Solutions of the 1D Time-Indep. Schr. Eq'n

Now we're going to actually solve the time-indep. Schrödinger eq'n for some specific potentials, sticking to one space dimension for the time being.

We'll be systematic, starting with potentials that don't have bound states, then moving on to ones that do. Typically we'll have the potential defined in various regions in x, and we'll have to find sol'ns for ψ in each region, then match them up at the boundaries.

Comment re/ differential eq'ns: Note that the time-indep. S.E. is a 2nd-order ordinary diff. eq'n. It's solution therefore has 2 arbitrary constants (mathematically, that's because in principle you have to integrate twice to get a sol'n, generating two constants of integration). The conditions on ψ, viz

$$\psi, \frac{d\psi}{dx} \quad \text{finite, continuous, single-valued}$$

$$\text{and} \quad \int_{\text{all } x} \psi^* \psi \, dx = 1$$

will determine the constants.

We'll start by considering the sol'ns for constant potential, and we'll get the behavior we talked about in the previous chapter.

Constant potential : $V = V_0$ General sol'n

We'll look at 3 cases:

i) $V = 0$

ii) $V = V_0, \quad E > V_0$

iii) $V = V_0, \quad E < V_0$

$\boxed{i)\ V=0}$ is just a free particle. It has wave fn

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

and ψ satisfies

$$\left.-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi\right\}$$

Now, we know that a plane wave sol'n exists with $\quad \Psi = Ae^{i(kx-\omega t)} \quad$ where $\omega = E/\hbar$

That means $\psi = Ae^{ikx} \quad$ & $\quad \frac{d\psi}{dx} = Aik\,e^{ikx} = ik\psi$

& $\frac{d^2\psi}{dx^2} = -k^2\psi$

So $\quad \frac{\hbar^2}{2m}k^2 = E \quad$ & $\quad k = \frac{\sqrt{2mE}}{\hbar} \quad$ & $\quad p = \hbar k$

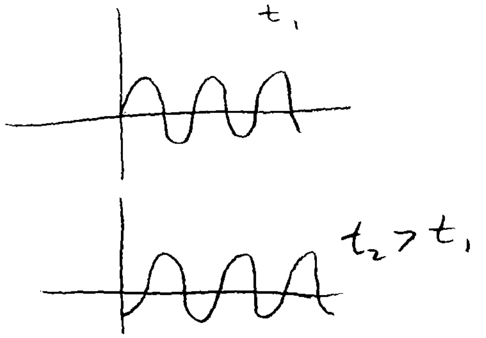
This sol'n $\quad \Psi = Ae^{i(kx-\omega t)} \quad$ is a $\longrightarrow$

traveling wave: the nodes of its real part ($\sim \cos(kx-\omega t)$) appear when

$$(kx-\omega t) = (n+\tfrac{1}{2})\pi, \quad n = \text{any integer}$$

$\Rightarrow \quad k x_{node} = \omega t + (n+\tfrac{1}{2})\pi$

$\Rightarrow$ the nodes move in the direction of increasing x.



$\Rightarrow$ This sol'n is a wave traveling in the $+x$ direction

But wait! When we solved $\frac{\hbar^2 k^2}{2m} = E$ for k, we only took the positive solution. We could also have $-\frac{\sqrt{2mE}}{\hbar}$. Let's define k to be positive, so the sol'n w/ a minus sign looks like

$$\Psi = B e^{i(-kx-\omega t)}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

This sol'n is just as good; physically it's a wave traveling in the $-x$ direction.

We have to conclude, then, that the general (3.4) sol'n is

$V=0, E>V$ $\boxed{\psi(x) = Ae^{ikx} + Be^{-ikx}}$, $\boxed{k = \sqrt{2mE}/\hbar}$

+ they both have the same time dep. $e^{-i\omega t} = e^{-iEt/\hbar}$

So the whole sol'n is

$$\Psi(x,t) = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}$$

and we get two arbitrary constants, as promised.

$\boxed{\text{ii) } V=V_0;\ E>V_0}$ Well, this case is really just like (i) with the energy shifted up. We still have

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

but now

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi$$

but that's just

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E-V_0)\psi$$

which is the <u>same</u> as the <u>free eq'n</u> on p. 3.2 with $E \to E-V_0$. So we expect similar sol'ns

$\psi \sim e^{\pm ikx}$ but with different k. Let's

take $\psi = Ae^{+ikx}$ + find k.

$$\frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{as above, so the S.E. becomes}$$

$$\frac{\hbar^2 k^2}{2m}\psi = (E - V_0)\psi$$

So $\frac{\hbar^2 k^2}{2m} = E - V_0$ or $k = \frac{\sqrt{2m(E-V_0)}}{\hbar}$, & notice

$E - V_0 > 0$ so k is real and everything works okay.

Again, we can have both signs on the square root, so we have

$$\boxed{\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \frac{\sqrt{2m(E-V_0)}}{\hbar}} \qquad E > V_0$$

Now recall that $e^{ikx} = \cos kx + i\sin kx$, so for both i) and ii) we get oscillating solutions, as advertised in the previous chapter for cases where $E > V$.

iii) $V = V_0$, $E < V_0$ This is the classically disallowed region. Classically, we'd have $\psi = 0$ here. But in QM, we can find a sol'n, so

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

and

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \underbrace{(E - V_0)}_{<0}\psi$$

Now the second derivative of ψ has the same sign as ψ itself. What has this behavior?

A real exponential! But suppose we didn't know this? We've already done the math in part ii): Nothing we did there required k to be real. (I commented that it was, but the math didn't care.) So let's just follow through the math, with one difference: let's use $\varkappa$ (= kappa) instead of k for the time being. So try

$$\psi = Ae^{i\varkappa x}$$

& we get $\frac{\hbar^2\varkappa^2}{2m} = E - V_0$ + $\varkappa = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

but $E - V_0 < 0$, so $\varkappa$ is imaginary! Write

$$\varkappa = iK \qquad \text{where } K = \frac{\sqrt{2m(V_0-E)}}{\hbar} \text{ is real.}$$

Then we have

$$\psi = Ae^{i(iK)x} = Ae^{-Kx},$$

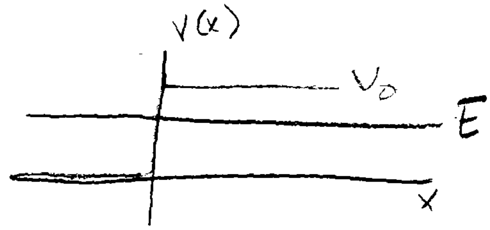
a real exponential. Again we can have both signs in the exponential, so the general sol'n is

$$\boxed{\psi(x) = Ae^{-Kx} + Be^{+Kx}, \quad K = \frac{\sqrt{2m(V_0-E)}}{\hbar}}, \quad E < V_0$$

and we've found a quantum mechanical sol'n in the classically disallowed region. Note that K no longer has the same rel'n to p as for the free particle.

Step potential ($E < V_0$)

Now for our first application. Let's take a step potential:



$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases}$$

and take total energy $E < V_0$, and the particle incident from $x<0$.

Aside: This is of course an idealization: in real life the potential would be continuous. But it's not a bad approximation in many cases.

Classically, what would happen? The particle would come along from $x<0$, hit the barrier, + bounce back, and never have a chance of reaching $x>0$.

Quantum mechanically, we just solve the S. E. and see. In fact we know the general sol'ns; we just have to match them up. So

$x<0$: $\psi(x) = Ae^{ik_1x} + Be^{-ik_1x}$ $\quad k_1 = \frac{\sqrt{2mE}}{\hbar}$

$x>0$: $\psi(x) = Ce^{k_2x} + De^{-k_2x}$ $\quad k_2 = \sqrt{2m(V_0-E)}$

Now we use the conditions on $\psi, \frac{d\psi}{dx}$ to find the constants. ψ is already single-valued, as it will be for most of our examples.

- ψ finite : No problem for $x<0$, but for $x \to +\infty$, $e^{K_2 x}$ blows up, so we must have

$$C = 0$$

- $\frac{d\psi}{dx}$ finite : guaranteed now that $C=0$ (this happens a lot)

- ψ continuous: Applying this at $x=0$:

$$\boxed{A + B = D}$$

- $\frac{d\psi}{dx}$ continuous : Applying this at $x=0$:

$$iK_1 A - iK_1 B = -K_2 D$$

$$\Rightarrow \quad \boxed{A - B = \frac{iK_2}{K_1} D}$$

So we can solve for A & B in terms of D. Adding the boxed eq'ns gives

$$A = \tfrac{1}{2}\left(1 + \frac{iK_2}{K_1}\right) D$$

and subtracting gives

$$B = \tfrac{1}{2}\left(1 - \frac{iK_2}{K_1}\right) D$$

and the sol'n is

$$\psi(x) = \begin{cases} \frac{D}{2}\left(1+\frac{iK_2}{K_1}\right)e^{iK_1 x} + \frac{D}{2}\left(1-\frac{iK_2}{K_1}\right)e^{-iK_1 x} & x > 0 \\ D e^{-K_2 x} & x < 0 \end{cases}$$

Comments

— Now we would find D from the normalization condition, and we'd run into the usual plane wave problem where the integral is infinite. We can fix that with box normalization or another method, but let's not evaluate it at all. Turns out we can get away w/not evaluating it + still extract physics info.

