The Schrödinger Equation

de Broglie: $\lambda = \frac{h}{p}$; $E = \hbar\omega$ $p = \hbar k$

"particle waves"

Let's see if we can find any insight from Classical Physics

Classical 1D motion under the influence of a potential

$$E = K + V(x)$$

↑ kinetic energy

$$E = \frac{1}{2} m \dot{x}^2 + V(x) \qquad (1)$$

E is a constant if there are no dissipative forces

So, $\frac{d}{dt}(1) =$

$$0 = \frac{1}{2} 2m \dot{x} \ddot{x} + \frac{\partial V}{\partial x} \dot{x} \qquad (2)$$

One solution... $\dot{x} = 0$ (Statics)
$\dot{x} \neq 0$ (Dynamics)

dynamic eq'n

$$m\ddot{x} + \frac{dV}{dx} = 0 \qquad (2)$$

$$\frac{dV}{dx} \equiv -F(x)$$

$$m\ddot{x} - F = 0 \quad \text{or} \quad F = ma \qquad \left.\begin{matrix}\\ \\ \end{matrix}\right\} \text{Newton's Laws} \quad (3)$$

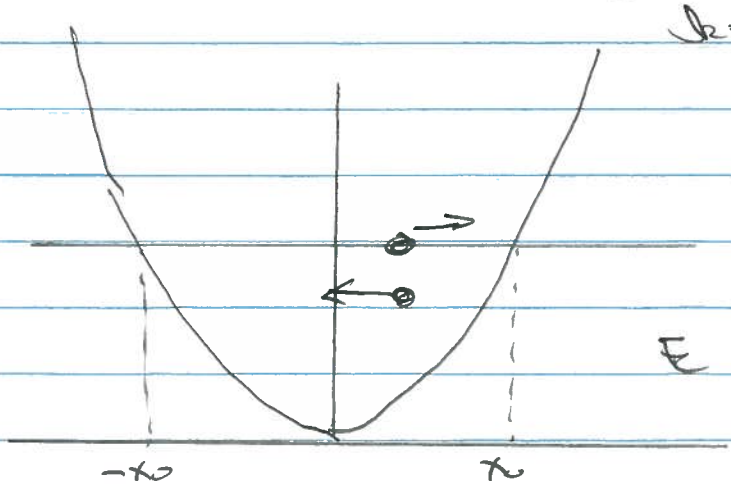
2nd order differential eq'n in x
yields $x(t)$, $p(t)$ "exactly"

Demonstration

The harmonic oscillator

$$V(x) = \tfrac{1}{2}kx^2 \quad ; \quad F = -kx$$

k = spring constant



particle moves back and forth

E constant, K & V constantly exchanging

Solve eq. (2)

$$m\ddot{x} + kx = 0 \qquad k, m \text{ +ve}$$

$$\ddot{x} + \frac{k}{m}x = 0 \qquad \text{let } \omega = \sqrt{\frac{k}{m}}$$

$$\ddot{x} + \omega^2 x = 0 \quad (3)$$

ω^2 is +ve. $\quad x = A\cos\omega t + B\sin\omega t \quad (4)$

Need 2 boundary conditions

Let's choose At $t=0$ $x=0$ (5)

(5) in (4) $\Rightarrow \quad 0 = A \quad (6)$

So $\quad x = B\sin\omega t$

At $t=0 \quad v = v_0$

$$\dot{x} = B\omega\cos\omega t$$

$$v_0 = B\omega \quad ; \quad B = \frac{v_0}{\omega}$$

So $\quad x = \frac{v_0}{\omega}\sin\omega t$

What is E?

$$E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2$$

$$x = \frac{v_0}{\omega}\sin\omega t \qquad \dot{x} = v_0\cos\omega t$$

So $$E = \frac{1}{2}mv_0^2\cos^2\omega t + \frac{1}{2}k\frac{v_0^2}{\omega^2}\sin^2\omega t \qquad \omega^2 = \frac{k}{m}$$

$$= \frac{1}{2}mv_0^2\cos^2\omega t + \frac{1}{2}mv_0^2\sin^2\omega t$$

$$= \frac{1}{2}mv_0^2$$

$$\boxed{E = \frac{1}{2}mv_0^2}$$ makes sense

Average value of K?

The period τ_0 is defined by how long the particle takes to

Recall $$x = \frac{v_0}{\omega}\sin\omega t$$

return to starting point with same speed at $\omega\tau_0 = 2\pi$

$$\tau_0 = \frac{2\pi}{\omega}$$

Average value of K?

$$\langle K \rangle = \frac{1}{\tau_0} \int_0^{\tau_0} dt \; \frac{1}{2} m \dot{x}^2$$

$$= \frac{1}{\tau_0} \int_0^{\tau_0} dt \; \underbrace{\frac{1}{2} m v_0^2}_{=E} \cos^2 \omega t$$

Let $\theta = \omega t$ $\qquad 2\pi = \omega \tau_0$

$$\langle K \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta \cos^2 \theta$$

$$= \frac{1}{2}$$

$$\langle K \rangle = E/2$$

By CoE $\qquad E = \langle K \rangle + \langle V \rangle$

So $\qquad \langle V \rangle = \frac{1}{2} E$

K & V share the energy equally in time

Finally, what is the classical "turning point" x_0?

From $x = \frac{v_0}{\omega} \sin \omega t$

$|x|_{max}$ when $\sin \omega t = \pm 1$ ← error in notes

So $x_0 = \frac{v_0}{\omega}$

The complete solution

$$x = \frac{v_0}{\omega} \sin \omega t$$

$$\dot{x} = v_0 \cos \omega t$$

$\omega^2 = \frac{k}{m}$ ← given

v_0 – given, related $E = \frac{1}{2} m v_0^2$, $x_0 = \frac{v_0}{\omega}$

$$\langle K \rangle = \langle V \rangle = E/2$$

The complete solution to the classical harmonic oscillator

$x = \frac{v_0}{\omega}\sin\omega t$; $E = \frac{1}{2}mv_0^2$ (total energy)

$p = mv_0\cos\omega t$; $\langle K\rangle = \langle V\rangle = E/2$

$\omega^2 = \frac{k}{m}$ ← given ; $\tau_0 = \frac{2\pi}{\omega}$ (period)

$x_0 = v_0/\omega$

Some other results

If you can not see the mass moving, the most you can say about it is

time average

$\langle x\rangle = 0$ (avg position is at origin)

$\langle p\rangle = 0$ (not going anywhere)

What about $\langle x^2\rangle$ $\langle p^2\rangle$?

$$\langle x^2\rangle = \frac{1}{\tau_0}\int_0^{\tau_0} dt\; x^2(t) = \frac{1}{\tau_0}\int_0^{\tau_0} dt\; \frac{v_0^2}{\omega^2}\sin^2\omega t$$

$$= x_0^2\,\frac{1}{\tau_0}\int_0^{\tau_0} dt\,\sin^2\omega t = x_0^2\,\frac{1}{\omega\tau_0}\int_{\theta=\omega t}^{\omega\tau_0} d\theta\,\sin^2\theta$$

$$= x_0^2\,\frac{1}{2\pi}\int_0^{2\pi} d\theta\,\sin^2\theta = \frac{x_0^2}{2}$$

($\omega\tau_0 = 2\pi$)

$$\langle x^2 \rangle = \frac{x_0^2}{2}$$

{ note: easier to have done $\langle x^2 \rangle = 2k \langle \frac{1}{2} k x_0^2 \rangle = kE$ }

$$\langle p^2 \rangle = \frac{1}{\tau_0} \int_0^{\tau_0} dt\, p^2(t) = \frac{1}{\tau_0} \int_0^{\tau_0} dt\, m^2 v_0^2 \cos^2 \omega t$$

$$= m^2 v_0^2 \frac{1}{2\pi} \int_0^{2\pi} d\theta \cos^2 \theta$$

$$= \frac{1}{2} m^2 v_0^2$$

$$\langle p^2 \rangle = \frac{1}{2} m^2 v_0^2$$

{ note: easier to say $\langle p^2 \rangle = 2m \langle \frac{p^2}{2m} \rangle = 2m \frac{1}{2} E = mE$ }

Classical uncertainty relationship?

$$(\Delta p)(\Delta x) = \left[\left(\langle p^2 \rangle - \langle p \rangle^2 \right) \left(\langle x^2 \rangle - \langle x \rangle^2 \right) \right]^{1/2}$$

$$= \left[\langle p^2 x^2 \rangle \right]^{1/2}$$

$$= \left[\frac{1}{2} m v_0^2 \; \frac{1}{2} x_0^2 \right]^{1/2}$$

$$= \left[m \left[\frac{1}{2} m v_0^2 \right] \frac{1}{k} \left[\frac{1}{2} k x_0^2 \right] \right]^{1/2}$$

($\frac{1}{2} m v_0^2 = E$, $\frac{1}{2} k x_0^2 = E$)

$$= \frac{E}{\omega}$$

$$\boxed{\Delta p \Delta x = \frac{E}{\omega}}$$

Quantum Mechanics

photons

quantum mechanics — small things, e^-, γ etc p, n, nuclei, atoms — how they move, interact with each other

"Derive" Schrödinger's equation

Recall our wave representation of a particle

$$A(x,t) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dk\, A(k)\, e^{i(kx - \omega(k)t)} \quad (1)$$

{ gosh, I'm getting tired of writing this, over and over again! }

And, now, for Schrödinger's stroke of genius
{ They don't give away Nobel prizes for nothing! }

Consider $\left\{ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - i\hbar\frac{\partial}{\partial t} \right\}$ operating on (1)

$$\left\{ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - i\hbar\frac{\partial}{\partial t} \right\} A(x,t) =$$

$$\frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dk\, A(k) \left\{ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - i\hbar\frac{\partial}{\partial t} \right\} e^{i(kx - \omega(k)t)}$$

$$= \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dk\, A(k) \left(\frac{\hbar^2 k^2}{2m} - \hbar\omega(k) \right) e^{i(kx - \omega(k)t)}$$

$= 0$! for each k component

because $\frac{\hbar^2 k^2}{2m} - \hbar\omega(k) = K - E$ for each k component.

