with time.

3. These states have a definite energy; i.e. uncertainty ΔE=0.

The next lecture topics demonstrate these 3 points.

Plan of this section: First show that E is real if $\Psi = u(x)e^{-iEt/\hbar}$.

Then show why E being real is important.

To show the condition under which E is real, begin by assuming that E could be complex.

Then show that E - $E^* = 0$, i.e., $E = E^*$, so E must be real.

Recall probability density $\rho_{\Pr ob} = \Psi * \Psi = u * ue^{iE^*t/\hbar}e^{-iEt/\hbar} = u * ue^{-i(E-E^*)t/\hbar}$.

Recall probability current $J_{\Pr ob} = \dfrac{\hbar}{2im}\left[\Psi * \dfrac{\partial\Psi}{\partial x} - \dfrac{\partial\Psi *}{\partial x}\Psi\right]$.

Recall the 1-dimensional continuity equation for probability: $\dfrac{\partial\rho_{\text{Prob}}}{\partial \text{t}} + \dfrac{\partial J_{\text{Prob}}}{\partial x} = 0$.

Generalize this to 3 dimensions: $\dfrac{\partial\rho_{\text{Prob}}}{\partial \text{t}} + \vec{\nabla} \cdot \vec{J}_{\text{Prob}} = 0$.

Substitute ρ_{Prob} and J_{Prob} and take ∂/∂t: $\frac{-i}{\hbar}(E-E^*)u^*ue^{-i(E-E^*)t/\hbar}+\vec{\nabla}\cdot\vec{J}=0.$

Integrate over all space: $\frac{-i}{\hbar}(E-E^*)e^{-i(E-E^*)t/\hbar}\int_{Vol}u^*ud(Vol)=-\int_{Vol}\vec{\nabla}\cdot\vec{J}d(Vol).$

(Use the Divergence Theorem ($\int_{\text{Vol}}\vec{\nabla}\cdot\vec{V}d(Vol)=\int_{Area}\vec{V}\cdot d\vec{A}$))

$$=-\int_{r\to\infty}\vec{J}\cdot d\vec{A}$$

But Ψ must be square integrable: $\int\Psi^*\Psi d(Vol)<\infty$, so $\Psi(r\to\infty)\to 0.$

So J, being proportional to Ψ, also $\to 0$ as r $\to\infty$. So $\int_{r\to\infty}\vec{J}\cdot d\vec{A}=0.$

So lefthand side of the equation, $\frac{-i}{\hbar}(E-E^*)e^{-i(E-E^*)t/\hbar}\int_{Vol}u^*ud(Vol)=0$

$(E-E^*)=0$

$E=E^*,\quad E$ is real.

Outline

I. Stationary States
II. If Ψ is a stationary state, its ΔE=0.
III. Degeneracy
IV. Required properties of eigenfunctions
V. Solving the time-independent Schroedinger Equation when V=0
VI. Solving the time-independent Schroedinger Equation for a Barrier Potential

I. Stationary States

Recall that Ψ is separable as u(x)T(t), then

$\Psi = u(x)e^{-iEt/\hbar}$.

If E were complex $(E = E_R + iE_I)$, then we would have

$\Psi = u(x)e^{-i(E_R + iE_I)t/\hbar}$.

Then $\underbrace{\Psi^*\Psi}$ would be $u^*u\,\underbrace{e^{-2tE_I/\hbar}}$.

i.e., Probability of locating the particle would be time-dependent.

Expectation values $f(x) = \dfrac{\int \Psi^* f(x)\Psi\,dx}{\int \Psi^*\Psi\,dx}$ of all the properties of Ψ would involve $e^{-2tE_I/\hbar}$ too.

But since E is real when $\Psi = u(x)T(t)$, Probability, expectation values $\neq f(t)$.

So once we know something about the state, it remains true for ever.

These are called stationary states.

II. If Ψ is a stationary state, its ΔE=0

Recall when Ψ=u(x)T(t), this leads to

- the Time-dependent Schroedinger Eq: $T = e^{-iEt/\hbar}$
- the Time-independent Schroedinger Eq: $\underbrace{\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V\right)}_{\substack{\downarrow \\ \text{Hamiltonian } H}} u = Eu$

$$\text{Notice } \langle H \rangle = \int \Psi^* H \Psi \, dx = \int u^* e^{+iEt/\hbar} H u e^{-iEt/\hbar} \, dx = \int u^* \underbrace{Hu}_{\substack{\downarrow \\ Eu}} dx = E \underbrace{\int u^* u \, dx}_{\substack{\downarrow \\ 1}} = E$$

$$\text{Also } \langle H^2 \rangle = \int \Psi^* H^2 \Psi \, dx = \int u^* H \underbrace{Hu}_{\substack{\downarrow \\ Eu}} dx = E \int u^* \underbrace{Hu}_{\substack{\downarrow \\ Eu}} dx = E^2 \underbrace{\int u^* u \, dx}_{\substack{\downarrow \\ 1}} = E^2$$

Then $\Delta E \equiv \langle E^2 \rangle - \langle E \rangle^2 = 0.$

III. Degeneracy

If 2 states of the same system have the same energy, we call them degenerate.
Example: the rightward and leftward traveling components of the free particle Ψ:

$$\Psi = \delta\left[\cos\left(kx \pm \omega t\right) \pm i\sin\left(kx \pm \omega t\right)\right] \Rightarrow \delta e^{\pm i\left(kx \pm \omega t\right)}$$

$$\delta e^{+i\left(kx - \omega t\right)}: \quad \text{traveling rightward}$$

$$\delta e^{-i\left(kx + \omega t\right)}: \quad \text{traveling leftward}$$

IV. Required properties of eigenfunctions

-in addition to being square integrable-

(1) Recall Probability density(x,t)=$\Psi^*\Psi$. This means Ψ is related to the probability of locating an object at (x,t).

By definition of probability, no probability can be > 100%, and especially, no probability can be infinite.

So Ψ must be finite in amplitude.

(2) Recall $\langle p\rangle = \int \Psi^* \left(-i\hbar \frac{\partial \Psi}{\partial x} \right) dx.$

Momentum in the physical world cannot be infinite, so

$d\Psi/dx$ must be finite.

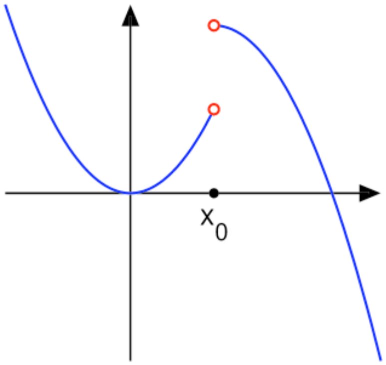
(3) Recall the Schroedinger Equation

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

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

In the physical world, V, E, and m cannot be infinite, so

$d^2\Psi/dx^2$ must be finite.



(4) Recall the continuity relations:

If a variable (Ψ) is discontinuous,
then its first derivative is infinite at the discontinuity.

So conversely, if dΨ/dx is finite, then Ψ is continuous.

We already showed this. This is not really new information but it deserves emphasis.

(5) Similarly, if $d^2\Psi/dx^2$ is finite, then dΨ/dx is continuous.

(6) If the amplitude of Ψ represents information about a physical object, Ψ must be single-valued (i.e, one value at each x, not necessarily same value at all x).

(7) If Ψ is single-valued, dΨ/dx is single-valued.