— Look at the form of the wave function for $x < 0$:

$e^{ik_1 x}$ $\Leftrightarrow$ **incident** wave moving to right

$e^{-ik_1 x}$ $\Leftrightarrow$ **reflected** wave moving to left.

We can quantify the extent to which the wave is reflected from the potential, with the reflection and transmission coefficients. In the homework you show that for a plane wave the current density $\vec{J}$ is $\vec{J} = \vec{v}\cdot\psi^*\psi$. (This current density has units of particle/m²/sec + is also known as flux, or probability flux)

Now define

$$R = \text{reflection coefficient} = \frac{|\text{flux of reflected wave}|}{|\text{flux of incident wave}|}$$

$$= \frac{|\vec{J}_{reflected}|}{|\vec{J}_{incident}|}$$

In this example,

$$|\vec{J}|_{incident} = \frac{\hbar k_1}{m} A^* A$$

$$|\vec{J}|_{reflected} = \frac{\hbar k_1}{m} B^* B$$

So $$R = \frac{B^*B}{A^*A} = \frac{\frac{1}{2}\left(1+\frac{ik_2}{k_1}\right)D^* \frac{1}{2}\left(1-\frac{ik_2}{k_1}\right)D}{\frac{1}{2}\left(1-\frac{ik_2}{k_1}\right)D^* \frac{1}{2}\left(1+\frac{ik_2}{k_1}\right)D} = 1$$

Similarly, define

$$T = \text{transmission coefficient} = \frac{|\vec{J}_{transmitted}|}{|\vec{J}_{incident}|}$$

Now transmitted means to $x > 0$, so we have to find the current corresponding to $\psi(x>0.)$ Recall

$$\vec{J} = \frac{\hbar}{2mi}\left[\Psi^* \vec{\nabla}\Psi - (\vec{\nabla}\Psi^*)\Psi\right]$$

Now $\Psi(x>0) = De^{-k_2 x} e^{-iEt/\hbar}$, and since we're in 1D, $\vec{\nabla} \to \hat{x}\frac{d}{dx}$. Now note

$$\Psi^* \vec{\nabla}\Psi - (\vec{\nabla}\Psi^*)\Psi = \hat{x}\underbrace{\left[\psi^* \frac{d\psi}{dx} - \left(\frac{d\psi^*}{dx}\right)\psi\right]}_{-k_2\psi^*\psi + k_2\psi^*\psi = 0!}$$

There is no transmitted current, hence no transmission coefficient:

$$T = 0$$

In fact, it is generally true that

$$T + R = 1$$

and neither T nor R can be bigger than 1 (which just says you can't reflect or transmit more of the wave than you started with).

— Look at the wave function for $x < 0$ again. In the course of calculating R, notice we showed that the magnitudes of A & B are equal, so let's pursue that by writing the exponentials in ψ in terms of sin & cos. From the bottom of p. 3.8,

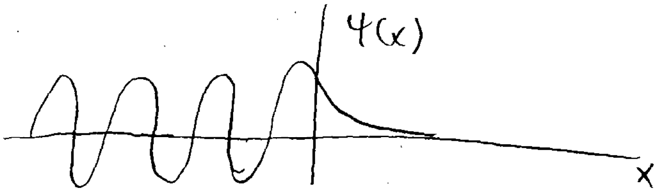
$$\psi(x<0) = \frac{D}{2}\left[\left(1+\frac{ik_2}{k_1}\right)(\cos k_1x + i\sin k_1x) + \left(1-\frac{ik_2}{k_1}\right)(\cos k_1x - i\sin k_1x)\right]$$

$$= \frac{D}{2}\left[2\cos k_1x - 2\frac{k_2}{k_1}\sin k_1x + \cancel{\frac{ik_2}{k_1}\cos k_1x(1-1)}^{\,0}\right]$$

$$= D\cos k_1x - D\frac{k_2}{k_1}\sin k_1x$$

Now mutiply by the time dependence $e^{-iEt/\hbar}$ & note that the locations of the nodes are indep. of time, i.e. we have a standing wave.
This is a general result: two traveling waves in the opposite direction w/ the same magnitude add to give a standing wave.

— What's happening for $x > 0$? The particle has some probability to be found at $x > 0$.



It falls off exponentially. This is called penetration of the classically excluded region. It doesn't happen for classical particles, but it does for classical waves. Penetration distance Δx is when $\psi \to \frac{1}{e}$ of its value at 0, i.e., $k_2 x = 1 \Rightarrow \boxed{\Delta x = \frac{1}{k_2}}$

— Ex. This step potential is actually an okay description for conduction electrons in a block of copper. The electrons are pretty much free inside the block, but the potential is $+V_0 > E$ outside. This keeps the electrons inside the metal. The min. energy to remove the electron (= work function) $\Rightarrow V_0 - E = 4\,eV$. Find dist Δx that electron can penetrate outside block.

well,
$$\Delta x = \frac{1}{k_2} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

$\frac{kg\,m^2}{sec} * \frac{sec}{kg\,m} = m$

$$= \frac{10^{-34}\text{ joule sec}}{\sqrt{2 * 9\times10^{-31}\,kg * 4\,eV * \frac{1.6\times10^{-19}\text{ joule}}{eV}}}$$

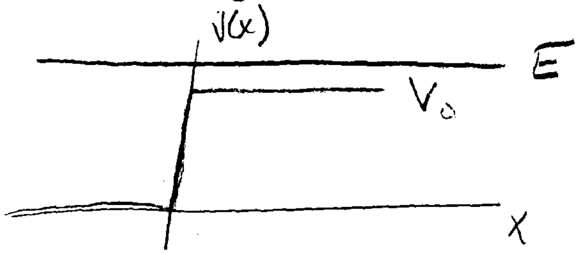
$$\simeq 10^{-10}\,m \sim 1\,\text{Å}$$

$\Rightarrow$ atomic dimensions $\Rightarrow$ it can matter in atomic systems!

— Notice that we found solutions without any restrictions being placed on the energy $\Rightarrow$ any $E > 0$ is allowed and we have a continuum

Step Potential ($E > V_0$)

Now take $E > V_0$ so the particle is allowed everywhere even classically. Assume the particle is incident to the right fr / $x < 0$,



"so we know we have oscillating sol'ns everywhere:

$$x < 0: \quad \psi(x) = A e^{ik_1 x} + B e^{-ik_1 x} \qquad k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$x > 0: \quad \psi(x) = C e^{ik_2 x} + D e^{-ik_2 x} \qquad k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

(Note that the wiggles are faster, i.e. k is bigger, for $x < 0$.)

Classically, the particle would feel a force when it went across the step due to the change in potential, but it would keep going to $x > 0$; none of it would be reflected.

Quantum mechanically, it'll be different, as usual.

Now we use the conditions on the wave function (3.14)
to learn about $A, B, C, + D$.

First, consider the D term in $\psi(x>0)$. It represents a wave traveling to the left (e^{-ik_2x}). But the incident wave is traveling to the right, so the D term would have to be a reflected wave. But there's nothing to reflect from, so there can be no reflected wave, hence we must have

$$D = 0$$

Now we go to continuity of ψ and of $d\psi/dx$.

- ψ continuous at $x = 0$: $\Rightarrow$

$$A + B = C$$

- $\frac{d\psi}{dx}$ continuous at $x=0$ $\Rightarrow$

$$ik_1 A - ik_1 B = ik_2 C$$

or

$$(A-B) = \frac{k_2 C}{k_1}$$

Now the book uses these eq'ns to solve for A (instead of C in analogy w/ the previous case); this will be convenient so we will too.

We get $2A = \left(1+\frac{k_2}{k_1}\right)C$ or

$$C = \left(\frac{2k_1}{k_1+k_2}\right)A$$

and $B = C - A$

$$B = \left(\frac{k_1-k_2}{k_1+k_2}\right)A$$

so the wave function is

$$x<0 \quad \psi(x) = Ae^{ik_1x} + A\left(\frac{k_1-k_2}{k_1+k_2}\right)e^{-ik_1x} \qquad k_1 = \sqrt{2mE}/\hbar$$

$$x>0 \qquad = \frac{2k_1A}{(k_1+k_2)}e^{ik_2x} \qquad k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

Comments

— Again (as in the previous example), we could in principle find A from box normalization, but we don't need to here.