$= 0$ since there are no external forces

Voila! (One Nobel Prize!)

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

This is the equation that describes the dynamics of a non-relativistic particle without influence of external forces.

It is called the 1D time-dependent Schrödinger eq'n.

So, how did Schrö.. guess at (2)?

Probably he saw that $-i\hbar\frac{\partial}{\partial x}$ drew down a $\hbar k$ in (1). So, as an operator

$$\boxed{p = -i\hbar\frac{\partial}{\partial x} \qquad (3)}$$

$$K = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Also, the energy operator

$i\hbar \frac{\partial}{\partial t}$ by the same reasoning

As an operator

$$\boxed{E = i\hbar \frac{\partial}{\partial t}} \quad (4)$$

Then it was just a matter of writing

$\frac{p^2}{2m} = E$; in the absence of external forces

Some conventions

Instead of $\psi(x,t)$, it is common to use the symbol $\Psi(x,t)$. It's just convention

Thus $$\frac{-\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} = \frac{i\hbar \partial \Psi(x,t)}{\partial t} \quad (5)$$

Adding in the effect of external forces

By analogy with classical physics

$$\frac{p^2}{2m} + V = E \qquad \text{(Classical)}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x,t)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \qquad (6)$$

(Quantum)

norm

We wish to identify the solutions to (6) as single particles. Thus we choose the norm to be

$$1 = \int_{-\infty}^{\infty} dx\, \Psi^*(x,t)\Psi(x,t) \qquad (7)$$

IMPORTANT CONCEPT

This is the only connection we have between

1 particle, and a wave that is, in principle, distributed over all space.

Note. (7) $\Rightarrow$ no time dependence.
One can prove this is the case if $V(x,t)$ is real.

(7) also implies

The integral (7) must exist, i.e. $\Psi(x,t)$ must be "square integrable" in the $|\Psi(x,t)|^2$ sense.

Probability density

$$P(x,t)\,dx \equiv \Psi^*(x,t)\Psi(x,t)\,dx \qquad (8)$$

CRITICALLY IMPORTANT CONCEPT

Our interpretation of $P(x,t)$ is that of it telling where the $|\text{amplitude}|^2$ of the wave is the strongest, and more likely to interact with another wave's amplitude, or potential, at x.

It is not an expression of where the particle is likely to be. [The particle is everywhere, simultaneously!] Unfortunately, Krane makes this mistake, as do some older quantum mechanics texts.

Where is the wave going?

Continuity equation

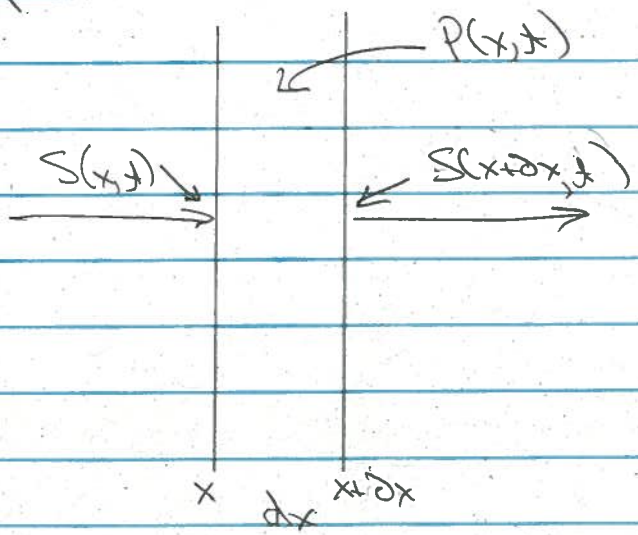
If the potential $V(x,t)$ is real, it can be shown that

$$\frac{\partial P(x,t)}{\partial t} + \frac{\partial}{\partial x} S(x,t) = 0 \qquad (9)$$

when the probability current density, $S(x,t)$ is given by

$$S(x,t) = -\frac{\hbar}{m} \underbrace{\mathrm{Im}}_{\text{correction}} \left[\psi(x,t) \frac{\partial}{\partial x} \psi^*(x,t) \right] \qquad (10)$$

Interpretation



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

change in Prob

diff between what goes in and goes out

The derivation of (9) ⇒ (10) with a bonus! (optional)

From (8) $P = \psi^* \psi$ (dependence on x,t will be left implicit)

$\frac{\partial}{\partial t}$ (8) ⇒ $\frac{\partial P}{\partial t} = \left(\frac{\partial \psi^*}{\partial t}\right)\psi + \psi^* \frac{\partial \psi}{\partial t}$ (11)

From (6)

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} V\psi \qquad (12)$$

(12)* ⇒ $$\frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar} V^*\psi^* \qquad (13)$$

(13) & (12) → (11) ⇒

$$\frac{\partial P}{\partial t} = -\frac{i\hbar}{2m}\left[\frac{\partial^2 \psi^*}{\partial x^2}\right]\psi + \frac{i}{\hbar} V^*\psi^*\psi$$

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

$$= \underbrace{\frac{i\hbar}{2m}\left[\psi^*\frac{\partial^2 \psi}{\partial x^2} - \left(\frac{\partial^2 \psi^*}{\partial x^2}\right)\psi\right]}_{-\frac{\partial}{\partial x}\left(\left(\frac{\partial \psi^*}{\partial x}\right)\psi - \psi^*\frac{\partial \psi}{\partial x}\right)} - \frac{i}{\hbar}\underbrace{\left[\psi^*(V - V^*)\psi\right]}_{2i\,\mathrm{Im}V}$$

$2i\,\mathrm{Im}\,\psi\left(\frac{\partial}{\partial x}\psi^*\right)$

$$= \frac{\partial}{\partial x}\underbrace{\frac{\hbar}{m}\mathrm{Im}\,\psi\left(\frac{\partial \psi^*}{\partial x}\right)}_{\equiv -S(x,t)} + \frac{2}{\hbar}\psi^*\,\mathrm{Im}V\psi$$

$$\boxed{\frac{\partial P}{\partial t} + \frac{\partial S}{\partial x} = \frac{2}{\hbar}\psi^*\,\mathrm{Im}V\psi} \quad (14)$$

Note: this assumed that V was not a directionally sensitive operator

If V is real

$$\frac{\partial P}{\partial t} + \frac{\partial S}{\partial x} = 0 \qquad \text{QED}$$

end of optional part

Summary of results up to now

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(x,t) + V(x,t)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \qquad (1)$$

time-dependent SE in 1D with external forces

$$P(x,t)\,dx = \Psi^*(x,t)\Psi(x,t)\,dx \qquad (2)$$

Probability Density

can model absorbtion, probability generation

$$\frac{\partial P(x,t)}{\partial t} + \frac{\partial}{\partial x}S(x,t) = \frac{2}{\hbar}\Psi^*(x,t)\left[\Sigma_m V(x,t)\right]\Psi(x,t) \qquad (3)$$

$= 0$ if V is real

$$S(x,t) = -\frac{\hbar}{m}\left\{\Psi(x,t)\frac{\partial}{\partial x}\Psi^*(x,t)\right\}^{\text{Im}} \qquad (4)$$

Probability current density

Properties of $\Psi(x,t)$

To be a proper wavefunction

1.) $\Psi(x,t)$ must be normalized

i.e. $$\int_{-\infty}^{\infty} dx\, \Psi^*(x,t)\Psi(x,t) = 1 \qquad (5)$$

[V must be real, in this case]

Note: if $\Psi(x,t)$ is a "candidate" wavefunction, it can only be a proper wavefunction if we can normalize it

$$|N|^2 = \frac{1}{\int_{-\infty}^{\infty} dx\, \phi^*(x,t)\phi(x,t)}$$

and $\Psi(x,t) = N\phi(x,t)$

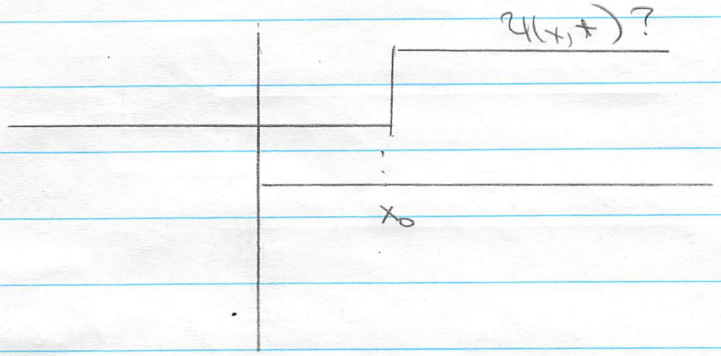
2.) $\Psi(x,t)$ must be continuous everywhere

3.) $\frac{\partial}{\partial x}\Psi(x,t)$ must be continuous everywhere

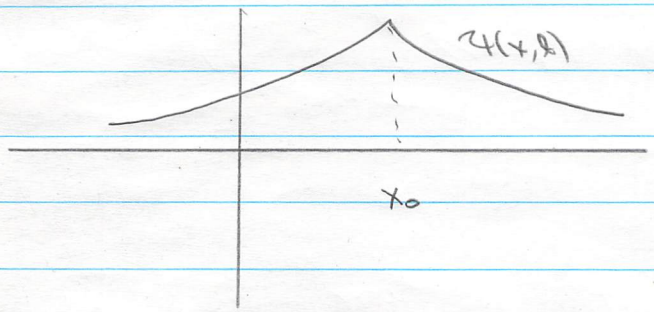
(except at the boundaries of infinite potentials)

Note: From (3)(4) we see if 2.) & 3.) do not hold, we can produce a source or sink of probability.