V. Solving the time-independent Schroedinger Equation when $V = 0$

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

Plug in 0:

One can check by substitution that 2 possible solutions are

$\psi_1 = e^{i\left(\frac{\sqrt{2mE}}{\hbar}\right)x}$ and $\psi_2 = e^{-i\left(\frac{\sqrt{2mE}}{\hbar}\right)x}$.

So the general solution is the linear combination

$$\psi_{\text{general, time-indep, free particle}} = Ae^{i\left(\frac{\sqrt{2mE}}{\hbar}\right)x} + Be^{-i\left(\frac{\sqrt{2mE}}{\hbar}\right)x}.$$

Notice since this is a free particle (V=0), the E here is $\mathrm{E}_{\text{kinetic}}$ only.

But $\mathrm{E}_{\text{kinetic}} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$, so $\frac{\sqrt{2\mathrm{mE}}}{\hbar}$ is really $\frac{1}{\hbar}\sqrt{2m\frac{\hbar^2 k^2}{2m}} = k$.

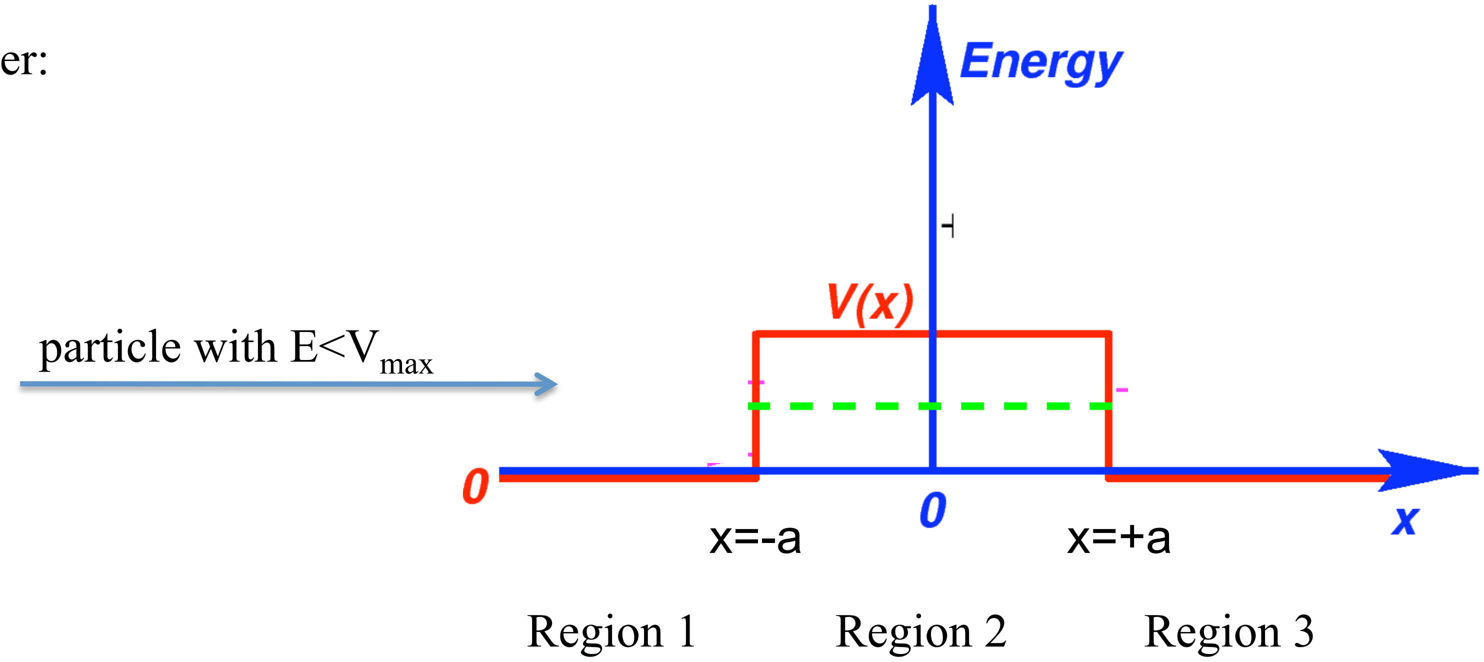
So $\psi_{\text{general, time-indep, free particle}} = Ae^{ikx} + Be^{-ikx}$.

To get the time-dependent solution, just multiply by $e^{-iEt/\hbar}$:

$\psi_{\text{general, free particle}} = (Ae^{ikx} + Be^{-ikx})e^{-iEt/\hbar}$.

VI. Solving the Time-independent Schroedinger Equation for a Barrier Potential

Consider:



The procedure to solve this:

(a) Solve the Time-indep Schroedinger Eq separately in each of the 3 regions.

(b) Incorporate initial conditions.

(c) Make sure that 3 solutions join smoothly at boundaries between regions (this is the continuity requirement on ψ and dψ/dx).

(d) Normalize the final ψ over the full range $-\infty < x < +\infty$.

Notes	**Region 1**	**Region 2**	**Region 3**
	$V = 0$	$V = V_0$	$V = 0$
Time-indep Schr Eq becomes:	$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$	$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = (E - V_0)\psi$	$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$
Solution to Schr Eq is:	$\psi_{\text{Reg 1}} = Ae^{ik_1x} + Be^{-ik_1x}$	$\psi_{\text{Reg 2}} = Fe^{ik_2x} + Ge^{-ik_2x}$	$\psi_{\text{Reg 3}} = Ce^{ik_1x} + De^{-ik_1x}$
where	$k_1 = \frac{\sqrt{2mE}}{\hbar}$	$k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$	k same as in Region 1

Focus on the meaning of $$k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

Notice we are considering the case where E <V_0, so (E-V_0) is a negative number, so this √ is intrinsically imaginary. To show the imaginary nature explicitly, write

$$k_2 = \frac{\sqrt{2m(-1)(V_0 - E)}}{\hbar} \quad = i\underbrace{\frac{\sqrt{2m(V_0 - E)}}{\hbar}}_{\downarrow}$$

call this K_2, so $k_2 = iK_2$

This means that in Region 2, the ψ components are real decaying exponentials, e.g.

$$Fe^{ik_2x} = Fe^{i(iK_2)x} = Fe^{-K_2x}$$

Now apply initial conditions:

Assume incident wave comes from the left: this is Ae^{ik_1x}.
It can reflect at the x=-a boundary, so in Region 1 there can also be a leftward-going wave: this is Be^{-ik_1x}.

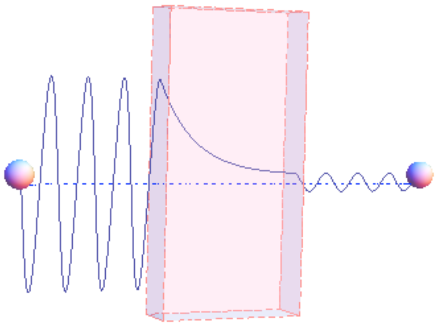
The wave can be transmitted through the x=-a boundary (Fe^{ik_2x}),
then reflected at the x=+a boundary (Ge^{-ik_2x}). So in Region 2 there are both leftward and rightward going waves.

Transmit rightward through the x=a boundary into Region 3 (Ce^{ik_1x}).

In Region 3 there is no way to develop a leftward-traveling wave since there is no boundary to cause reflection there. So $D = 0$.