— Again we have, for **$x<0$**, both the incident wave (e^{ik_1x}) and a reflected wave (e^{-ik_1x}). [Classically, there would be no reflected wave – it would just keep going.] For **$x>0$**, we have the transmitted wave (e^{ik_2x}). The reflection and transmission coefficients are

— Notice T & R are symmetric under exchange (3.17)
of $k_1 \leftrightarrow k_2$, i.e., they don't change. That means you'd get the same T & R if the particle was incident from the right. The change in ψ is only ~~because~~ of the discontinuity in V, not the fact that it increases.

We can combine the results of the two steps to find T & R for any value of E. We have

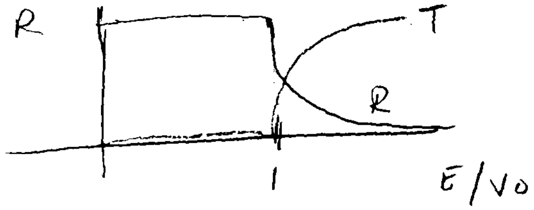
$$R = 1 \qquad E < V_0$$

$$= \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \qquad E > V_0$$

Now, if we substitute for the k's, we find (as you will show in the homework),

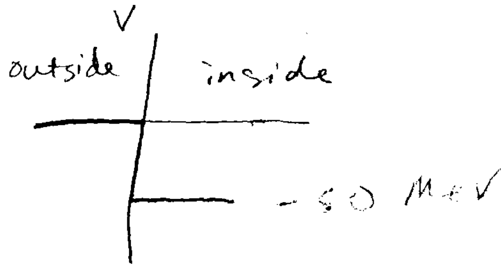
$$R = \left(\frac{1 - \sqrt{1 - V_0/E}}{1 + \sqrt{1 + V_0/E}}\right)^2 \qquad E/V_0 > 1$$

where we've written in terms of the dim'less ratio V_0/E.
Note that we only get $R < 1$ for $E/V_0 > 1$.



& we get T fr/ $T = 1 - R$

Ex A nucleus looks like a step potential to a neutron:



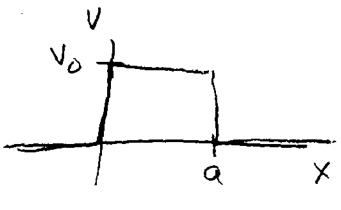
Suppose a neutron has kinetic energy $K = 5$ MeV, typical fr/ fission + is incident on a nucleus. What's the prob. that the neutron'll be reflected instead of going in?

Well, this is just like the step coming fr/ the right, + we can use the same reflection coeff. The step is 50 MeV, and the energy E is 50+5 MeV = 55 MeV

$$\Rightarrow R = \left(\frac{1 - \sqrt{1 - 50/55}}{1 + \sqrt{1 - 50/55}} \right)^2 = 0.29$$

Barrier Potential

Here's where we see real measurable effects of the penetration into the classically forbidden region. Let the potential be



$$V(x) = V_0 \qquad 0 < x < a$$
$$= 0 \qquad x < 0, x > a$$

Classically, if a particle comes in fr/ $x < 0$, if $E > V_0$ it keeps going, and if $E < V_0$ it gets reflected. In QM, both can happen in both regions; in particular, if $E < V_0$ there's some probability the particle gets through.

We know the sol'ns in each region:

$$x<0: \quad \psi(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

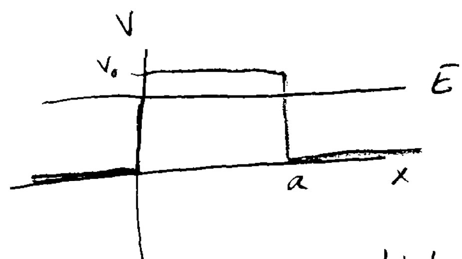
$$x>a \quad \psi(x) = Ce^{ik_1x} + De^{-ik_1x}$$

same k_1 $\qquad k_1 = \frac{\sqrt{2mE}}{\hbar}$

+ if particle is incident fr/ left, we won't have traveling wave going <u>to</u> left for $x>a$, so

$$D=0.$$

Now, for the region $0<x<a$ where the barrier is, we consider two cases:



i. $E<V_0$

This is the one where classically, the particle could never get through. The sol'n here is exponential:

$$0<x<a \quad \psi(x) = Fe^{-k_2x} + Ge^{+k_2x} \qquad k_2 = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

Note that we can't set $G=0$, because x doesn't $\to\infty$ in this region, so the G term doesn't blow up. We have to keep both.

So we require continuity of ψ + $\frac{d\psi}{dx}$ at $x=0$ + $x=a$ + we get relations among the coeff's. When we do this, we find for the transmission coeff

$$T = \frac{v_1 C^* C}{v_1 A^* A} = \left[1 + \frac{\left(e^{k_2 a} + e^{-k_2 a}\right)^2}{16 \frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)} \right]^{-1}$$

$E < V_0$

$$= \left[1 + \frac{\sinh^2 k_2 a}{4 \frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)} \right]^{-1}$$

$$\sinh x = \frac{e^x - e^{-x}}{2}$$

~~Bu~~

Note that T is not 0 — the particle has a finite probability of being found past the barrier! When the particle makes it through, this is called tunneling. We'll discuss some physical examples

ii) $E > V_0$

Now every region is classically accessible, & we have oscillatory sol'ns everywhere. So $x < 0$ & $x > a$ are the same as above (modulo boundary conditions), but for $0 < x < a$:

$$\psi(x) = F e^{ik_3 x} + G e^{-ik_3 x} \qquad k_3 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

Now for the transmission coeff. we get

$$T = \left[1 - \frac{\left(e^{ik_3 a} - e^{-ik_3 a}\right)^2}{16 \frac{E}{V_0}\left(\frac{E}{V_0} - 1\right)} \right]^{-1} = \left[1 + \frac{\sin^2 k_3 a}{4 \frac{E}{V_0}\left(\frac{E}{V_0} - 1\right)} \right]^{-1}$$

Notice that this T has oscillations. Also, for $K_3 a = n\pi$, $T=1$ + there's no reflection. Since K_3 depends on energy, this says that for given combinations of energy + thickness of barrier, the particle is always transmitted with no reflection. This is exactly analogous to reflection of light in thin films — for certain comb. of wave length ($\Leftrightarrow k$) + thickness, all the light gets through.

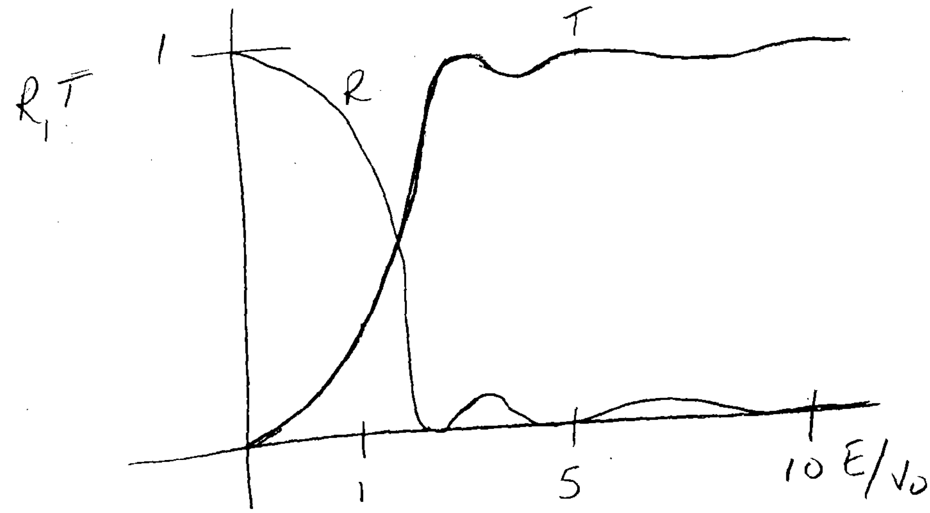
This condition $K_3 a = n\pi$ says that an integral or half-integral no. of deBroglie wavelengths fit in the barrier. When this happens you get destructive interference btwn the reflections at $x=0$ + $x=a$, + all you're left with is the transmitted wave.