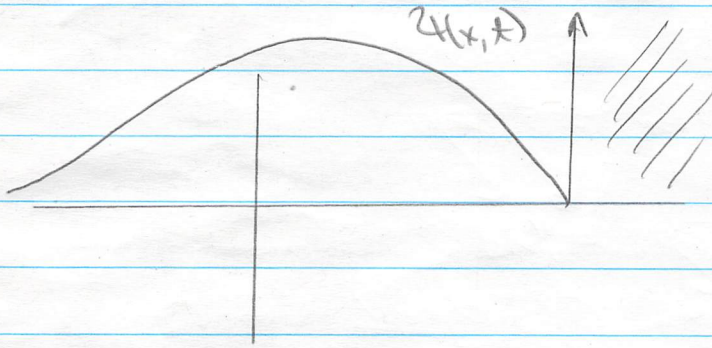
examples



not a proper wf
ψ(x,t) is discontinuous
at x_0



not a proper wf
ψ'(x,t) discontinuous
at $x = x_0$



is a proper wf if ψ(x,t) is normalizable

$$\psi(x,t) = \frac{N e^{-\frac{iE_0}{\hbar}t}}{[a^2+x^2]^{1/4}}$$

is not a proper wf since

$$\int_{-\infty}^{\infty} dx \; \frac{1}{[a^2+x^2]^{1/2}} \to \infty$$

Note $$\int_{-x_0}^{x_0} dx \; \frac{1}{[a^2+x^2]^{1/2}} = \log\left[\frac{[x_0 + \sqrt{a^2+x_0^2}\,]^2}{a^2}\right]$$

$\to \infty$ if $x_0 \to \infty$

$$\psi(x,t) = \frac{N}{[a^2+x^2]^{1/2}} e^{-i\frac{E_0}{\hbar}t}$$

$$\int_{-\infty}^{\infty} dx \frac{1}{(a^2+x^2)} = \frac{\pi}{|a|}$$

$$\Rightarrow \psi(x,t) = \sqrt{\frac{|a|}{\pi}} \frac{e^{-i\frac{E_0}{\hbar}t}}{(a^2+x^2)^{1/2}}$$ is a proper wavefunction

example

If $\psi(x,t) = \sqrt{\frac{|a|}{\pi}} \frac{e^{-i\frac{E_0}{\hbar}t}}{(a^2+x^2)^{1/2}}$ ⑥

what is $V(x,t)$?

From ①, if $\psi(x,t)$ is known

$$V(x,t) = \frac{i\hbar \frac{\partial}{\partial t}\psi(x,t) + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)}{\psi(x,t)}$$ ⑦

let $\psi(x,t) = C e^{-i\frac{E_0}{\hbar}t} f(x)$ $C = \sqrt{\frac{|a|}{\pi}}$ ⑧

$$f = (a^2+x^2)^{-1/2}$$

⑧ → ⑦ ⇒

$$V(x,t) = \frac{E_0 f + \frac{\hbar^2}{2m} f''}{f}$$

$$V(x,t) = E_0 + \frac{\hbar^2}{2m}\frac{f''}{f}$$

$$f = (x^2+a^2)^{-1/2}$$

$$f' = -\tfrac{1}{2}(2x)(x^2+a^2)^{-3/2}$$

$$= -x(x^2+a^2)^{-3/2}$$

$$f'' = -(x^2+a^2)^{-3/2} - x\left(-\tfrac{3}{2}\right)(2x)(x^2+a^2)^{-5/2}$$

$$= -(x^2+a^2)^{-3/2} + 3x^2(x^2+a^2)^{-5/2}$$

$$= \frac{-(x^2+a^2)+3x^2}{(x^2+a^2)^{5/2}} = \frac{-a^2+2x^2}{(x^2+a^2)^{5/2}}$$

$$\frac{f''}{f} = \frac{a^2-2x^2}{(x^2+a^2)^2} = \frac{3a^2-2(x^2+a^2)}{(x^2+a^2)^2}$$

$$\frac{f''}{f} = -\frac{3a^2}{(x^2+a^2)^2} + \frac{2}{(x^2+a^2)}$$

$$\Rightarrow \quad V(x,t) = V(x) = E_0 + \frac{\hbar^2}{2m}\left\{\frac{2}{(x^2+a^2)} - \frac{3}{(x^2+a^2)^2}\right\}$$

(9)

Sketch

General Classes of Problems

A) E is monoenergetic is all regions of space

If there is only one energy in a given region of space, then we can write

$$\psi(x,t) = u(x) e^{-i\frac{E}{\hbar}t} \qquad (9)$$

(9) → (1) ⇒

$$-\frac{\hbar^2}{2m} e^{-i\frac{E}{\hbar}t} u''(x) + V(x,t) u(x) e^{-i\frac{E}{\hbar}t} = E e^{-i\frac{E}{\hbar}t} u(x) \qquad (10)$$

The $e^{-i\frac{E}{\hbar}t}$ cancel out to leave

$$-\frac{\hbar^2}{2m} u'' + V(x,t) u = E u \qquad (11)$$

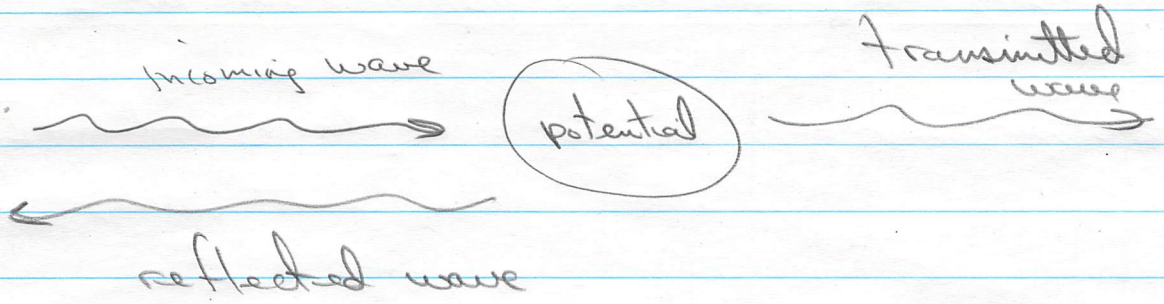
Since $V(x,t) = E + \frac{\hbar^2}{2m}\frac{u''}{u}$

we see that V can not be dependent on time either.

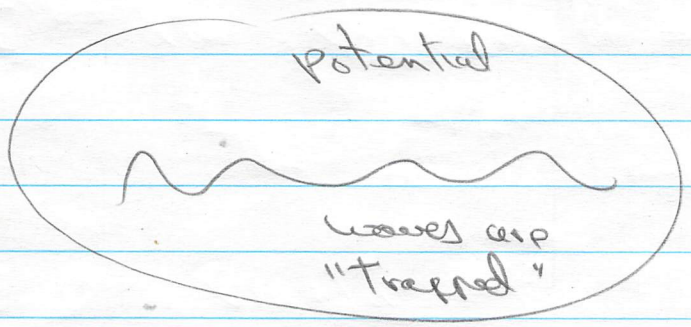
So A) Monoenergetic E, steadystate problems

$$-\frac{\hbar^2}{2m} u'' + V(x) u = E u \qquad (12)$$

A1) Unbound problems



A2) Bound problems

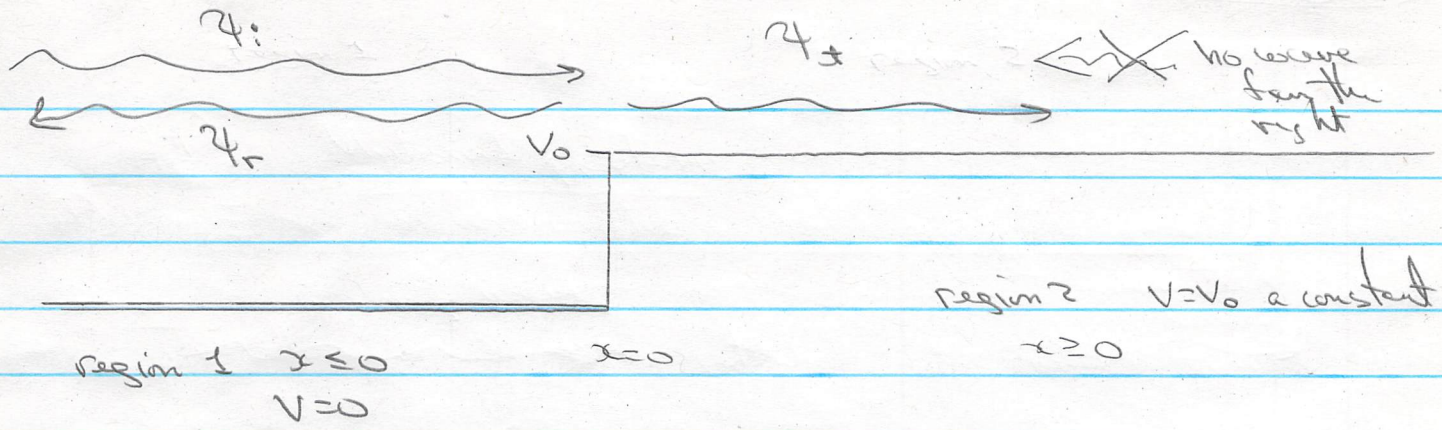


We'll focus initially on A1

Unbound, steady state, monoenergetic problems

example

Scattering of a wave on a barrier



Given 1) A particle is incident from the left, its wave function is

$$\psi_i = A e^{ik_1 x} e^{-i\frac{E}{\hbar}t}$$

↑ incident

E is known
A is known,
and it is assumed to be defined so that the wave function over all space is properly normalized.