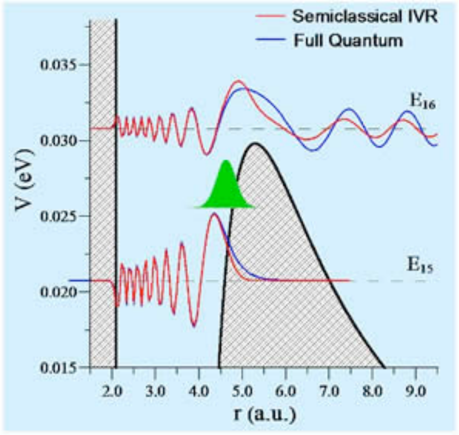
Boundary Condition #	implies
$1:\ \psi$ is continuous at x = -a	$Ae^{ik_1(-a)}+Be^{-ik_1(-a)}=Fe^{ik_2(-a)}+Ge^{-ik_2(-a)}$
$2:\ \dfrac{\partial\psi}{\partial x}$ is continuous at x = -a	$ik_1Ae^{ik_1(-a)}-ik_2Be^{-ik_1(-a)}=ik_2Fe^{ik_2(-a)}-ik_2Ge^{-ik_2(-a)}$
$3:\ \psi$ is continuous at x = +a	$Fe^{ik_2(a)}+Ge^{-ik_2(a)}=Ce^{ik_1(a)}$ (Remember $D=0$.)
$4:\ \dfrac{\partial\psi}{\partial x}$ is continuous at x = +a	$ik_2Fe^{ik_2(a)}-ik_2Ge^{-ik_2(a)}=ik_1Ce^{ik_1(a)}$

We have 4 equations and 5 unknowns (A, B, C, F, and G).
Solve for B, C, F, and G in terms of A.
Then get A by normalizing.
This produces the complete wavefunction. What it looks like:



←wave with E<V_0 decays inside the barrier

wave with E>V_0 is amplified above the barrier→



Outline

I. Reflection and Transmission Coefficients
II. The response of a particle to being trapped in a square well potential
III. Energy of a particle trapped in a square well

I. Reflection and transmission coefficients

Consider 2 questions:

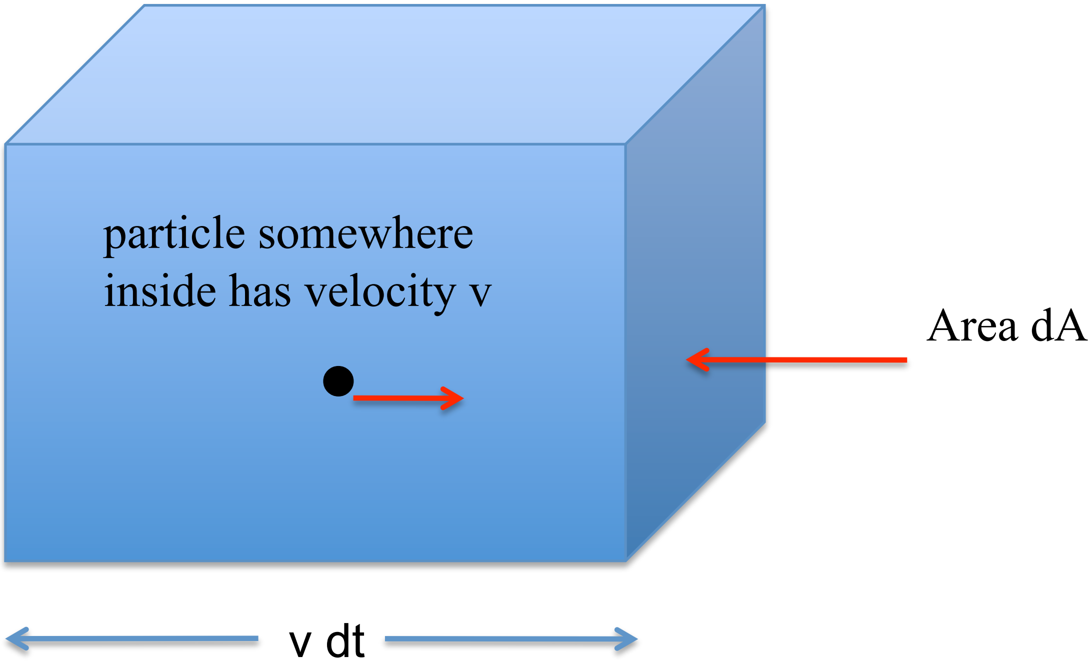
1. What is the probability that the original particle is transmitted past any particular boundary?

2. What is the probability that it is reflected at any particular boundary?

Recall probability density $\rho(x,t) = \psi^*\psi$.
This is the probability per location x and time t; i.e., the probability that the particle is located AT point x if one tries to observe it at time t.
Now suppose the particle has velocity v, and you want to know its

"probability flux": probability density PER SECOND that the particle crosses location x, heading in a particular direction.

Consider a volume:



Choose the orientation of the volume so the particle is moving parallel to the edge "v dt".

If the particle is somewhere in the box at t = 0, and has velocity v, then by the time dt, the particle is guaranteed to have crossed through dA. The probability that this will happen is (Probability per unit volune that particle is in box) × (Volume of box)

$$(\psi^*\psi) \qquad \times (v\ dt\ dA)$$

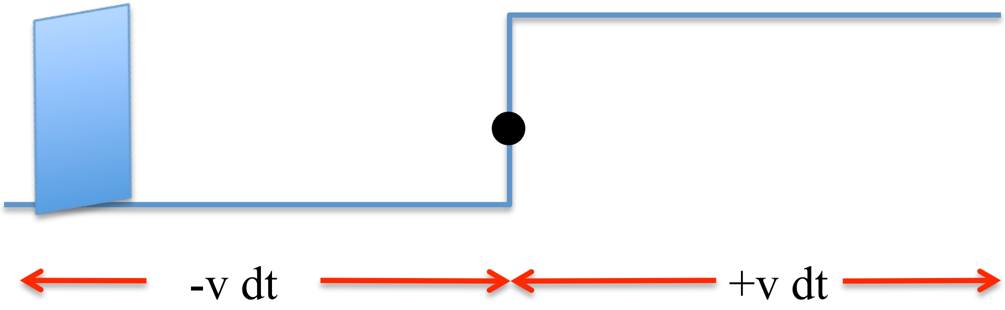
So the probability of crossing dA during dt per unit volume per unit area is

$$\text{Probability Flux} \quad = \psi^*\psi\ v.$$

Now consider a specific particle of velocity =v, approaching step potential V. It passes through dA on its way there:

Define the probability of an initial pass through dA as P(I), "probability of incidence upon the step".

At the moment when it reaches x=-a, there is
some probability that it reflects P(R) and some probability that it is transmitted P(T).
If it reflects, then some time later it will pass through dA at x=-vdt, traveling leftward.
If it is transmitted, then some time later it will pass through dA at x=+vt, traveling rightward.