We can once again ~~combine~~ the results for $E < V_0$ + $E > V_0$ in terms of E/V_0. Notice that all of the dimensionful stuff, besides $E + V_0$, appears in

$$Ka = \sqrt{\left(\frac{2mV_0 a^2}{\hbar^2}\right)\underbrace{\left(1-\frac{E}{V_0}\right)}_{\text{or } \left(\frac{E}{V_0}-1\right)}}$$

dimless; take it $= 9$

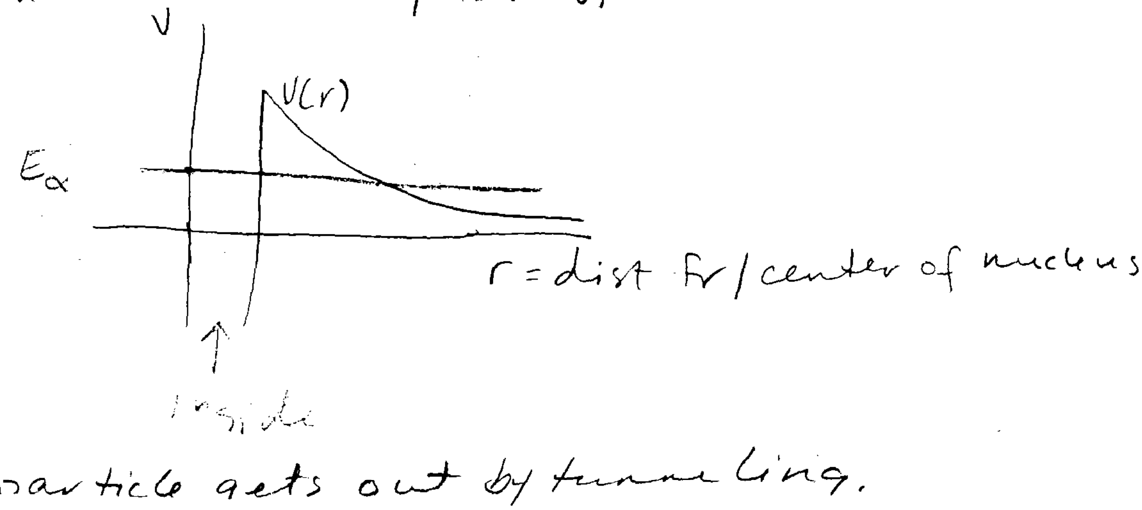
Then



Barrier penetration: Examples

1) Aluminum wires: Join wires by twisting together, but outside of wire reacts w/ air & forms layer of alum. oxide = barrier to electrons. They get through by barrier penetration (layer is thin)

2) α decay of U^{238}: U^{238} can decay radioactively by emitting an α particle. Classically this is forbidden; the potential looks like this, w/ E of the α particle smaller than the peak V.



The α particle gets out by tunneling.

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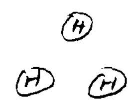
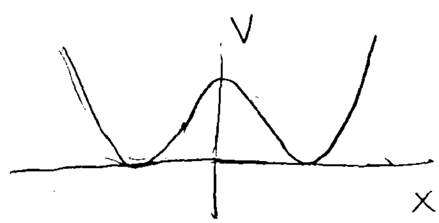
3) NH_3 inversion. The ammonia molecule has two equivalent equilibrium configurations. The 3 H atoms are in a plane, like



Then the N atom can go in the middle either just above or just below the plane of the H's. It can't go in between, though. The potential, as a function of the distance from the plane, looks to the N like



If the N atom starts on one side, it ends up tunneling to the other. In fact, it keeps going back + forth with such regularity (and high frequency — 2×10^{10} Hz in the ground state) that it was used as a standard for the first atomic clocks.

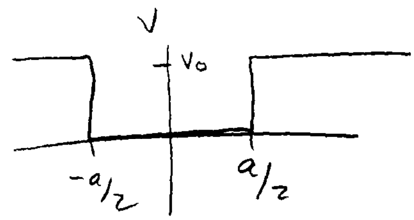
Square Well potential

Now let's flip the barrier upside down: 

Finally, this can give us bound states when $E < V_0$.

Classically it doesn't of course — if you're inside the well, you can have any energy at all. Not so in QM.

So, we have the potential



$$V(x) = \begin{cases} V_0 & x < -a/2,\ x > +a/2 \\ 0 & -a/2 < x < +a/2 \end{cases}$$

K, we'll take $E < V_0$ *

So the sol'n is

$-\frac{a}{2} < x < \frac{a}{2}$ $\quad \psi(x) = A e^{ik_1 x} + B e^{-ik_1 x}$ $\qquad K_1 = \frac{\sqrt{2mE}}{\hbar}$

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

+ we made the switch to sin + cos because the symmetry of the potential tells us the particle is equally likely to be traveling in the +x as the -x direction, which gives standing waves, i.e. straight sines + cosines. It'll turn out to be more convenient to solve the problem this way.

Mathematically, they're completely equivalent, which you can show by writing $A + B$ in terms of $A' + B'$: $\quad A = \frac{A' + B'}{2} \quad B = \frac{B' - A'}{2i}$

* $E > V_0$ is a lot like the barrier case, except the high + low freq. wiggles are in different regions.

$x < -\frac{a}{2}$ $\quad \psi = Ce^{k_2 x} + De^{-k_2 x}$ $\qquad k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

$x > +\frac{a}{2}$ $\quad \psi = Fe^{k_2 x} + Ge^{-k_2 x}$

Now we use finiteness of ψ to get $D = F = 0$
$\Rightarrow$ outside the well, the wave function falls exponentially.

Now we have to match up the values of ψ & $\frac{d\psi}{dx}$ at the edges of the well. That'll give us 4 equations:

$$\psi(x = -\tfrac{a}{2}),\ \psi(x = +\tfrac{a}{2})$$

$$\frac{d\psi}{dx}(x = -\tfrac{a}{2}),\ \frac{d\psi}{dx}(x = +\tfrac{a}{2})$$

and 4 unknowns: A', B', C, G.

Oops! There's one other equation, for the normalization of ψ! So we have 5 equations, + 4 unknowns; the system is overdetermined.

It turns out that we can find solutions to these equations only for certain values of E.

This is the same problem described earlier, where we have to match an oscillating function to decreasing exponentials on both sides:

 or 

etc.

Algebraically this turns out to be a mess.
The equations are worked out in Appendix H of
Eisberg + Resnick; You get a transcendental
eq'n you can't solve analytically. You have
to solve

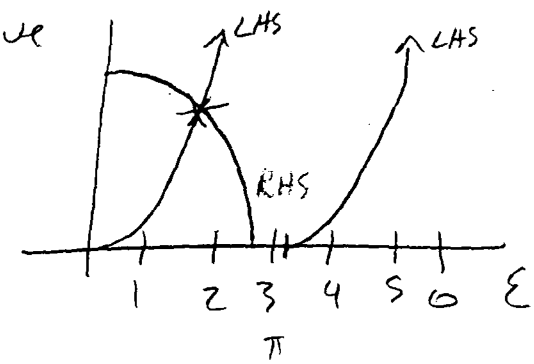
$$\varepsilon \tan \varepsilon = \sqrt{\frac{m V_0 a^2}{2\hbar^2} - \varepsilon^2} \quad \text{and} \quad -\varepsilon \cot \varepsilon = \sqrt{}$$

where $\varepsilon = \sqrt{\frac{m E a^2}{2\hbar^2}}$

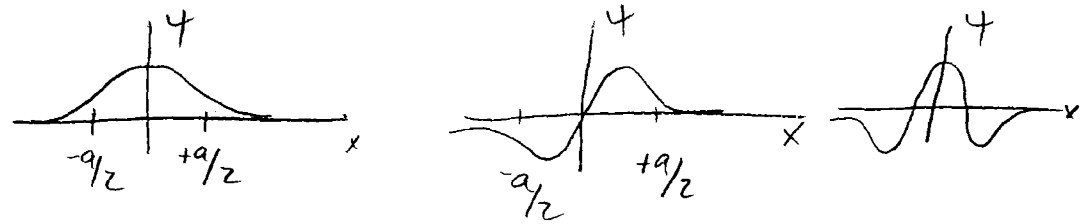
for E. Not so trivial — you have to do it
numerically. You can also do it graphically.
The eq'n has the form

$$\boxed{\text{function of } \varepsilon = \text{different function of } \varepsilon}$$

So if we plot them both vs ε, then where
they cross gives us possible ε's, which we can
then solve for E. So for example, using the
1st eq'n, we have



When you work it out, the first few sol'ns look like



+ The number of eigenfunctions depends on the depth of the well; specifically, it depends on how big V_0 is compared to $\frac{2\hbar^2}{ma^2}$.

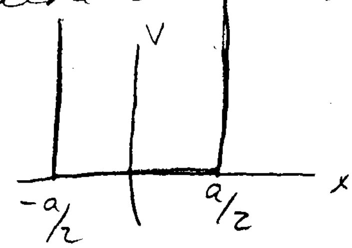
For $E > V_0$, there are no bound states, + all energies are allowed.

<u>Infinite Square Well (Particle in box)</u>

Things simplify mathematically if we take <u>$V_0 \to \infty$</u>.

Physically, that means the <u>walls</u> of the well are <u>impenetrable</u> — ψ is 0 everywhere outside.

$$V = \begin{cases} \infty & x < -\frac{a}{2},\ x > +\frac{a}{2} \\ 0 & -\frac{a}{2} < x < +\frac{a}{2} \end{cases}$$



<u>Any</u> state is now bound inside the well.