Since it is a monoenergetic problem, in region 2, from (11)

$$u = A e^{ik_1 x} + B e^{-ik_1 x} \qquad (13)$$

↑ reflected wave

$$-\frac{\hbar^2}{2m} u'' = -\frac{\hbar^2}{2m}(-k_1^2)\, u$$

Hence $\frac{\hbar^2 k_1^2}{2m} u = E u$ from (11)

$$\frac{\hbar^2 k_1^2}{2m} = E \qquad (14)$$

$$k_1 = \left[\frac{2mE}{\hbar^2}\right]^{1/2} \qquad (15)$$

In region (2)

can be different

$$u = C e^{ik_2 x} + D e^{-ik_2 x} \qquad (16)$$

Ce^{ik_2x}: transmitted wave

De^{-ik_2x}: no wave coming in from the right

(16) ⇒ (11) ⇒

$$\frac{\hbar^2 k_2^2}{2m} u + V_0 u = E u \qquad (16)$$

$$\Rightarrow \quad \frac{\hbar^2 k_2^2}{2m} = E - V_0$$

$$k_2 = \left[\frac{2m(E-V_0)}{\hbar^2}\right]^{1/2} \qquad (17)$$

Note: we will allow V_0 to be anything. But if $V_0 > E$, we must choose

$$k_2 = i\left[\frac{2m(V_0-E)}{\hbar^2}\right]^{1/2} \qquad (18)$$

Since $k_2 = +i\left[\ \right]^{1/2}$

means that $\psi_+ = Ce^{-\left[\frac{2m(V_0-E)}{\hbar^2}\right]^{1/2}}$

a decaying exponential

With this understanding, we can solve for any constant potential. We just have to use complex numbers.

Set up the solution

		ψ	ψ'
(19)	region 1	$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$	$\psi_1' = Aik_1e^{ik_1x} - Bik_1e^{-ik_1x}$
(20)	region 2	$\psi_2 = Ce^{ik_2x}$	$\psi_2' = Cik_2e^{ik_2x}$

Apply continuity conditions

$\psi_1(0) = \psi_2(0) \Rightarrow$ (19) = (20) $\quad A + B = C$ (21)

$\psi_1'(0) = \psi_2'(0) \Rightarrow \quad k_1A - k_1B = k_2C$ (22)

Solve for B & C (A is known)

k_2(21) − (22) $\Rightarrow \quad A(k_2 - k_1) + (k_2 + k_1)B = 0$

$$B = \left(\frac{k_1 - k_2}{k_1 + k_2}\right) A \qquad (23)$$

k_1(21) + (22) $\Rightarrow$ $\qquad 2k_1 A = (k_1 + k_2) C$

$$C = \frac{2k_1 A}{k_1 + k_2} \qquad (24)$$

check $\quad C - B = \frac{2k_1 A}{k_1 + k_2} - \frac{k_1 - k_2}{k_1 + k_2} A = \frac{k_1 + k_2}{k_1 + k_2} A = A$ ✓

$$k_2 C + k_1 B = \frac{2k_1 k_2 A}{k_1 + k_2} + \frac{k_1 (k_1 - k_2)}{k_1 + k_2} A$$

$$= \frac{k_1 k_2 + k_1^2}{(k_1 + k_2)} A = k_1 A \quad ✓$$

So, our complete solution is

$$\psi = A \left\{ e^{ik_1 x} + \left(\frac{k_1 - k_2}{k_1 + k_2}\right) e^{-ik_1 x} \right\} \qquad x \le 0$$

$$= A \frac{2k_1}{k_1 + k_2} e^{ik_2 x} \qquad x \ge 0 \qquad (25)$$

$$k_1 = \left[\frac{2mE}{\hbar^2}\right]^{1/2}, \quad k_2 = \left[\frac{2m(E - V_0)}{\hbar^2}\right]^{1/2}$$

Analyze the scattering of a monoenergetic wave (E is constant)

Wave, $Ae^{ik_1 x}$, incident from the left ($x \Rightarrow -\infty$)
on a potential of the form (time independent problem)
There is no wave incident from the right ($x \Rightarrow +\infty$)

Region 1 $V = 0 \quad x \leq 0$

Region 2 $V = V_0$, an arbitrary constant, for $x \geq 0$

From the Time-independent 1D SE

$$-\frac{\hbar^2}{2m} u'' + V u = E u \qquad (1)$$

If $V = V_0$, the solutions are of the form $e^{\pm ikx}$

$$\left(e^{\pm ikx}\right)'' = -k^2 e^{\pm ikx} \qquad (2)$$

(2) $\Rightarrow$ (1) $\Rightarrow$

$$\left(\frac{\hbar^2 k^2}{2m}\right) e^{\pm ikx} = (E - V_0) e^{\pm ikx}$$

or $$\frac{\hbar^2 k^2}{2m} = E - V_0$$

$$k = \left[\frac{2m(E-V_0)}{\hbar^2}\right]^{1/2} \qquad (3)$$

So, for region 1 $k_1 = \left[\frac{2mE}{\hbar^2}\right]^{1/2}$

$k_2 = \left[\frac{2m(E-V_0)}{\hbar^2}\right]^{1/2}$ (4)

Since $E>0$ k_1 is real

Since V_0 is arbitrary k_2 can be complex

If $V_0 \leq E$ $\Rightarrow$ V_0 is real k_2 is real

Else k_2 is complex

The solutions

	u (reflected wave)	u'
Region 1	$u_1 = Ae^{ik_1x} + Be^{-ik_1x}$	$u_1' = ik_1(Ae^{ik_1x} - Be^{-ik_1x})$
Region 2	$u_2 = Ce^{ik_2x}$	$u_2' = ik_2Ce^{ik_2x}$

(5)

Apply continuity $u_1(0) = u_2(0)$; $u_1'(0) = u_2'(0)$

$u_1(0) = u_2(0) \Rightarrow$ $A + B = C$ (6)

$u_1'(0) = u_2'(0) \Rightarrow$ $k_1A - k_1B = k_2C$ (7)

Solve for B & C in terms of A

k_2 (6) − (7) ⇒

$$(k_2 - k_1)A + (k_2 + k_1)B = 0$$

$$B = \left(\frac{k_1 - k_2}{k_1 + k_2}\right) A \qquad (8)$$

k_1 (6) + (7) ⇒

$$2k_1 A = (k_1 + k_2)C$$

$$C = \frac{2k_1}{(k_1 + k_2)} A \qquad (9)$$

on your own: . . .
check
$A + B = C$
$k_1(A - B) = k_2 C$

So, our complete solution is:

(10)

$$\begin{cases} u(x) = u_1(x) = A\left\{e^{ik_1 x} + \left(\frac{k_1 - k_2}{k_1 + k_2}\right) e^{-ik_1 x}\right\} & \text{for } x \le 0 \\ u_2(x) = A\left(\frac{2k_1}{k_1 + k_2}\right) e^{ik_2 x} & \text{for } x \ge 0 \end{cases}$$

(note k_2 can be complex)

What does this mean

Recall our definition of probability current

$$S = \frac{-\hbar}{m} \mathrm{Im}\left\{ \Psi(x,t) \frac{\partial}{\partial x} \left(\Psi^*(x,t) \right) \right\}$$

For time independent problems

$$\Psi(x,t) = u(x) e^{-i(E/\hbar)t}$$

$$\frac{\partial}{\partial x} \Psi^*(x,t) = u'(x) e^{i(E/\hbar)t}$$

$$S(x) = -\frac{\hbar}{m} \mathrm{Im}\left\{ u(x) \left(u^*(x) \right)' \right\}$$

Evaluate the incident, reflected & transmitted current

incident $$S_i(x) = -\frac{\hbar}{m} \mathrm{Im}\left\{ A e^{ik_1 x} \left(A^* e^{-ik_1 x} \right)' \right\}$$

cancel; real is real

$$= -\frac{\hbar}{m} \mathrm{Im}\left\{ |A|^2 e^{ik_1 x} (-ik_1) e^{-ik_1 x} \right\}$$

$$= \frac{\hbar}{m} |A|^2 \mathrm{Im}\{ik_1\}$$

incident $$\boxed{S_i(x) = \frac{\hbar k_1}{m} |A|^2} \quad (11)$$

note: $\frac{\hbar k_1}{m} |A|^2 \Rightarrow \frac{\text{momentum}}{\text{mass}}$

$\Rightarrow$ velocity

reflected $\quad S_r(x) = -\frac{\hbar}{m} \mathrm{Im}\left\{ B e^{-ik_1 x} \left(B^* e^{ik_1 x} \right)' \right\}$

"...show..."

$$\boxed{S_r = -\frac{\hbar k_1}{m} |B|^2} \qquad (12)$$

note sign: reflected wave is going to the left

transmitted wave

$$S_t(x) = -\frac{\hbar}{m} \mathrm{Im}\left\{ C e^{ik_2 x} \left(C^* e^{-ik_2^* x} \right) \right\}$$

recall, k_2 can be complex!

$$= -\frac{\hbar}{m} \mathrm{Im}\left\{ |C|^2 e^{ik_2 x} (-ik_2^*) e^{-ik_2^* x} \right\}$$

$$= \frac{\hbar}{m} \mathrm{Im}\left\{ |C|^2 \, i k_2 \, e^{i(k_2 - k_2^*)x} \right\}$$

($|C|^2$: real)

$$\frac{\hbar}{m} \mathrm{Im}\{ik_2\} |C|^2 e^{-\mathrm{Im}(k_2)x}$$

($e^{-\mathrm{Im}(k_2)x}$: real)

$$\boxed{S_t(x) = \frac{\hbar}{m} \mathrm{Re}(k_2) |C|^2 e^{-\mathrm{Im}(k_2)x}} \qquad (13)$$

(case a) k_2 is real (requires $E \geq V_0$; V_0 real)

$$S_x = \frac{\hbar}{m} k_2 |C|^2 \qquad (14a)$$

(case b) $V_0 > E$ and V_0 is real

$\Rightarrow$ k_2 is pure imaginary

$\Rightarrow$ $S_x = 0$ (14b)

optional info

(case c) $\Rightarrow$ V_0 is complex (k_2 is mixed)

$$S_x(x) = \frac{\hbar}{m} \mathrm{Re}(k_2) |C|^2 \, e^{-\mathrm{Im}(k_2)x} \qquad (14c)$$

Can model S_x increasing or decreasing with x.