Define Reflection Coefficient $\equiv \dfrac{P(R)}{P(I)} \equiv "R^2" = \dfrac{\psi^*_{reflected}\psi_{reflected}v_{reflected}}{\psi^*_{incident}\psi_{incident}v_{incident}}$

To substitute into this, recall 2 things:

(1) In the region $x < \text{-}a,\ \psi = \underbrace{Ae^{ik_1x}} + \underbrace{Be^{-ik_1x}}$

leftward-going reflected particle = $\psi_{\text{reflected}}$

rightward-going incident particle = ψ_{incident}

(2) $mv = p = \hbar k$, so $v = \hbar k/m$

$$\left.\begin{aligned} k_{refleced} &= k_1,\ \text{so v}_{\text{reflected}} = \hbar k_1 / m \\ k_{incident} &= k_1,\ \text{so v}_{\text{incident}} = \hbar k_1 / m \end{aligned}\right\}\ \text{these are equal.}$$

Now substitute to get:

$$\text{R}^2 = \frac{B*e^{+ik_1x}Be^{-ik_1x}\dfrac{\hbar k_1}{m}}{A*e^{ik_1x}Ae^{-ik_1x}\dfrac{\hbar k_1}{m}} = \frac{B*B}{A*A}$$

We can similarly define

$$\mathrm{T}^2 \equiv \frac{\psi^*_{transmitted}\psi_{transmitted}v_{transmitted}}{\psi^*_{incident}\psi_{incident}v_{incident}}$$

Notice for transmission from Region 1 to Region 2,

$$\left.\begin{aligned} v_{transmitted} &= \frac{\hbar k_2}{m} \\ v_{incident} &= \frac{\hbar k_1}{m} \end{aligned}\right\} \text{they do NOT cancel}$$

However from Region 1 to Region 3, $\mathrm{v}_{\mathrm{inc}} = v_{trans} = \hbar k_1 / m$

Substituting all of the above into T^2 for transmission from Region 1 to Region 3 yields

$$\mathrm{T}^2 = \frac{(2k_1K_2)^2}{(k_1^2 + K_2^2)^2 \sinh^2 2K_2a + (2k_1K_2)^2}.$$

The fact that this is nonzero even when E < V_0 is called "tunneling."

Recall $\sinh x = \dfrac{e^{x} - e^{-x}}{2}$.

Consider the case where $\underbrace{\mathrm{V}_0 - E}_{\downarrow} >> 0$ (particle is far below the height of the barrier)

$\mathrm{K}_2 \quad >> 0$

AND $\quad$ a>>0 $\quad$ (barrier is very wide)

Then $\sinh\ 2K_2 a = \dfrac{e^{2K_2 a} - e^{-2K_2 a}}{2} \to \dfrac{e^{2K_2 a}}{2}$

so $\sinh^2 2K_2 a \to \dfrac{e^{4K_2 a}}{4}$

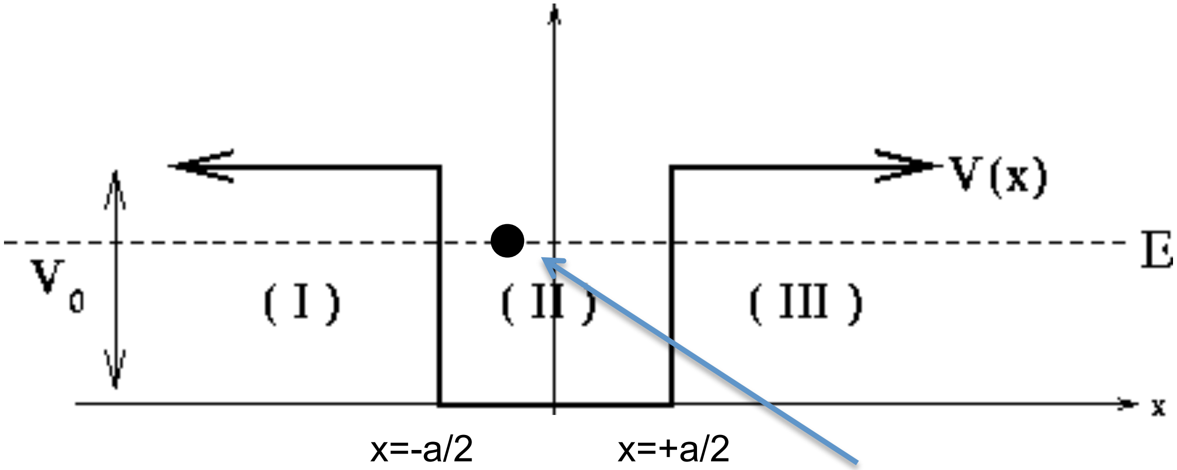
Then $$T^2 \to \frac{(2k_1 K_2)^2}{(k_1^2 + K_2^2)\dfrac{e^{4K_2 a}}{4} + (2k_1 K_2)^2} \to \frac{1}{\left[\dfrac{k_1^2 + K_2^2}{(2k_1 K_2)^2}\right]\dfrac{e^{4K_2 a}}{4} + \cancel{1}} \approx e^{-4K_2 a}$$

neglect

Since exp is a rapidly varying function, transmission depends sensitively on the magnitudes of $(\mathrm{V}_0 - E)$ and a. This fact is useful in designing electronic devices.

II. The response of a particle to being trapped in a square well potential

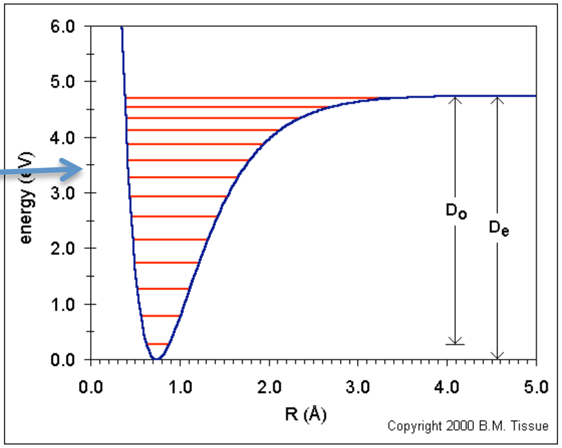
Consider:



a particle with energy $E<V_0$ is in the well.

How did the particle get in there in the first place, if $E<V_0$?

This is an approximation to the situation of a proton bound in a nucleus or an electron bound in an atom. (They are not really square.)



Perhaps before it was bound (i.e., trapped down in the well), it was in the vicinity of $–a/2<x<+a/2$, had $E>V_0$, then lost some energy ("gave up binding energy")/

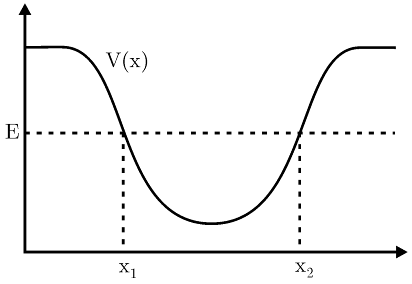
Goal for this section:

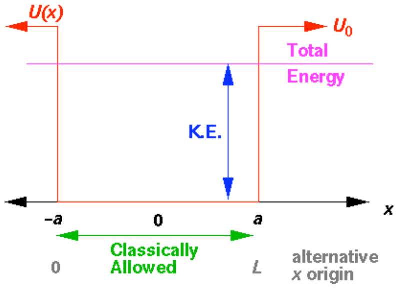
(1) Find the ψ of the particle. Remember: once we know ψ, we know everything it is possible to know about the particle in this situation. Everything is encoded in ψ.
(2) Learn that if a potential has a shape that can bind a particle, then the particle can NOT have arbitrary energy.

restrict it to a limited region

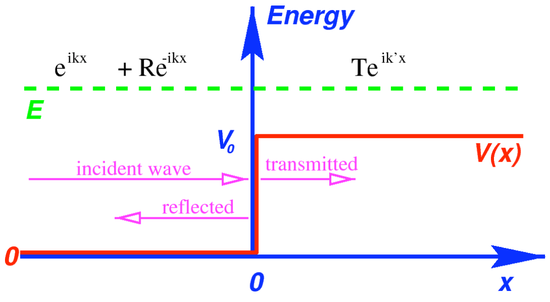
The particle must have an energy selected from a limited set of allowed energies.