The general sol'n is (again, it's most convenient to use sines + cosines)

$-\frac{a}{2} < x < \frac{a}{2}$ $\quad \psi(x) = A\sin kx + B\cos kx$

+ $\psi = 0$ outside

<u>Aside</u> Notice that $\psi \to 0$ outside actually follows from the sol'n to the finite square well. we had e.g. for large x, $\psi = Ge^{-k_2 x}$
But $k_2 = \frac{\sqrt{2m(V_0-E)}}{\hbar}$. As $V_0 \to \infty$, $k_2 \to \infty$, and $\psi \to 0$

Continuity of ψ:

$x = -\frac{a}{2}$ $\quad \psi(\frac{-a}{2}) = -A\sin\frac{ka}{2} + B\cos\frac{ka}{2} = 0$

$x = +\frac{a}{2}$ $\quad \psi(+\frac{a}{2}) = A\sin\frac{ka}{2} + B\cos\frac{ka}{2} = 0$

Adding + subtracting these eq'ns gives

$$A\sin\frac{ka}{2} = 0 \quad + \quad B\cos\frac{ka}{2} = 0$$

and <u>both</u> of these must be satisfied.

Now, sin + cos can't simultaneously be 0, so we must have

i) $\cos\frac{ka}{2} = 0$ and $A = 0$
$\Rightarrow \frac{ka}{2} = \frac{n\pi}{2}$, $n = 1, 3, 5\ldots$ $\Rightarrow K = \frac{n\pi}{a}$ $n = 1, 3, 5, \ldots$

or ii) $\sin\frac{ka}{2} = 0$ and $B = 0$
$\Rightarrow \frac{ka}{2} = m\pi$, $m = 1, 2, 3 \ldots$ or $K = \frac{n\pi}{a}$ $n = 2, 4, 6\ldots$

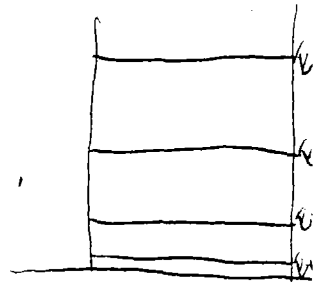
So we have sol'ns

i) $\psi_n(x) = B_n \cos k_n x$ $\quad K_n = \frac{n\pi}{a}$, $n = 1, 3, 5\ldots$

ii) $\psi_n(x) = A_n \sin k_n x$ $\quad K_n = \frac{n\pi}{a}$, $n = 2, 4, 6\ldots$
(note $n=0$ gives $\psi=0$)

(3.29)

If we go back and write the expressions for k in terms of E, we find



$$\boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\pi^2 \hbar^2 n^2}{2ma^2}} \qquad n = 1, 2, 3, \ldots$$

$\Rightarrow$ the energy is quantized.

Comments

- Note that since $E \propto n^2$, the energy levels are not evenly spaced.
- Also, since $E \propto \frac{1}{a^2}$, the smaller the box, the bigger the energy. And $E \propto \frac{1}{m}$, so the lighter the particle, the bigger the energy
- The minimum energy is $E_1 = \frac{\hbar^2 \pi^2}{2ma^2}$, not 0

$\Rightarrow$ the particle cannot have zero energy. This follows from the uncertainty principle. If the particle is confined to the box, its uncertainty in x is $\Delta x \simeq a \Rightarrow \Delta p \gtrsim \frac{\hbar}{2a}$. Can't have $E = 0$ because that would mean $\Delta p = 0$.

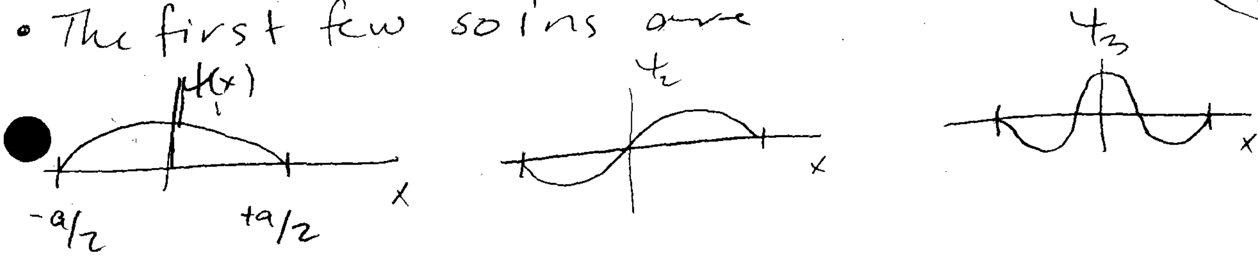
For min energy E_1, $|\vec{p}_1| \simeq \sqrt{2mE_1} = \pi \hbar / a$.

Standing wave $\Rightarrow$ particle moving back + forth equally likely, so $\Delta p \simeq 2p_1 = 2\pi\hbar/a$

$\Rightarrow \Delta x \Delta p \simeq 2\pi\hbar > \hbar/2$ as req'd by unc. princ.

Minimum energy is called zero point energy.

• The first few sol'ns are



They look like the square well, except there's no ψ beyond $x = \pm \frac{a}{2}$

• We didn't use $\frac{d\psi}{dx}$ continuous – in fact it's not continuous at $x = \pm a/2$ for any of the sol'ns we found! You can show this explicitly, and also it's obvious from the graphs of ψ.

Is this a problem? No – $\frac{d\psi}{dx}$ must be continuous only if V is finite. So back to the Schrodinger eq'n

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[E - V]\psi$$

If V is finite (and so is E), $\frac{d^2\psi}{dx^2}$ must also be finite. But $\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left(\frac{d\psi}{dx}\right)$, and if $\frac{d\psi}{dx}$ has a finite derivative, then it's continuous. I.e.

$$\frac{d}{dx}(\text{thing}) = \text{finite} \Leftrightarrow \text{thing is continuous}$$

(Infinite derivative can mean a finite change in zero distance: $\frac{\Delta \text{thing}}{\Delta x} \to \infty$ if $\Delta x = 0$.)

(3.31)

- Alternate derivation: we can find the energies by requiring that half-integer numbers of de Broglie wavelengths fit into the box:

$$n\left(\frac{\lambda}{2}\right) = a \quad \Rightarrow \quad \lambda = \frac{2a}{n}$$

Recall $p = h/\lambda = \frac{2\pi\hbar}{\lambda} = \frac{2\pi\hbar n}{2a} = \frac{\pi\hbar n}{a}$

Now, potential energy = 0 so all energy is kinetic:

$$E = \frac{p^2}{2m} = \frac{\pi^2\hbar^2 n^2}{2ma^2}$$

Ex: Before discovery of the neutron, people thought the nuclei of atoms were a combination of protons and electrons. (For atomic number Z and weight A, it was A protons and $A-Z$ electrons. This gives the correct mass and charge because the electron's mass is small compared to the proton's.) But an estimate of the zero-point energy of an electron in a box the size of a nucleus gives an energy way to big for the electron to actually be bound.

For $m = 10^{-30}\,kg$ + $a = 10^{-14}\,m$ (typical for a nucleus),

$$E = \frac{\pi\hbar^2}{2ma^2} \simeq \frac{10 \times 10^{-68}\ \text{joule}^2\,\text{sec}^2}{2 \times 10^{-30}\,\text{kg} \times 10^{-28}\,\text{m}^2} \simeq \frac{10^{-9}}{2}\ \text{joule}$$

$$= \frac{10^{-9}\ \text{joule}}{2} \times \frac{1\,\text{eV}}{1.6 \times 10^{-19}\ \text{joule}} \sim 10^9\,\text{eV} = 10^3\,\text{MeV}$$

Oops, relativistic. More detailed calc still gives [illegible] too big

Parity

Now we'll discuss explicitly a feature of the wave functions of the bound states we've discussed: they (the wave functions) are either symmetric or anti-symmetric. This is a consequense of the fact that the potentials themselves were symmetric.

Ex: Particle in box

$$\psi_1(x) = B_1 \cos\frac{\pi x}{a} \qquad \psi_1(-x) = \psi_1(x) \quad \text{"even parity"}$$

$$\psi_2(x) = A_2 \sin\frac{2\pi x}{a} \qquad \psi_2(-x) = -\psi_2(x) \quad \text{"odd parity"}$$

We can show this explicitly. Let's go back to the Schrödinger eq'n, and we'll use the 3-D version.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\,\psi(\vec{r})$$

Now we'll do what's called a parity transformation: take $\boxed{\vec{r} \to -\vec{r}}$ (In 1-D, that means $x \to -x$. In 3-D, it's $x \to -x$, $y \to -y$, $z \to -z$.) Now we assume the potential V is symmetric, that is

$$V(-\vec{r}) = V(\vec{r})$$

Now, under this transformation, if $x \to -x$,
then $\frac{\partial}{\partial x} \to -\frac{\partial}{\partial x}$, etc. So $\vec{\nabla} \to -\vec{\nabla}$ (or in 1-D, $\frac{d}{dx} \to -\frac{d}{dx}$).
But $\nabla^2 \equiv \vec{\nabla}\cdot\vec{\nabla} \to (-\vec{\nabla}\cdot-\vec{\nabla}) = \nabla^2$: it doesn't change.