In NERS 311 I will only consider Cases a & b

In NERS 312, 14c is the basis of the optical model of the nucleus.

So don't forget your quantum mechanics next year

Reflection & Transmission Coefficients (Case D & B)

Reflection coefficient

$$R = \left| \frac{S_r}{S_i} \right| \quad \text{(15)}$$

absolute value to the correct directional signs

(11) (12) → (15) ⇒

$$R = \left| \frac{S_r}{S_i} \right| = \left| \frac{-\frac{\hbar k_2}{m}|B|^2}{\frac{\hbar k_1}{m}|A|^2} \right| = \frac{|B|^2}{|A|^2} \quad \text{(16)}$$

(8) ⇒ (16) ⇒

recall k_1 is real, k_2 is either pure real $V_0 \leq E$ or pure imaginary $V_0 > E$

$$R = \frac{(k_1 - k_2^*)(k_1 - k_2)}{(k_1 + k_2^*)(k_1 + k_2)} = \frac{k_1^2 - k_1(k_2 + k_2^*) + |k_2|^2}{k_1^2 + k_1(k_2 + k_2^*) + |k_2|^2}$$

$$R = \frac{k_1^2 - 2k_1 \mathrm{Re}(k_2) + |k_2|^2}{k_1^2 + 2k_1 \mathrm{Re}(k_2) + |k_2|^2} \quad \text{(17a)}$$

$$= \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \quad \text{(17b)} \quad \text{if } V_0 \leq E$$

$$= 1 \quad \text{(17c)} \quad \text{if } V_0 > E$$

Transmission Coefficient

$$T = \left| \frac{S_t}{S_i} \right| \quad \leftarrow \text{absolute value} \qquad (18)$$

Case A) if k_2 is real

(14a) ÷ (9) ⇒ (16) ⇒

$$T = \left| \frac{\cancel{\frac{\hbar}{m}} k_2 |C|^2}{\cancel{\frac{\hbar}{m}} k_1 |A|^2} \right|$$

$$T = \frac{k_2}{k_1} \frac{(2k_1)^2}{(k_1+k_2)^2} \qquad (19a)$$

If Case B) k_2 is pure imaginary

(14b) ⇒ $T = 0$ (19b)

What is $T+R$?

Case A) (19a) ÷ (17b) ⇒

$$T+R = \frac{(k_1-k_2)^2}{(k_1+k_2)^2} + \frac{4k_1k_2}{(k_1+k_2)^2} = 1$$

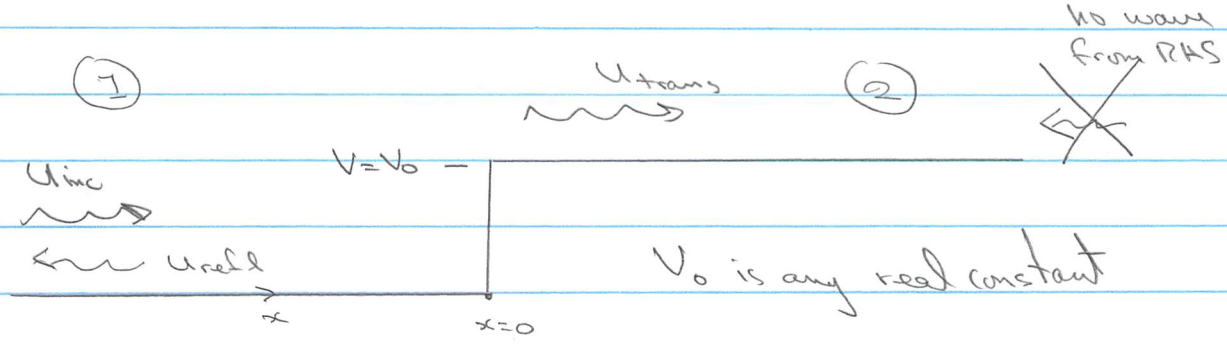
Case B) (19b) + (17c) ⇒ $T+R=1$

$T+R=1 \Rightarrow$ probability is conserved for any real potential

(Aside. If V_0 is complex, probability is <u>not</u> conserved.)

Page 99 is missing!

2D barrier scattering



region (1): $\psi_1(x) = \psi_{inc}(x) + \psi_{refl}(x)$

$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$ (1)

$k_1 = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$ (2)

region (2): $\psi_2(x) = \psi_{trans}(x) = Ce^{ik_2x}$ (3)

$k_2 = \left[\frac{2m(E-V_0)}{\hbar^2}\right]^{1/2}$ (4)

Note: If $E < V_0$ $\quad k_2 = i\left[\frac{2m(V_0-E)}{\hbar^2}\right]^{1/2}$

Since, by definition $i = \sqrt{-1}$

— apply continuity relationships at $x=0$

$\psi_1(0) = \psi_2(0) \Rightarrow \quad A + B = C$ (5)

$\psi_1'(0) = \psi_2'(0) \Rightarrow \quad ik_1(A-B) = ik_2C$ (6)

- solve for B & C in terms of A

$k_1 \times (5) + (6)$ / ; $\Rightarrow \quad 2k_1 A = (k_1 + k_2) C$

$\therefore \quad C = \left(\frac{2k_1}{k_1 + k_2}\right) A \qquad (7)$

similarly

$k_2 \times (5) - (6)$ / ; $\Rightarrow \quad (k_2 - k_1) A + (k_2 + k_1) B = 0$

$\therefore \quad B = \left(\frac{k_1 - k_2}{k_1 + k_2}\right) A \qquad (8)$

---

check note: (7) & $(8) \rightsquigarrow (5)$

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

(7) & $(8) \rightsquigarrow (6)$ /;

$k_1 A - \frac{k_1 (k_1 - k_2)}{k_1 + k_2} A = \frac{2 k_1 k_2}{k_1 + k_2} A$

✓

- extract the reflection & transmission coefficients using

$$T = \left| \frac{S_{trans}}{S_{inc}} \right| \quad (9)$$

$$R = \left| \frac{S_{refl}}{S_{inc}} \right| \quad (10)$$

Recall the derivation for a wave

$$S = -\frac{\hbar}{m} \mathrm{Im}\{u\, u^{*\prime}\} \quad (11)$$

For a generic plane wave

$$u = N e^{\pm i k x}$$

(k can be complex)

N: norm constant

$$u^* = N^* e^{\pm i k^* x}$$

$$u^{*\prime} = N^* (\mp i k^*)\, e^{\pm i k^* x}$$

$$S = -\frac{\hbar}{m} \mathrm{Im}\left\{ N e^{\pm i k x} (\mp i k) N^* e^{\pm i k^* x} \right\}$$

$$= \pm \frac{\hbar}{m} |N|^2 \, \mathrm{Im}\left\{ ik \, e^{\pm i(k-k^*)x} \right\}$$

$(k-k^* = 2ik_I)$

$$k = k_R + ik_I$$

$$= \pm \frac{\hbar}{m} |N|^2 e^{\mp 2k_I x} \, \mathrm{Im}(ik)$$

$$\boxed{S = \pm \frac{\hbar}{m} |N|^2 k_R e^{\mp 2k_I x}} \qquad (12)$$

So, for our situation

$$S_{inc} = |A|^2 \frac{\hbar k_1}{m} \qquad (13)$$

If $E > V_0$ (k_2 is real)

$$S_{refl} = -|B|^2 \frac{\hbar k_1}{m} \qquad (14)$$

$$S_{trans} = |C|^2 \frac{\hbar k_2}{m} \qquad (15)$$

(14) ÷ (13) → (10) ÷ (12) with (8) ⇒

$$R = \left| \frac{-|B|^2 \frac{\hbar k_1}{m}}{|A|^2 \frac{\hbar k_1}{m}} \right| = \frac{|B|^2}{|A|^2} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 \qquad (16) \qquad (\text{for } E > V_0)$$

(15) ÷ (13) → (9)' ÷ (12) with (7) ⇒

$$T = \left|\frac{S_{trans}}{S_{inc}}\right| = \frac{|C|^2 \frac{\hbar k_2}{m}}{|D|^2 \frac{\hbar k_1}{m}} = \frac{k_2}{k_1}\frac{4k_1^2}{(k_1+k_2)^2} = \frac{4k_1k_2}{(k_1+k_2)^2}$$

$$T = \frac{4k_1k_2}{(k_1+k_2)^2} \quad (17)$$

note: Using (16) ÷ (17)