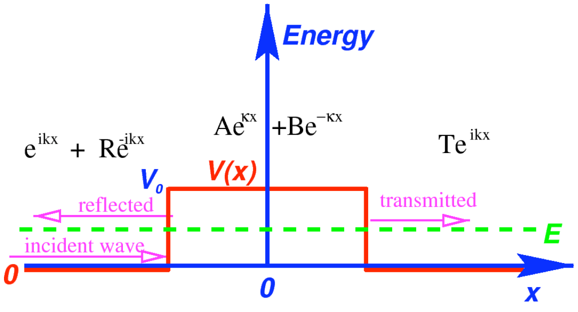
Examples of potentials that can bind particles:



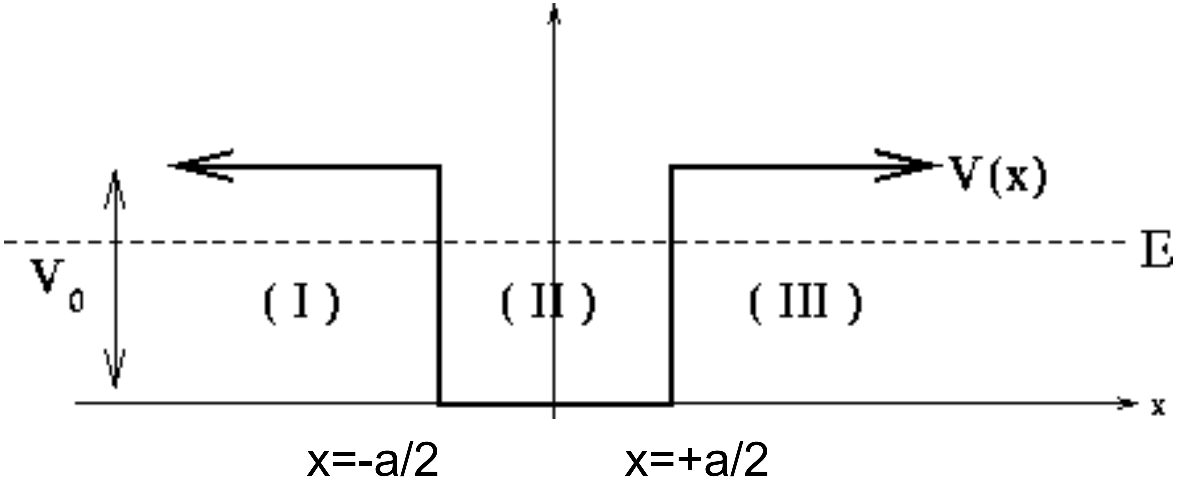


Examples of potentials that do NOT bind particles:





The method to find ψ...



...is almost identical to the method for the Barrier Potential:

(a) Write the Schroedinger Equation for each region
(b) Solve the Schroedinger Equation for each region
(c) Match ψ's at boundaries to find A, B, C, D, etc.

The discovery we will make is that energy E of the particle cannot be arbitrary. It has to be treated like A, B, C etc. That is: only particular values of E will allow ψ to satisfy the boundary conditions.

Notes	**Region 1**	**Region 2**	**Region 3**
	$V = V_0$	$V = 0$	$V = V_0$
Time-indep Schr Eq becomes:	$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi_0 = E\psi$	$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$	$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V_0\psi = E\psi$
Solution to Schr Eq is:	$\psi_{\text{Reg 1}} = De^{ik_2 x} + Ce^{-ik_2 x}$	$\psi_{\text{Reg 2}} = He^{ik_1 x} + Je^{-ik_1 x}$	$\psi_{\text{Reg 3}} = Ge^{ik_2 x} + Fe^{-ik_2 x}$
where	$k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$	$k_2 = \frac{\sqrt{2mE}}{\hbar}$	k_2 same as in Region 1

Recall (Goswami, Appendix F):

$e^{\pm ikx} = \cos kx \pm i \sin kx$

So $\psi_{\text{Region 2}} = H\cos k_1 x + iH\sin k_1 x + J\cos k_1 x - iJ\sin k_1 x$

$$= \underbrace{(H+J)}_{\substack{\downarrow \\ \text{call this "}B\text{"}}}\cos k_1 x + \underbrace{i(H-J)}_{\substack{\downarrow \\ \text{call this "}A\text{"}}}\sin k_1 x$$

So we can rewrite $\psi_{\text{Region 2}}$ as

$\psi_2 = A\sin k_1 x + B\cos k_1 x$

Also as previously, k_2 is intrinsically imaginary so define the real number K_2 such that $k_2 = iK_2$.

$$\text{Then}: \ \psi_1 = De^{-K_2x} + Ce^{+K_2x}$$

$$\psi_3 = Ge^{-K_2x} + Fe^{+K_2x}$$

Now apply boundary conditions

(1) Initial conditions. Whereas for the barrier potential we might say "particle is travelling rightward", here the particle is bound: not traveling.

(2) ψ must be finite everywhere. This was true automatically for previous shapes of V so we did not explicitly consider it. Her we have to enforce it.

To guarantee ψ finite as x ➔ -∞, D must =0.

To guarantee ψ finite as x ➔ +∞, F must =0.

(3) ψ continous at x=-a/2➔

$$A\sin\left[k_1\left(\frac{-a}{2}\right)\right] + B\cos\left[k_1\left(\frac{-a}{2}\right)\right] = Ce^{K_2\left(\frac{-a}{2}\right)}$$

Use $\sin(\text{-}x) = \text{-}\sin x$ and $\cos(\text{-}x) = \cos x$

$$A\sin\left(\frac{k_1a}{2}\right) + B\cos\left(\frac{k_1a}{2}\right) = Ce^{\frac{-K_2a}{2}}$$

"Eq. 1"

(4) $\dfrac{\partial\psi}{\partial \mathrm{x}}$ is continuous at x = -a / 2 $\Rightarrow$

$$Ak_1\cos\left[k_1\left(\frac{-a}{2}\right)\right]+Bk_1\left\{-\sin\left[k_1\left(\frac{-a}{2}\right)\right]\right\}=CK_2e^{K_2\left(\frac{-a}{2}\right)}$$

$$Ak_1\cos\frac{k_1a}{2}+Bk_1\sin\frac{k_1a}{2}=CK_2e^{\frac{-K_2a}{2}} \qquad \text{"Eq. 2"}$$

(5) ψ is continuous at x=+a/2 $\Rightarrow$

$$A\sin\frac{k_1a}{2}+B\cos\frac{k_1a}{2}=Ge^{\frac{-K_2a}{2}} \qquad \text{"Eq. 3"}$$

(6) $\dfrac{\partial\psi}{\partial \mathrm{x}}$ is continuous at x=+a/2 $\Rightarrow$

$$Ak_1\cos\frac{k_1a}{2}+Bk_1\left\{-\sin\frac{k_1a}{2}\right\}=G(-K_2)e^{-K_2\left(\frac{a}{2}\right)}$$

$$Ak_1\cos\frac{k_1a}{2}-Bk_1\sin\frac{k_1a}{2}=-GK_2e^{\frac{-K_2a}{2}} \qquad \text{"Eq. 4"}$$

We have 4 equations and 4 unknowns (A, B, C, G).