So under the parity transformation, the S.E. becomes

$$-\frac{\hbar^2}{2m}\nabla^2 \psi(-\vec{r}) + V(\vec{r})\psi(-\vec{r}) = E\,\psi(-\vec{r})$$

and the only thing that has changed is we have
$\psi(-\vec{r})$ instead of $\psi(\vec{r})$. That means

$\psi(\vec{r})$ and $\psi(-\vec{r})$ satisfy the same Schrödinger eq'n for the same energy.

Unless there is more than one wave function with the same energy (when that happens it's called degeneracy), that means $\psi(-\vec{r})$ must be some constant multiple of $\psi(\vec{r})$:

$$\psi(-\vec{r}) = c\psi(\vec{r})$$

But now do the parity transf. on this eq'n ($\vec{r} \to -\vec{r}$)

$$\Rightarrow \quad \psi(\vec{r}) = c\,\psi(-\vec{r})$$

Substituting for $\psi(-\vec{r})$ on the RHS, we get

$$\psi(\vec{r}) = c^2\psi(\vec{r})$$

So we must have $c^2 = 1 \Rightarrow c = \pm 1$

$c = +1 \Rightarrow \psi(-\vec{r}) = \psi(\vec{r})$ even parity

$c = -1 \Rightarrow \psi(-\vec{r}) = -\psi(\vec{r})$ odd parity.

In 1-D, there is no degeneracy for bound-states w/ well-behaved potentials. Therefore you get energy eigenstates that are symmetric or antisymmetric if the potential is symmetric for bound states in 1D.

Correspondence Principle (Bohr, 1923)

Let's go back briefly to the development of quantum theory, when quantization had been discovered (as in the Bohr atom), but the Schrödinger eq'n wasn't around yet.

One of the puzzles the quantum physicists had to solve was how to connect quantum results to classical results – classical physics was known to work well in some regimes, so the quantum results had better match what happened classically. Bohr postulated that the classical limit is the limit of large quantum numbers. This led to the

Correspondence principle, which says that

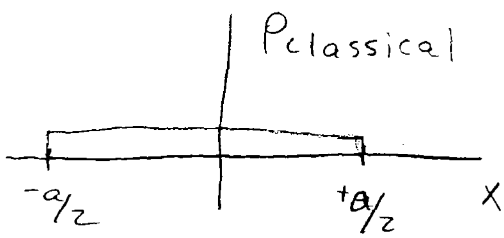
- $\boxed{\text{Quantum predictions for physical systems must match classical predictions in the limit of very large quantum numbers.}}$

There's another part, not so important for our purposes at the moment, that says

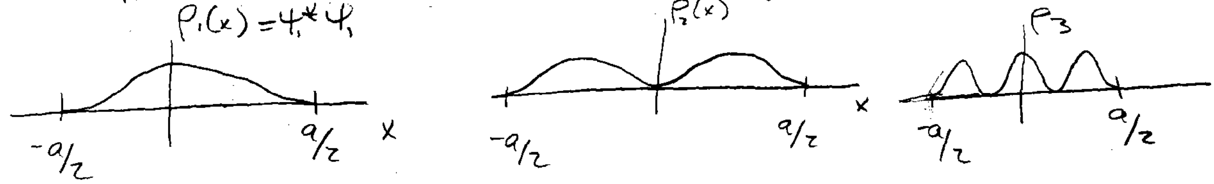
> any selection rules necessary to obtain correspondence in the classical (large-n) limit apply for all values of n.

Now let's go back to the particle in the box, and compare quantum and classical probability densities.

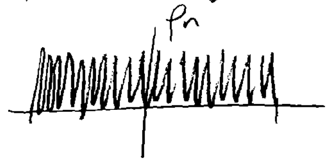
Classically, the particle bounces back + forth in the box with constant speed. It's equally likely to be found anywhere in the box, so its probability density is flat;



The QM prob. density is of course given by $\psi^*\psi$:



These look nothing like the classical density. But look what happens for large quantum numbers: the wiggles get very close together.



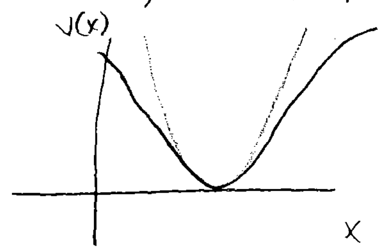
Now, for high n, the fractional $= \frac{E_{n+1}-E_n}{E_n}$ separation in adjacent energy levels becomes small (it $\to 0$ as $n \to \infty$), which means that they look continuous – you can't resolve the discreteness. That's good, because classically the energy is continuous. The other consequence is that you can't resolve the wiggles in the probability density – it looks flat, just like the classical density.

Simple Harmonic Oscillator

Now we're going to solve the S.E. for a continuous potential: $V(x) \propto x^2$, the simple harmonic oscillator. This is a good example for several reasons:

a) We can solve it analytically – and it's one of the few that we can

b) It's a good approximation for most potentials that have a minimum, if you stay close enough to the minimum, i.e. if you consider small oscillations:



Aside: To see this mathematically, think Taylor series expansion, + for simplicity take the min to be at $x=0$. Then

$$V(x) = V(0) + V'(0)\,x + \frac{V''(0)}{2}x^2 + \frac{V'''(0)}{3!}x^3 + \dots$$

- $V(0)$ is just a constant, + we can shift the energy scale to make it 0.
- $V'(0) = 0$ if x is a minimum
- $V''(0)$ is a number – call it C

- $V'''(0)\, x^3$ and higher powers of x can be neglected compared to the x^2 term if we stick to small x. (If it's exactly a harmonic oscillator potential, then the higher terms are identically 0.)

$\Rightarrow$ That leaves us with

$$V(x) \simeq \frac{c}{2} x^2$$

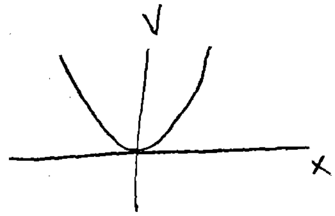
end of Aside

c) It's a good approximation and the starting point for studying most systems w/ oscillations (this pretty much follows from b, actually). Some examples:
   - vibration of atoms in diatomic molecules
   - acoustic + thermal properties of solids which come from atomic vibrations
   - magnetic properties of solids when they come from vibrations in orientation of nuclei
   - electrodynamics of quantum systems with vibrating EM waves.

In general, any system that executes small vibrations about a position of stable equilibrium. (stable equilibrium $\Leftrightarrow$ minimum of potential).

So consider the potential

$$V(x) = \frac{c}{2} x^2$$



(We're not using the standard classical notation $\frac{1}{2}kx^2$ because we're using k for other things in QM.)

Classically, what happens? Let's review. The particle experiences a restoring force

$$F = -\frac{dV}{dx} = -cx$$

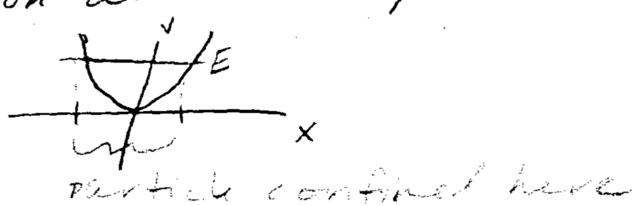
so the eq'n of motion is

$$\frac{d^2x}{dt^2} = -cx$$

And the sol'n is the well-known simple harmonic motion

$$x = A\cos(\omega t + \varphi)$$

where $\omega = \sqrt{\frac{c}{m}} = 2\pi\nu$ is the angular frequency of the motion. Any energy is allowed, and the motion is confined to a finite region determined by E



Quantum Mechanically, we already know qualitatively what will happen. Since V increases indefinitely with $|x|$, the only possible solutions are

- bound states with quantized energy.

We know that within the classical limits of the motion, $E > V$ and the sol'ns are oscillatory; outside, the wave function (or its magnitude) must fall off to 0 as $|x| \to \infty$. Finally, we know that, because the potential is symmetric, we will find energy eigenstates with definite parity – they'll be symmetric or antisymmetric about $x=0$ (and as with the square well, we'll find that the symmetric sol'ns make up one class and the antisymm. another when we solve the eq'n).

So we're going to follow Appendix I of Eisberg and Resnick and work through the gory details of finding the solution analytically. The technique is a standard one for solving differential equations, and we'll use it again for the hydrogen atom. It's a bit involved, so here's an outline of the plan.