$$R + T = \frac{(k_1-k_2)^2}{(k_1+k_2)^2} + \frac{4k_1k_2}{(k_1+k_2)^2}$$

$$= \frac{k_1^2 - 2k_1k_2 + k_2^2 + 4k_1k_2}{k_1^2 + 2k_1k_2 + k_2^2}$$

$$= 1$$

$$R + T = 1$$

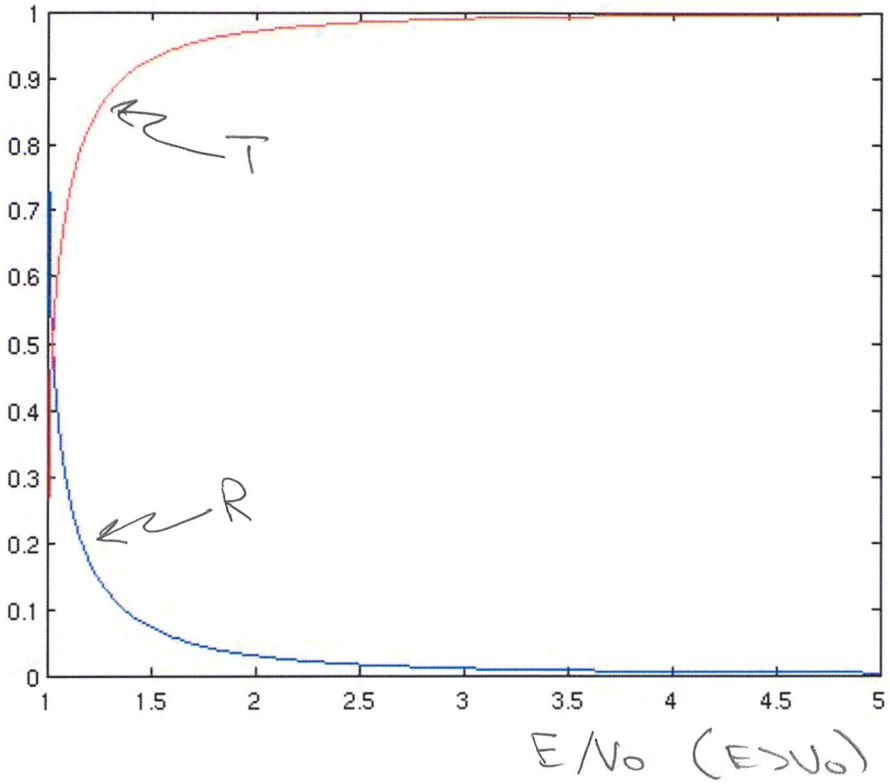
Plot R & T as a fn of E/V_0 $(E > V_0)$

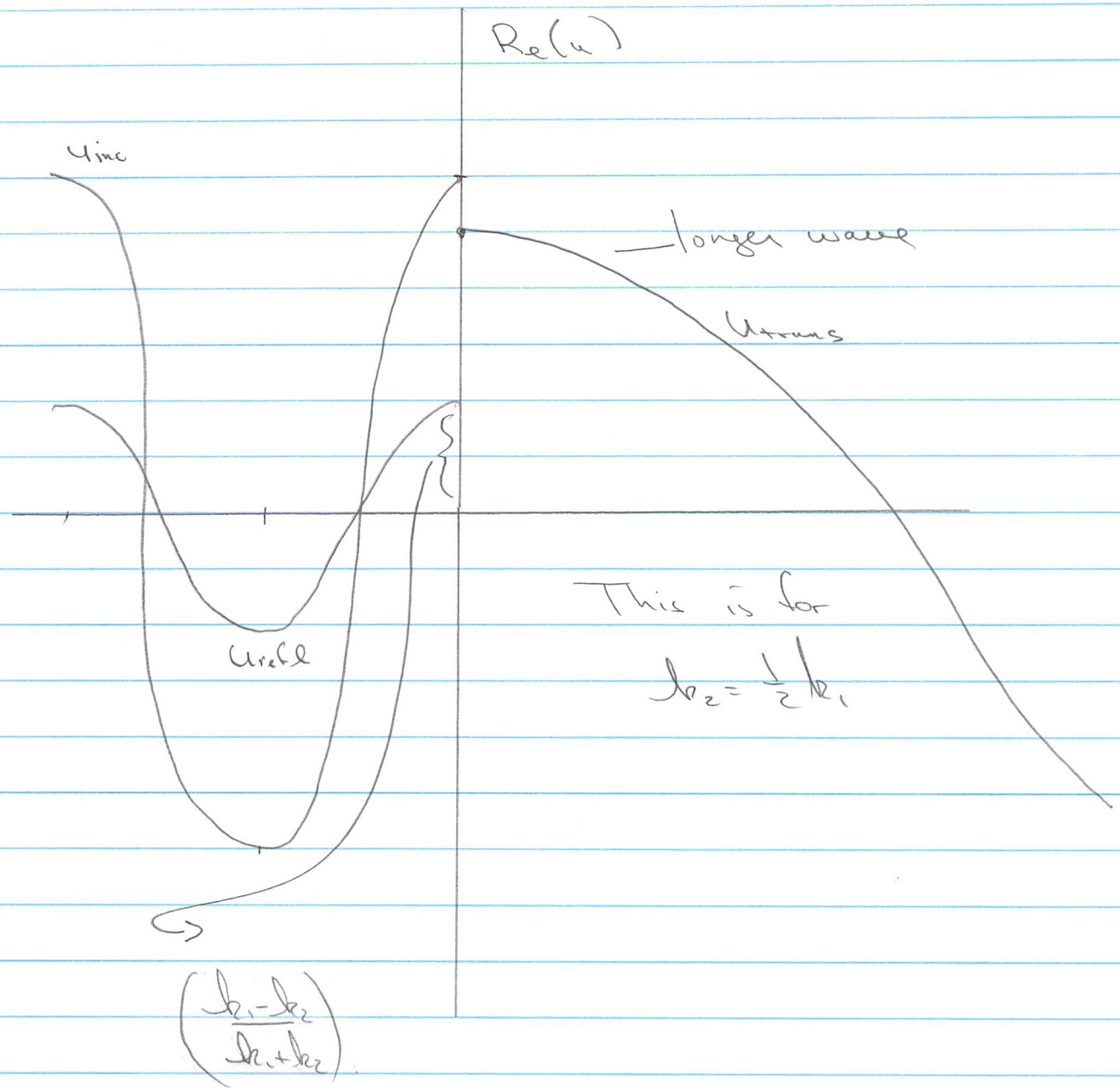
using (2) & (4)

$$R = \frac{\left(\sqrt{E} - \sqrt{E-V_0}\right)^2}{\left(\sqrt{E} + \sqrt{E-V_0}\right)^2} \quad (18)$$

$$T = \frac{4\sqrt{E}\sqrt{E-V_0}}{\left(\sqrt{E} + \sqrt{E-V_0}\right)^2} \quad (19)$$

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Re(u)
u_inc
longer wave
u_trans
u_refl
This is for
$k_2 = \frac{1}{2} k_1$
$\left(\frac{k_1 - k_2}{k_1 + k_2}\right)$

Case $V_0 > E$

Here we know from (12) that

$$k_2 = k_R + i k_I$$

$$= i \left(\frac{2m(V_0 - E)}{\hbar^2} \right)^{1/2}$$

$$k_R = 0 \; ; \qquad k_I = \left(\frac{2m(V_0 - E)}{\hbar^2} \right)^{1/2} \quad (20)$$

Recall (7) $\quad C = \dfrac{2k_1}{k_1 + k_2}$

$$|C|^2 = \frac{4k_1^2 |A|^2}{|k_1 + k_2|^2} = \frac{4k_1^2 |A|^2}{(k_1^2 + k_I^2)}$$

Recall (8) $\quad B = \dfrac{(k_1 - k_2)}{(k_1 + k_2)} A$

$$= \left(\frac{k_1 - i k_I}{k_1 + i k_I} \right) A$$

$$|B|^2 = \left(\frac{k_1^2 + k_I^2}{k_1^2 + k_I^2} \right) |A|^2 = |A|^2 \quad (21)$$

From (12)

$$S = \pm \frac{\hbar}{m} |N|^2 k_R e^{\mp 2k_I x}$$

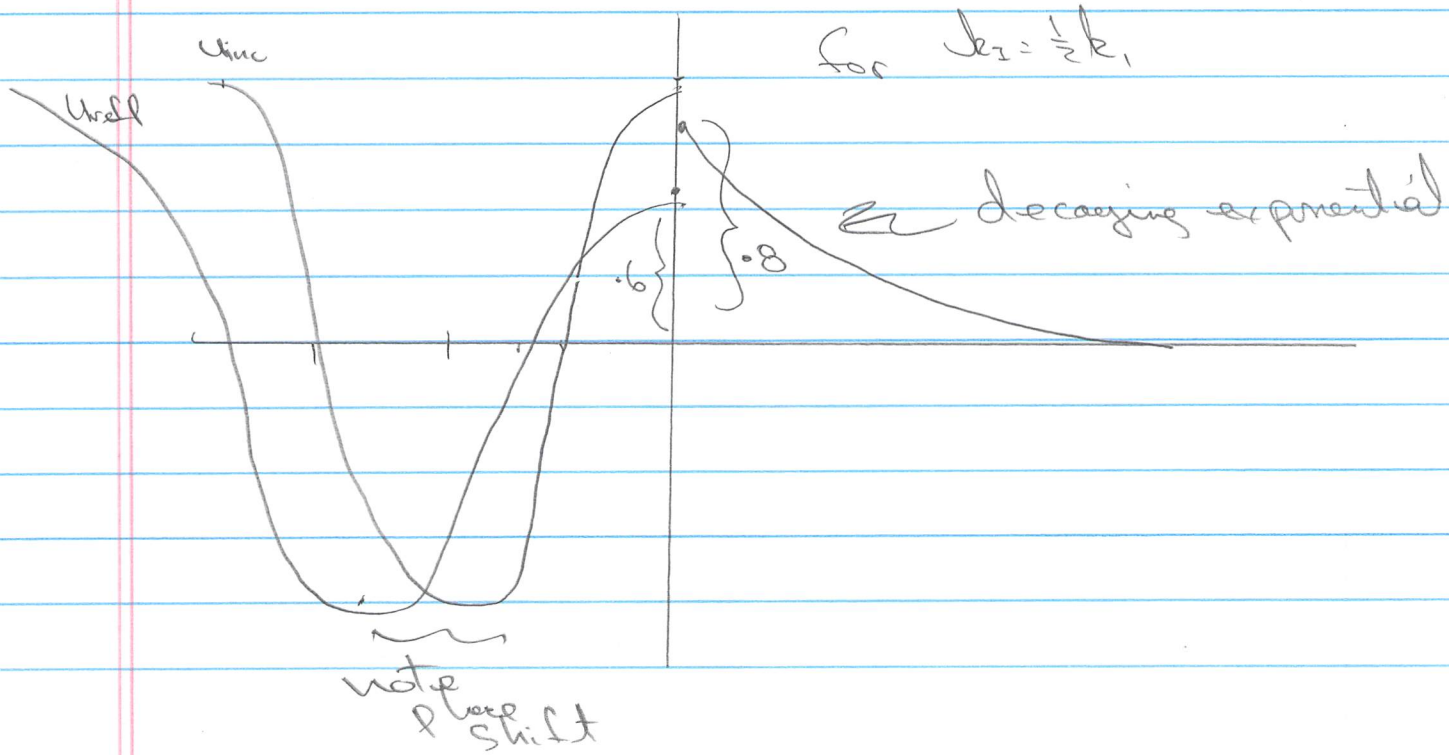
In region (1) k_1 is pure real

$$\therefore S_{refl} = -\frac{\hbar k_1}{m}|B|^2 = -\frac{\hbar k_1}{m}|A|^2 \quad (21)$$