We could solve for the unknowns immediately, however it is easier to convert the equations to a different form:

Subtract Eq 3 - Eq 1 to get:

$$2A\sin\frac{k_1 a}{2} = (G-C)e^{-\frac{K_2 a}{2}} \qquad \text{Eq. 5}$$

Add Eq 1 + Eq 3 to get

$$2B\cos\frac{k_1 a}{2} = (G+C)e^{-\frac{K_2 a}{2}} \qquad \text{Eq. 6}$$

Subtract Eq 2-Eq 4 to get:

$$2Bk_1\sin\frac{k_1 a}{2} = (G+C)K_2 e^{-\frac{K_2 a}{2}} \qquad \text{Eq. 7}$$

Add Eq 2 + Eq 4 to get:

$$2Ak_1\cos\frac{k_1 a}{2} = -(G-C)K_2 e^{-\frac{K_2 a}{2}} \qquad \text{Eq. 8}$$

(Still 4 independent equations, "Eqs. 5, 6, 7, and 8", for 4 unknowns.

Consider 2 possibilities:

Possibility #1

If B $\neq 0$ and (G + C) $\neq 0$

then it is permitted to divide $\frac{\text{Eq 7}}{\text{Eq 6}}$ which leads to

$$\frac{2Bk_1 \sin\frac{k_1 a}{2}}{2B\cos\frac{k_1 a}{2}} = \frac{(G+C)K_2 e^{-K_2 a/2}}{(G+C)e^{-K_2 a/2}} \text{ which leads to}$$

$$k_1 \tan\frac{k_1 a}{2} = K_2$$

Note, we do not care what values A and (G - C) have.

They could be zero.

Possibility #2

If A $\neq 0$ and (G - C) $\neq 0$

then it is permitted to divide $\frac{\text{Eq 8}}{\text{Eq 5}}$ which leads to

$$\frac{2\mathrm{A}\mathrm{k}_1 \cos\frac{k_1 a}{2}}{2A\sin\frac{k_1 a}{2}} = \frac{-(G-C)K_2 e^{-K_2 a/2}}{(G-C)e^{-K_2 a/2}} \text{ which leads to}$$

$$\mathrm{k}_1 \cot\frac{k_1 a}{2} = -K_2$$

Note, we do not care what values B and (G + C) have.

They could be zero.

For a given k_1, a, and K_2, it is mathematically impossible to have both relations simultaneously true. So we continue to treat them separately:

Possibility #1 ("Class 1")

Defined by: (1) A and $(G - C)$ can be anything;

so pick the simplest option: $A = G - C = 0$, and

(2) $k_1 \tan \frac{k_1 a}{2} = K_2$

Possibility #2 ("Class 2")

Defined by: (1) B and $(G + C)$ can be anything;

so pick the simplest option: $B = G + C = 0$, and

(2) $k_1 \cot \frac{k_1 a}{2} = -K_2$

- - - - - - - - - - - - - - Our goal: to use these conditions to relate A, C, and G to B -

If A = 0, then Eq 3 becomes:

$$\mathrm{B}\cos\frac{\mathrm{k}_1 a}{2} = Ge^{-K_2 a/2}, \text{ so}$$

$$\mathrm{G} = \mathrm{B}\cos\frac{\mathrm{k}_1 a}{2} e^{+K_2 a/2}$$

If G - C = 0, C = G, so

$$\mathrm{C} = \mathrm{B}\cos\frac{\mathrm{k}_1 a}{2} = Ge^{-K_2 a/2}$$

If B = 0, then Eq 3 becomes:

$$\mathrm{A}\sin\frac{\mathrm{k}_1 a}{2} = Ge^{-K_2 a/2}, \text{ so}$$

$$\mathrm{G} = \mathrm{A}\sin\frac{\mathrm{k}_1 a}{2} e^{+K_2 a/2}$$

If G + C = 0, C = -G, so

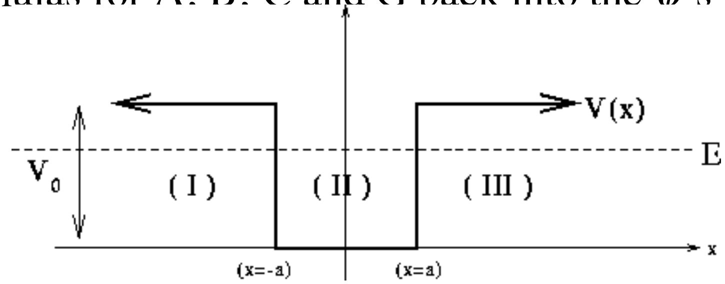
$$\mathrm{C} = -\mathrm{A}\sin\frac{\mathrm{k}_1 a}{2} = Ge^{-K_2 a/2}$$

- - - - - - - - - - - - - - - Now substitute these formulas for A, B, C and G back into the ψ's - - - - - - - - - - - - - - -

Recall $\psi_{\text{Region 1}} = Ce^{+K_2 x}$

$$\psi_{\text{Region 2}} = A\sin k_1 x + B\cos k_1 x$$

$$\psi_{\text{Region 3}} = Ge^{-K_2 x}$$



Class 1

$$\psi_1 = B\cos\frac{k_1 a}{2}e^{+K_2 a/2}e^{+K_2 x}$$

$$\psi_2 = B\cos k_1 x$$

$$\psi_3 = B\cos\frac{k_1 a}{2}e^{-K_2 a/2}e^{-K_2 x}$$

Class 2

$$\psi_1 = -A\sin\frac{k_1 a}{2}e^{+K_2 a/2}e^{+K_2 x}$$

$$\psi_2 = A\sin k_1 x$$

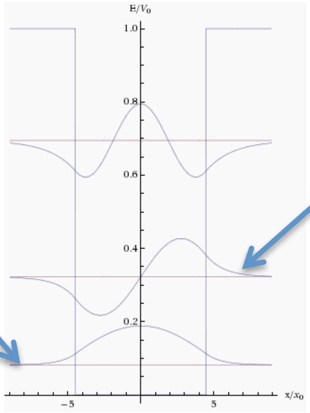
$$\psi_3 = A\sin\frac{k_1 a}{2}e^{+K_2 a/2}e^{-K_2 x}$$

- - - - - - - - The last step is to normalize to get A and B. We do not show that here.- - - - - - - - - -

Some important points:

(1) Terms that do not include "x" (such as $B\cos\frac{k_1 a}{2}e^{-K_2 a/2}$) are just complicated normalization coefficients. They are not variables once a and K_2 ($\propto m, E, V_0$) are known. Ignoring these terms, the structure of the ψ's is:

$$\left.\begin{array}{l}\psi_1 \sim e^{+K_2 x}\\ \psi_2 \sim \cos k_1 x\\ \psi_3 \sim e^{-K_2 x}\end{array}\right\}$$



$$\left\{\begin{array}{l}\psi_1 \sim -e^{+K_2 x}\\ \psi_2 \sim \sin k_1 x\\ \psi_3 \sim e^{-K_2 x}\end{array}\right.$$

(2) The exponentials in Regions 1 and 3 are like those in the barrier potential.