We want to solve

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{C}{2}x^2\psi = E\psi$$

Plan: 1) First we'll simplify things algebraically by pulling some constants together into new parameters, and we'll rescale x while we're at it.

2) We can't solve the eq'n directly, so we'll factorize ψ like we did when separating the time-dep. S.E., only this time the factors will be

$$\psi(x) = \overbrace{\left[\psi(\text{large } x)\right]}^{\text{call this } G} * \overbrace{\left[\text{What's left over}\right]}^{\text{call this } H}$$

This isn't guaranteed to work, of course, and often it doesn't. But if we can find sol'ns of this form that satisfy the S.E., then it works.

3) We'll find the asymptotic form, $\overbrace{\psi(\text{large } x)}^{G}$, first. The S.E. will simplify in this limit, and we'll be able to solve it.

4) Then we'll put the factorized ψ back into the exact original S.E. to find "What's left over," H. To do this, we'll look for a power series sol'n, i.e. we'll assume H is a polynomial in x (actually in the rescaled version of x) and the S.E. will tell us what the coefficients of the powers of x are. In the process, a crucial

thing will happen — when we require that ψ is finite, we'll find that that means the energy will be quantized, and each allowed energy will correspond to a different form for ψ.

end of plan

So let's do it:

Step 1) The Schrödinger eq'n is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{C}{2}x^2\psi = E\psi$$

It'll turn out the classical oscillation frequency ν (recall $\omega = 2\pi\nu$) will play an important role, so use

$$\nu = \frac{1}{2\pi}\sqrt{\frac{C}{m}} \quad \Rightarrow \quad C = (2\pi\nu)^2 m$$

+ substitute for C in

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + 2\pi^2\nu^2 m x^2\psi = E\psi$$

Multiplying through by $\left(-\frac{\hbar^2}{2m}\right)$ + putting everything on the left-hand side,

$$\frac{d^2\psi}{dx^2} + \left[\frac{2mE}{\hbar^2} - \left(\frac{2\pi m\nu}{\hbar}\right)^2 x^2\right]\psi = 0$$

Now we give this and this a name:

$$\alpha \equiv \frac{2\pi m\nu}{\hbar} \quad \text{and} \quad \beta \equiv \frac{2mE}{\hbar^2}$$

Now the S.E. is

$$\frac{d^2\psi}{dx^2} + (\beta - \alpha^2 x^2)\psi = 0$$

Much simpler. But we want to do one more thing. Right now ψ is a function of x, a dimensionful variable. Let's rescale x so that it's dimensionless. Notice that α has dim's of inverse (length)^2:

$$[\alpha] = Kg^1 * \frac{1}{sec} * \frac{sec}{Kg\,m^2} = \frac{1}{m^2}$$

joule $= \frac{kg\,m^2}{sec^2}$

$[\hbar]$ = joul-sec

So $\sqrt{\alpha}\,x$ would be dimensionless. Call it u:

$$\boxed{u \equiv \sqrt{\alpha}\,x} = \left(\frac{2\pi\nu m}{\hbar}\right)^{1/2} x = \left(\frac{2\pi m}{2\pi\hbar}\sqrt{\frac{c}{m}}\right)^{1/2} = \frac{(Cm)^{1/4}}{\hbar^{1/2}}\,x$$

$$\Rightarrow x = \frac{u}{\sqrt{\alpha}}$$

Now we will find $\psi(u)$, but we need to change variables in the eq'n, which means writing $\frac{d^2\psi}{dx^2}$ in terms of $\frac{d^2\psi}{du^2}$. Now, $\frac{du}{dx} = \sqrt{\alpha}$, so

$$\frac{d\psi}{dx} = \frac{d\psi}{du}\frac{du}{dx} = \sqrt{\alpha}\,\frac{d\psi}{du}$$

$$\boxed{\text{or } \frac{d}{dx} = \frac{du}{dx}\frac{d}{du} = \sqrt{\alpha}\frac{d}{du} \qquad \frac{d^2}{dx^2} = \left(\frac{du}{dx}\right)^2 \frac{d^2}{du^2} = \alpha\frac{d^2}{du^2}}$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left(\frac{d\psi}{dx}\right) = \frac{du}{dx}\frac{d}{du}\left(\frac{d\psi}{dx}\right) = \sqrt{\alpha}\,\frac{d}{du}\left(\sqrt{\alpha}\,\frac{d\psi}{du}\right)$$

$$= \alpha\,\frac{d^2\psi}{du^2}$$

Now we stick this back into the SE:

$$\alpha \frac{d^2\psi(u)}{du^2} + \left(\beta - \alpha^2 \frac{u^2}{\alpha}\right)\psi(u) = 0$$

+ dividing through by α

$$\boxed{\frac{d^2\psi}{du^2} + \left(\frac{\beta}{\alpha} - u^2\right)\psi = 0}$$

and this is the simplified form of the S.E. in terms of the dimensionless variable u. We'll solve it for $\psi(u)$ then plug back in to get $\psi(x)$

Step 2) We still can't solve the S.E. directly for ψ, So we're going to write the sol'n as

$$\psi(u) = [\psi(\text{large } u)] * [\text{what's left over}]$$

$$\equiv G(u) * H(u)$$

and find G, then H given G. An important point is that this separation is only meaningful, i.e. G is really ψ(large u), if H varies much slower than G at large u. Both have to be finite of course.

So we're assuming $\psi(\text{large } u) \sim G(u)$

Step 3) Now find $G(u)$. What we're doing is finding the asymptotic behavior of ψ as $|u| \to \infty$, so we take the limit of the S.E. (p. 3.44) in this limit. Remember $\frac{\beta}{\alpha}$ is constant so we can neglect it compared to u^2 as $|u| \to \infty$.

$\Rightarrow$

$$\frac{d^2 G}{du^2} = u^2 G \qquad |u| \to \infty$$

Aside: α and β are gone. Does that mean that asymptotically the wave fn is indep of the parameters of the problem? Nope – there's α dependence built into u. Also, the overall normalization will depend on the form of ψ in the nonasymptotic region, which will surely depend on α + β.

A solution for G for $|u|$ large is

$$G \sim e^{\pm u^2/2}$$

since $\frac{dG}{du} = \pm u G$ and $\frac{d^2 G}{du^2} = \pm G + u^2 G \simeq u^2 G$ for u large. Now we have to get rid of the "+" sign in the exponential because it blows up, and G must be finite.

That means for large u the sol'n is

$$G(u) = Ae^{-u^2/2}$$

and we'll have to use H to get an exact sol'n for ψ that's good for all u.

Aside: Actually, we could've had

$$G = u^n e^{-u^2/2}$$

for any integer n (note that $e^{-u^2/2}$ falls off faster than any power of n, so it's still finite for $|u| \to \infty$):

$$\frac{dG}{du} = n u^{n-1} e^{-u^2/2} \pm u^{n+1} e^{-u^2/2} \simeq \pm u^{n+1} e^{-u^2/2}$$

$$\frac{d^2G}{du^2} \simeq \pm (n+1) u^n e^{-u^2/2} + u^{n+2} e^{-u^2/2}$$

$$\simeq u^{n+2} e^{-u^2/2} = u^2 G$$

This won't be a problem, because if we're missing a factor of u^n it'll show up in H in the exact solution.

Step 4) Now comes the messy algebra, but it'll reward us with an exact solution. We now need to find $H(u)$ using the exact S.E. So

$$\psi(u) = A\,e^{-u^2/2}\,H(u)$$

where A is a normalization constant (we could have absorbed it into H, but we keep it to be consistent with Eisberg and Resnick). This ψ has to satisfy the exact S.E.

$$\frac{d^2\psi}{du^2} + \left(\frac{\beta}{\alpha} - u^2\right)\psi = 0$$

We'll substitute to get an eq'n for $H(u)$, and we're not allowed to make approximations any more.

$$\frac{d\psi}{du} = -uAe^{-u^2/2}H(u) + Ae^{-u^2/2}\frac{dH}{du}$$

$$\frac{d^2\psi}{du^2} = -Ae^{-u^2/2}H + u^2Ae^{-u^2/2}H - uAe^{-u^2/2}\frac{dH}{du}$$

$$-uAe^{-u^2/2}\frac{dH}{du} + Ae^{-u^2/2}\frac{d^2H}{du^2}$$

$$= Ae^{-u^2/2}\left[(-1+u^2)H - 2u\frac{dH}{du} + \frac{d^2H}{du^2}\right]$$

So the S.E. becomes

$$Ae^{-u^2/2}\left[(-1+u^2)H - 2u\frac{dH}{du} + \frac{d^2H}{du^2}\right] + Ae^{-u^2/2}\left(\frac{\beta}{\alpha} - u^2\right)H = 0$$

giving us the differential eqn for H(u)

$$\boxed{\frac{d^2H}{du^2} - 2u\frac{dH}{du} + \left(\frac{\beta}{\alpha} - 1\right) H = 0}$$

Now this doesn't look any better than the original version, but it turns out to be solvable. We'll use the <u>power series technique</u>, i.e. assume that H can be written as a series in powers of u, & we'll use the S.E. to tell us what the coefficients are, So assume

$$H(u) = \sum_{l=0}^{\infty} a_l u^l = a_0 + a_1 u + a_2 u^2 + \ldots$$

Now we need derivatives;

$$\frac{dH}{du} = \sum_{l=0}^{\infty} l a_l u^{l-1} = a_1 + 2a_2 u + \ldots$$

$$\frac{d^2H}{du^2} = \sum_{l=2}^{\infty} (l-1) l a_l u^{l-2} = 2a_2 + 6a_3 u + \ldots$$

And notice when we plug into the S.E. we're going to get contrib's f/ diff a_l for the same power of u.