$$R = \left|\frac{S_{refl}}{S_{inc}}\right| = 1 \quad (22)$$

$$T = 0 \quad (23)$$

$$R + T = 1$$



The phase shift

for $V_0 > E$

$$B = \frac{k_1 - ik_2}{k_1 + ik_2} A$$

$$= e^{i\phi} A$$

$$e^{i\phi} = \frac{k_1 - ik_2}{k_1 + ik_2}$$

$$= \frac{(k_1 - ik_2)^2}{|k_1 + ik_2|^2} = \frac{k_1^2 - k_2^2 - 2ik_1k_2}{k_1^2 + k_2^2}$$

$$\cos\phi + i\sin\phi = \frac{k_1^2 - k_2^2 - 2ik_1k_2}{k_1^2 + k_2^2}$$

$$\left.\begin{aligned} \cos\phi &= \frac{k_1^2 - k_2^2}{k_1^2 + k_2^2} \\ \sin\phi &= \frac{-2k_1k_2}{k_1^2 + k_2^2} \end{aligned}\right\} \quad (24)$$

1D - time independent bound state problems in QM (one energy)

The time-indep one energy (monochromatic) 1D NR SE eq'n

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + V(x)u(x) = Eu(x) \qquad (1)$$

Simplest (but relevant) example to nuclear physics

$$V(x) = +\infty \quad \text{for} \quad x \le 0 \;\&\; x \ge L$$
$$0 \quad \text{for} \quad 0 \le x \le L$$

boundary conditions (bc)

$$u(x) = 0 \quad \text{for} \quad x \le 0 \;\&\; x \ge L \qquad (2)$$

$$-\frac{\hbar^2}{2m}u'' - Eu = 0$$

or

$$u'' + k^2 u = 0 \qquad (3)$$

$$k = \left[\frac{2mE}{\hbar^2}\right]^{1/2} \qquad (4)$$

Solutions: For this case it is more convenient to use sin's & cosine's

Solutions to (1)

$$u(x) = A\sin kx + B\cos kx \quad (5)$$

Apply bc (2) at the left boundary

$$u(0) = 0 \qquad B\cos(0) \Rightarrow B = 0$$
$$u(L) = 0 = A\sin kL \Rightarrow kL = n\pi \quad (6)$$
$$n = 1, 2, 3, 4, \ldots$$

So $k_2 = k_n \Rightarrow$

$$\frac{2mE_nL^2}{\hbar^2} = n^2\pi^2$$

$$\boxed{k_n = n\pi/L \qquad n = 1, 2, 3, \ldots \infty}$$
$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}} \quad (7)$$

So, bound state problems are "eigenvalue" problems where eigenfunctions have discrete energies associated with them.

Before we write down the solution, we must normalize the "eigenfunctions".

Norm

$$1 = \int_0^L dx |A|^2 \sin^2 k_n x \quad (8)$$

Let $\theta = k_n x = \frac{n\pi x}{L}$ (9)

(9) → (8) ⇒ $1 = \frac{|A|^2}{n\pi} \int_0^{n\pi L} d\theta \sin^2\theta$

$$= \frac{|A|^2}{n\pi}\left(\frac{n\pi L}{2}\right) = |A|^2 \frac{L}{2}$$

$$\Rightarrow A = \sqrt{\frac{2}{L}} \quad (10)$$

So, now we have our complete solution

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin k_n x$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad (11)$$

General Properties of Eigenfunctions

1) All bound state problems can be expressed in terms of eigenfunctions, each normalized to 1, each with a unique "eigenenergy". (eigen is German for "special")

2) The smallest eigenenergy is called the "ground state" energy

3) Eigenfunctions satisfy the property of orthogonality

i.e. $\int dx\, u_n^* u_m = 0 \qquad n \neq m$

and normality

$$\int dx\, u_n^* u_n = 1$$

Collectively, this is called

"orthonormality"

$$\int dx\, u_n u_m = \delta_{nm} \quad (12)$$

$$\delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases}$$ Kronecker's delta

Proof of orthonormality for our example

$$I_{nm} = \int dx\, u_n^* u_m \quad \text{(general)} \qquad = \quad \text{specific} \quad \frac{2}{L}\int_0^L dx \sin\frac{n\pi x}{L}\sin\frac{m\pi x}{L}$$

Let $\theta = \frac{\pi x}{L}$ $\qquad dx = \frac{L}{\pi} d\theta$

$$I_{nm} = \frac{2}{L}\cdot\frac{L}{\pi}\int_0^{\pi} d\theta \sin n\theta \sin m\theta$$

$$= \frac{2}{\pi}\cdot\frac{1}{2}\int_{-\pi}^{\pi} d\theta \sin n\theta \sin m\theta$$

$$= \frac{1}{\pi}\int_{-\pi}^{\pi} d\theta \left[\frac{e^{in\theta} - e^{-in\theta}}{2i}\right]\left[\frac{e^{im\theta} - e^{-im\theta}}{2i}\right]$$

$$-\frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \left\{ e^{i(n+m)\theta} - e^{i(n-m)\theta} - e^{i(m-n)\theta} + e^{-i(n+m)\theta} \right\}$$

$= 0$, always $\qquad = 0$ if $n \neq m$

$$= -\frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \left\{ 2\cos(n+m)\theta - 2\cos(n-m)\theta \right\}$$

$$= 0 \quad \text{if} \quad n \neq m$$

if $n = m$ $\qquad I_{nn} = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta = 1$ ⌐

$$I_{nm} = \delta_{nm}$$

Aside:
Kronecker δ function
$\delta_{nm} = 0$ if $n \neq m$
$= 1$ if $n = m$
} n, m are integers

A "composite" wavefunction can be made up of two or more (even an ∞ number) of eigenfunctions (question 4 on Q1)

e.g. if $\phi(x)$ is a candidate wf,

$\int_0^L dx\,|\phi(x)|^2$ must exist

Set $\int_0^L dx\,|\phi(x)|^2 = |N|^2$

Then

$$\psi(x) = \frac{1}{N}\phi(x)$$

$\psi(x)$ must vanish at $x=0, L$, finite everywhere, ψ, ψ' continuous everywhere

$\psi(x)$ is expressible as $\psi'(0), \psi'(L)$ maybe discontinuous

$$\psi(x) = \sum_{n=1}^{\infty} a_n u_n(x)$$

↑ wavefunctions

By orthonormality

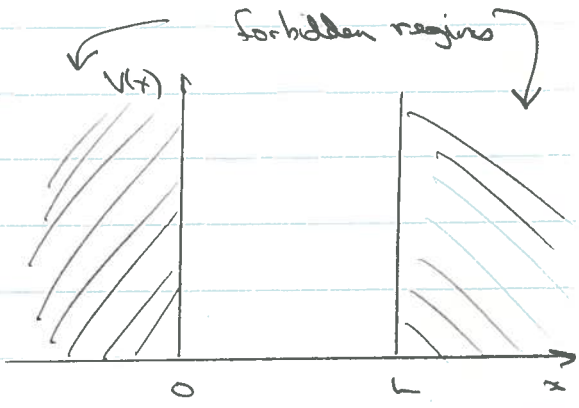
$$\int_0^L dx\, u_m^*(x)\psi(x) = \sum_{n=1}^{\infty} a_n \underbrace{\int_0^L dx\, u_m^* u_n}_{=\delta_{nm}}$$

$$= a_m$$

$$\boxed{a_m = \int_0^L dx\, u_m^* \psi}$$

Continuation of the infinite square well potential

Recall from last week ...



$$V(x) = \begin{cases} 0 & 0 \le x \le L \\ \to \infty & \text{otherwise} \end{cases} \quad (1)$$

The wavefunction must be = 0 in regions where the potential is infinite.