(3) In Region 2, the ψ can be either cos or sine. So the full time-dependent wave functions are

Class 1	Class 2
$\Psi_2 \sim \cos(k_1 x)e^{-iEt/\hbar}$	$\Psi_2 \sim \sin(k_1 x)e^{-iEt/\hbar}$

Notice: as t changes, x does not need to change to preserve the cosine or sine waveform---

so both cases are **standing waves:** the particle is trapped in the well, not traveling.

III. Energy of a particle trapped in a square well

The message of this section is:

A particle in a well cannot have any arbitrary energy. To satisfy all the boundary conditions, only certain energies are allowed.

How to find the allowed energies:

Recall that there are 2 classes of wavefunctions ψ supported by the square well. Each has its own relationship between k_1 and K_2:

Class 1

$$k_1 \tan\frac{k_1 a}{2} = K_2$$

Class 2

$$k_1 \cot\frac{k_1 a}{2} = -K_2$$

where:

$$k_1 \equiv \frac{\sqrt{2mE}}{\hbar} \quad \text{and} \quad K_2 \equiv \frac{\sqrt{2m(V_0 - E)}}{\hbar}.$$

Substitute for k_1 and K_2 and solve for E :

Class 1 (The Class 2 solutions will be computed as homework.)

$$\frac{\sqrt{2\mathrm{mE}}}{\hbar}\tan\left(\frac{a}{2}\frac{\sqrt{2mE}}{\hbar}\right)=\frac{\sqrt{2m(V_0-E)}}{\hbar}$$

Multiply through by $\frac{\mathrm{a}}{2}$:

$$\frac{a}{2}\frac{\sqrt{2\mathrm{mE}}}{\hbar}\tan\left(\frac{a}{2}\frac{\sqrt{2mE}}{\hbar}\right)=\frac{a}{2}\frac{\sqrt{2m(V_0-E)}}{\hbar}$$

$$\sqrt{\frac{mEa^2}{2\hbar^2}}\tan\left(\sqrt{\frac{mEa^2}{2\hbar^2}}\right)=\sqrt{\frac{mV_0a^2}{2\hbar^2}-\frac{mEa^2}{2\hbar^2}}$$

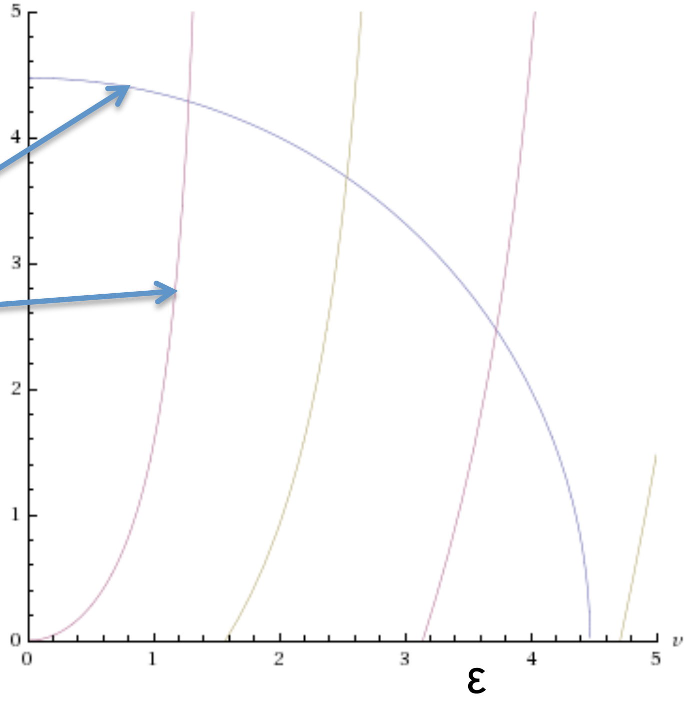
Define $\varepsilon\equiv\sqrt{\frac{mEa^2}{2\hbar^2}}$

$$\underbrace{\varepsilon\cdot\tan\varepsilon}_{\downarrow}=\underbrace{\sqrt{\frac{mV_0a^2}{2\hbar^2}-\varepsilon^2}}_{\downarrow}$$

Call this "p(ε)"

Call this "q(ε)"

Graph both p and q on the same plot, versus ε:



The meaning of the graph is: the points where the curves cross are the only values of ε for which $\mathrm{p}(\varepsilon) = \mathrm{q}(\varepsilon)$. That is, these are the only cases for which $k_1 \tan\frac{k_1 a}{2} = K_2$.

But $\varepsilon \equiv \sqrt{\frac{mEa^2}{2\hbar^2}}$, so $\mathrm{E} = \frac{2\hbar^2\varepsilon^2}{ma^2}$.

The only E's that this well permits, are the ones corresponding to the ε's at the intersections.

The "bottom line" in this example, the particle in the well can have one of only 3 possible energies (there are 3 intersection points). If you try to give it some energy other than those, it will not absorb it.

What is important about this energy result:
1.) A particle in a well cannot have arbitrary energy. It has a limited set of options.

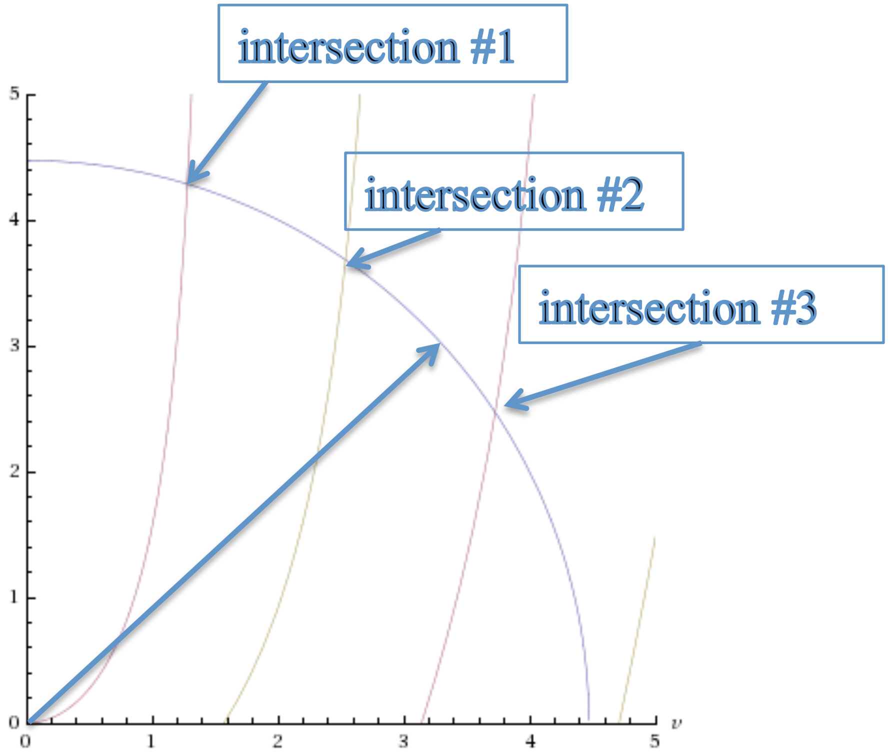
This well is a rough approximation to the nuclear potential that binds protons in a nucleus or the Coulomb potential that binds electrons in an atom.   So these permitted energies correspond to the allowed energy shells in which electrons. (Protons in the nucleus are restricted to shells too.)

2.) Consider the radius of the quarter-circle that is the graph of q(ε) versus ε.
The larger that radius is, the more intersections there will be: that is, the more allowed energy solutions that exist.