Substituting into the S.E.,

$$\underbrace{\sum_{l=2}^{\infty}(l-1)l\,a_l u^{l-2}}_{\sum_{l'=0}^{\infty}(l'+1)(l'+2)a_{l'+2}u^{l'}} - 2\sum_{l=0}^{\infty} l\,a_l u^l + \left(\frac{\beta}{\alpha}-1\right)\sum_{l=0}^{\infty} a_l u^l = 0$$

$l' = l-2 \Rightarrow$

~~because of factor of l in front~~

Now the l' here is a dummy variable; we can just call it l again. That means we can combine everything and write

$$\sum_{l=0}^{\infty}\left[(l+1)(l+2)a_{l+2} + \left(\frac{\beta}{\alpha}-1-2l\right)a_l\right]u^l = 0$$

Now, this has to be true for all possible values of u. The only way all those terms can add up to zero for all u is for the coefficients of <u>every</u> power of l to be zero. I.e.,

$$(l+1)(l+2)\,a_{l+2} + \left(\frac{\beta}{\alpha}-1-2l\right)a_l = 0$$

or

$$\boxed{a_{l+2} = \frac{-\left(\frac{\beta}{\alpha}-1-2l\right)}{(l+1)(l+2)}\,a_l}$$

This is called the recursion relation, and it tells you how to find $a_{\ell+2}$ if you know a_ℓ. So once you have a_0, that gives you all the even coefficients. Similarly, a_1 gives you all the odd ones. But it doesn't give you a_0 and a_1 — those are the two arbitrary constants the sol'n to a 2nd order differential eq'n must have.

<u>Aside</u> Why couldn't we just try a power series for the whole sol'n? instead of just for H It wouldn't work — we'd get a recursion rel'n w/ more than two coeff's, which we couldn't handle with our two allowed arbitrary constants.

Now do we just pick an a_0 and an a_1 and we're done? Nope. Turns out keeping the series arbitrary, w/ infinitely many odd and even terms, <u>doesn't give finite ψ</u>. To see this, look at the <u>large ℓ</u> behavior of the <u>ratio</u> of coefficients

$$\frac{a_{\ell+2}}{a_\ell} = \frac{-(\beta/\alpha - 1 - 2\ell)}{(\ell+1)(\ell+2)} \to \frac{2\ell}{\ell^2} \to \frac{2}{\ell}$$

Now, this is exactly the same as the expansion of e^{u^2}:

$$e^{u^2} = \sum_{i=0}^{\infty} \frac{1}{(i+1)!} u^{2i} = \sum_{\ell=2i} \frac{1}{(\ell/2+1)!} u^{\ell}$$

So the ratio of successive terms is

$$\frac{a_{l+2}}{a_l} = \frac{1}{l/2+1} \to \frac{1}{l/2} = \frac{2}{l},$$

same as above. That means for large u,

$H \to e^{u^2}$. Which means $\psi = GH \to e^{-u^2/2} e^{+u^2}$

$$= e^{+u^2/2}$$

$\Rightarrow$ it blows up! So we can't let the series have arbitrarily large powers of l. We can pick $a_0 = 0$ or $a_1 = 0$, then take $a_{l+2} \to 0$ for some value of l, call it n:

$$\frac{a_{l+2}}{a_l} = \frac{-\left(\frac{\beta}{\alpha} - 1 - 2l\right)}{(l+1)(l+2)} = 0 \quad \text{for } l = n$$

So $a_{n+2} = 0$ if

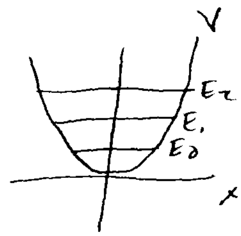
$$\boxed{\frac{\beta}{\alpha} = 2n+1 \qquad \begin{array}{l} a_1 = 0, \quad n = 0, 2, 4, \ldots \\ a_0 = 0, \quad n = 1, 3, 5, \ldots \end{array}}$$

and all the higher ones will be zero also. So we have functions $H_n(u)$ of order u^n. They're called the Hermite polynomials, So the sol'ns for the whole wave fn are

$$\boxed{\psi_n(u) = A_n e^{-u^2/2} H_n(u)}$$ simple harmonic oscillator

Now what about the eq'n for n? It says that β/α can't be arbitrary — it can only take on specific values, related to the integer n. But remember β is proportional to the energy $\Rightarrow$ E is quantized $\Leftrightarrow$ ψ finite. Specifically,

$$\frac{\beta}{\alpha} = \frac{2mE}{\hbar^2}\frac{\hbar}{2\pi m\nu} = \frac{2E}{h\nu} = 2n+1$$



$$\Rightarrow \boxed{E_n = h\nu\left(n + \tfrac{1}{2}\right)}$$

The eigenvalues are proportional to the classical oscillation freq. ν, and the zero point energy is $E_0 = \frac{h\nu}{2}$. Notice that the energy levels are evenly spaced.

The first few eigenfunctions are (recall $u = \frac{(Cm)^{1/4}}{\hbar^{1/2}} x$)

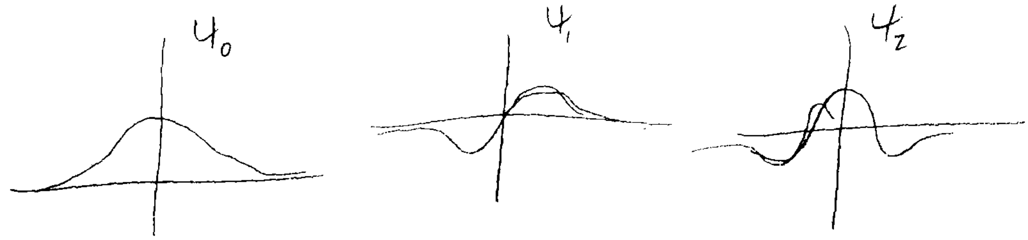
$$\psi_0 = A_0 e^{-u^2/2} \quad \leftarrow \text{(a gaussian)}$$

$$\psi_1 = A_1 u\, e^{-u^2/2}$$

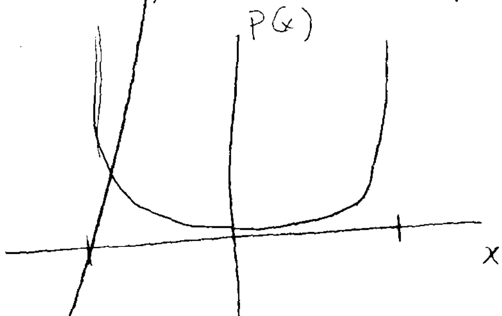
$$\psi_2 = A_2(1-2u^2)e^{-u^2/2}$$

$$\vdots$$

Notice that, as we expect for a symmetric potential, the wave functions have definite parity: even for even n, odd for odd n.

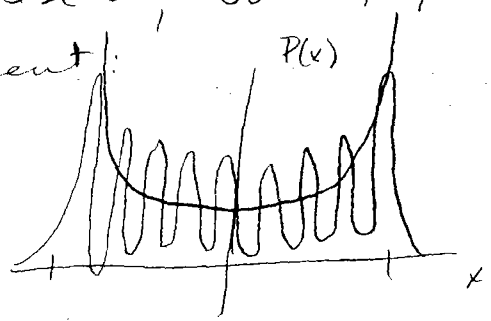


Now go back to the classical harmonic oscillator. Think about its behavior. The particle is moving fastest at the equilibrium position, and slowest near the limits of motion. Since it spends the most time in the regions where it's moving slowest, the particle's prob. density looks like (cf. fig. 5.3)



classical

Now obviously this doesn't look anything like the square of these, but if you go to higher n, things look different:



In the classical limit, at large n, you can't distinguish the wiggles and the classical + quantum probabilities look similar (see fig 5-19)

We've now seen lots of examples of sol'ns to the Schr. Eq'n in 1-Dim that illustrate the general properties we discussed early in the chapter. There is a very nice summary on p. 226 of the text.