The radius length is given by

$$\sqrt{\frac{mV_0a^2}{2\hbar^2}}$$

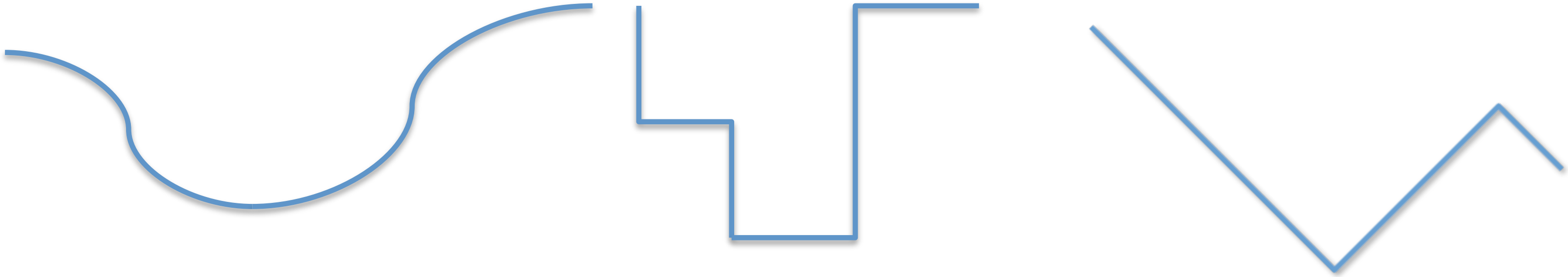
so larger a (well width) or larger V_0 (well depth) both produce more allowed energies.


intersection #1

intersection #2

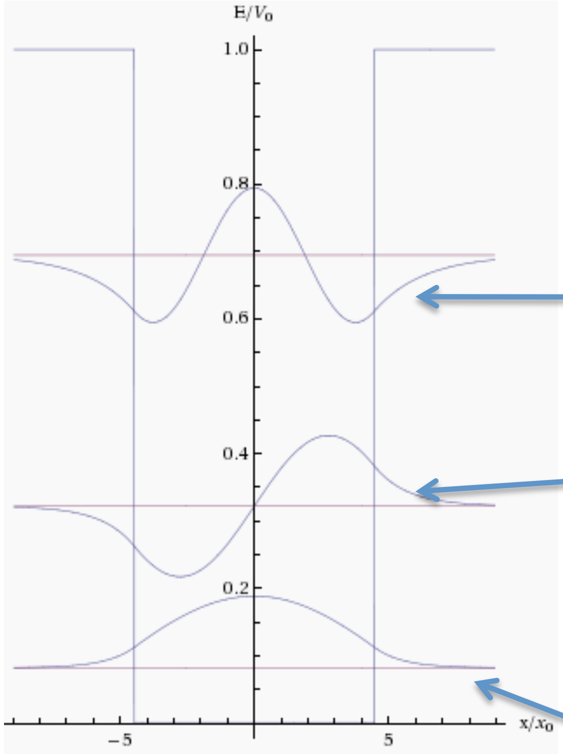
intersection #3

3.) The ability of the potential to limit the allowed energies of the particle is not unique to the square well. It is a property of any potential that binds a particle (i.e. limits it to a specific region of space). So we would get a limited set of allowed energies for potentials shaped like:



4.) The fact that the set of allowed energies is limited and that a particle cannot ramp up or down its energy in transitioning from one energy level to another is called "energy quantization."

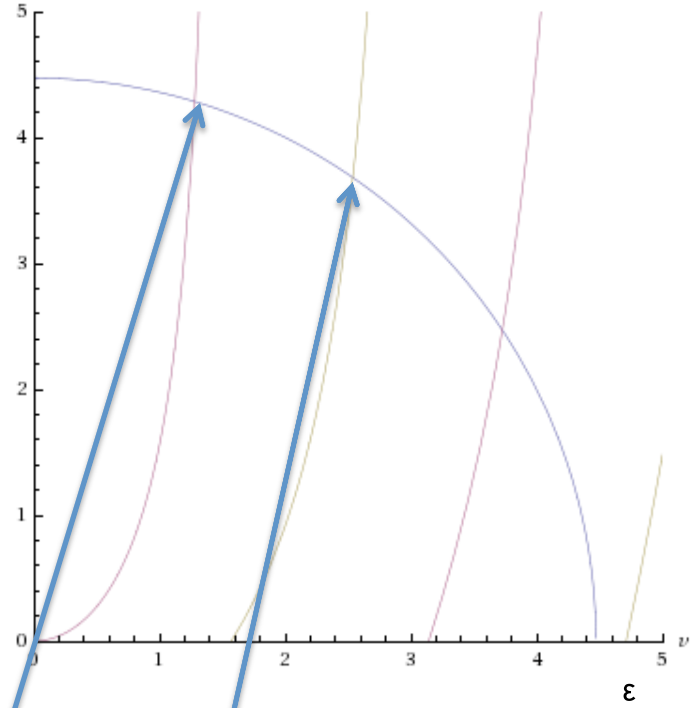
5.) There is a one-to-one association between allowed ψ's and allowed E's. Consider Class 1 (cosine) solutions only:



Class 1 E2, 3/2 cycle, etc.

next higher energy “Class 2 E1” is 1 cycle

lowest energy “Class 1 E1” is ½ cycle of cosine.



The Class 1 E’s come from here, where

ε_1 leads to Class 1 $E_1 = \dfrac{2\hbar^2\varepsilon_1}{ma^2}$

ε_2 leads to Class 1 $E_2 = \dfrac{2\hbar^2\varepsilon_2}{ma^2}$

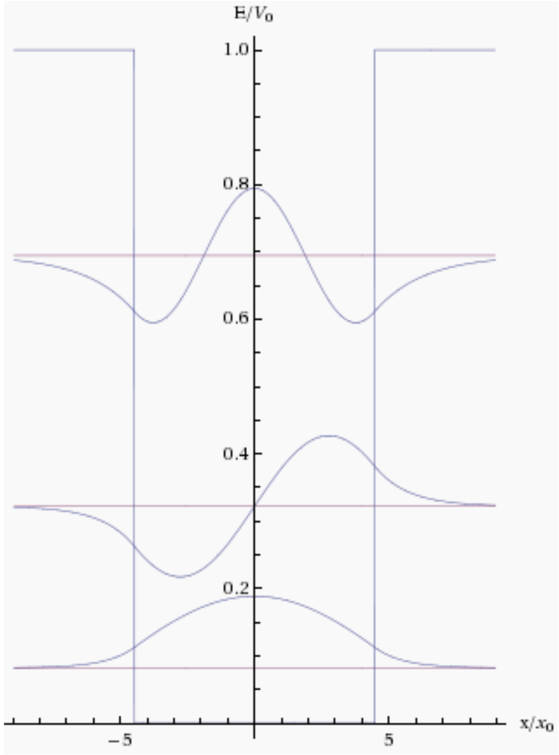
Notice higher energy goes with more cycles. This is reasonable as more cycles means higher frequency, and we know that E=hν.

Recall each ψ is called an eigenfunction of the Hamiltonian. The E that goes with it is called its eigenvalue or "eigenenergy."

6.) Recall we only plotted Class 1. We must not forget Class 2 solutions---these are defined by

$$k_1 \cot \frac{k_1 a}{2} = -K_2$$

The E's for Class 2 solutions are different from the E's for Class 1 solutions and interspersed with them:



Class 1 cosine

Class 2 sine

Class 1 cosine