Why? Let $V = V_0$ be very large in the region $x > L$

In this region $k^2 = \frac{2m(E - V_0)}{\hbar^2} = -K^2$ (2)

The SE there is $u'' - K^2 u = 0$

The solution there is of the form:

$$u = Ce^{-Kx} + De^{Kx} \quad (3)$$

We immediately see that we require

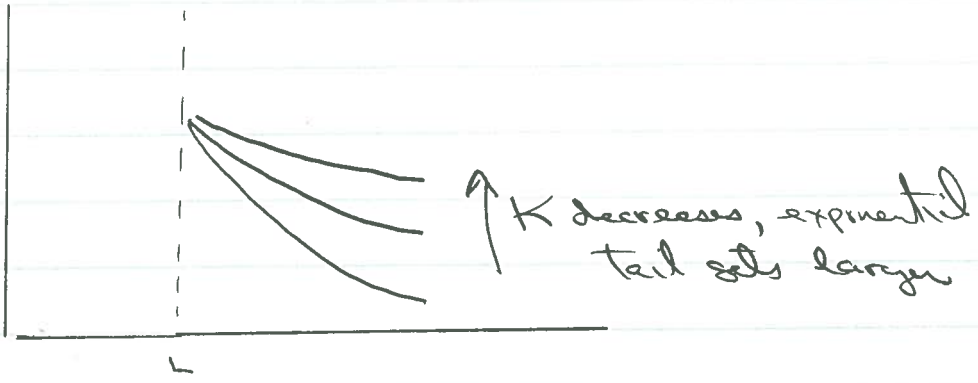
$$D = 0 , \quad (4)$$

otherwise u is not normalizable

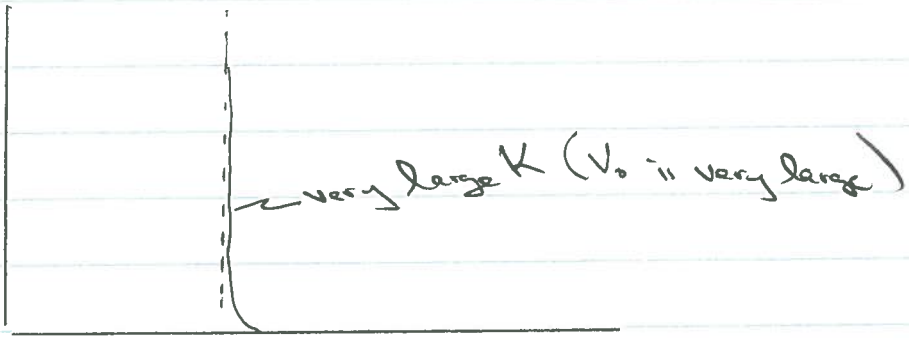
Therefore the soln there is

$$u = Ce^{-Kx} \quad (5)$$

Sketching for 3 different values of K



In the limit as $K \to \infty$, $u = 0$



Inside the limits $0 \le x \le L$, we discovered the complete sol'n to be a set of eigenfunctions

(6)
$$\begin{cases} u_n = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} & n = 1,2,3,\ldots \quad \leftarrow \text{eigenfunctions} \\ k_n = \frac{n\pi}{L} & \leftarrow \text{wave number (quantized)} \\ E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} & \leftarrow \text{energy} \end{cases}$$

Aside: Deriving E_n from u_n.
Since E_n is all kinetic

$$E_n = \int_{-\infty}^{\infty} dx\, u_n^* \underbrace{\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)}_{T_{op}} u_n \qquad \text{(general expression)}$$

$$= \int_0^L dx \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}$$

$$= \int_0^L dx \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \left(\frac{\hbar^2 n^2\pi^2}{2mL}\right) \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}$$

constant, comes outside

$$= \frac{\hbar^2 n^2\pi^2}{2mL^2} \int_0^L dx \underbrace{\sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}}_{u_n^*} \underbrace{\sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}}_{u_n}$$

$$= \frac{\hbar^2 n^2\pi^2}{2mL^2} (1) \text{ by the normalization}$$

$$E_n = \frac{\hbar^2 n^2\pi^2}{2mL^2} \qquad \text{QED}$$

Yet another example.

Construct an illustrative soln to the infinite square well, a composite

(7) $u = Nx(L-x)$

$u(0) = 0$ ✓

$u(L) = 0$ ✓

u' continuous ✓

u continuous ✓

normalizable? (Yes)

$$1 = \int_{-\infty}^{\infty} dx\, u^* u \qquad \text{general}$$

$$= |N|^2 \int_0^L dx\, x^2(L-x)^2$$

$$= |N|^2 L^5 \int_0^1 dz\, z^2(1-z)^2 \qquad (\text{using } z = x/L)$$

$$= |N|^2 L^5 \int_0^1 dz\, (z^2 - 2z^3 + z^4)$$

$$= |N|^2 L^5 \left\{ \frac{1}{3} - \frac{2}{4} + \frac{1}{5} \right\}$$

$$= \frac{|N|^2 L^5}{30}$$

$$N = \sqrt{\frac{30}{L^5}} \qquad (8)$$

$$u = \sqrt{\frac{30}{L^5}}\, x(L-x) \qquad (9)$$

E is totally kinetic, since $V = 0$ for $0 \le x \le L$

$$K = E = \int_{-\infty}^{\infty} dx\, u^* \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) u \qquad \text{general}$$

$$= \int_0^L dx \sqrt{\frac{30}{L^5}}\, x(L-x) \qquad \sqrt{\frac{30}{L^5}} \qquad u'' = -2\sqrt{\frac{30}{L^5}}$$

$$-\frac{\hbar^2}{2m} u'' = \frac{\hbar^2}{m} \sqrt{\frac{30}{L^5}}$$

$$= \frac{30}{L^5} \frac{\hbar^2}{m} \int_0^L dx\, x(L-x)$$

$$= \frac{30}{L^5} \frac{\hbar^2}{m} L^3 \int_0^1 dx\, z(1-z)$$

$$= \frac{30}{L^2} \frac{\hbar^2}{m} \underbrace{\int_0^1 dz\, (z - z^2)}_{= \frac{1}{6}}$$

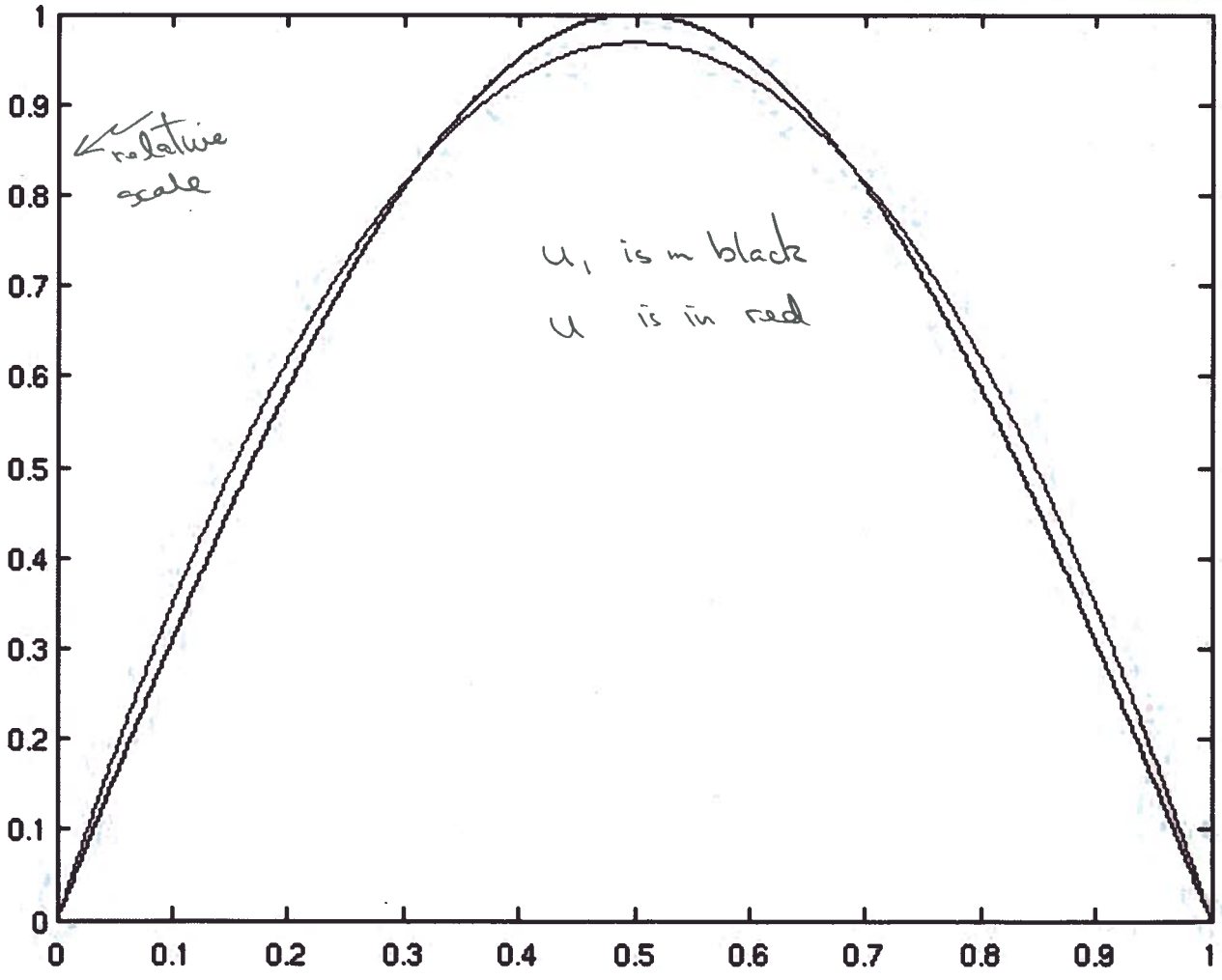
$$K = \frac{5\hbar^2}{mL^2} \quad (10)$$

cf K_n $\qquad K_1 = \frac{\hbar^2\pi^2}{2mL^2} = (4.9348)\frac{\hbar^2}{mL^2}$

$$K_2 = \frac{4\hbar^2\pi^2}{2mL^2} = \frac{2\hbar^2\pi^2}{mL^2}$$

19.7392

$u = \sqrt{\frac{30}{L^5}}\, x(L-x)$ is mostly u_1, with some higher n's thrown in.



As a composite set of eigenfunctions?

Before we do this, introduce Dirac's bra-ket notation.

$|n\rangle$ stands for $u_n(x)$ "ket"

$\langle m|$ stands for $u_m^*(x)$ "bra"

$\langle m|n\rangle$ stands for $\int_{-\infty}^{\infty} dx\, u_m^*(x)\, u_n(x)$

By orthonormality,

$\langle m|n\rangle = \delta_{mn}$ = 1 if $n = m$

= 0 if $n \neq m$

$\langle m|\hat{O}|n\rangle$ ← some operator stands for $\int_{-\infty}^{\infty} dx\, u_m^*(x)\, \hat{O}\, u_n(x)$

examples $\langle m|1|n\rangle = \delta_{mn}$

$\langle m|\hat{K}|n\rangle = \int_{-\infty}^{\infty} dx\, u_m^*(x) \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) u_n(x)$

↑ KE operator

$= \underbrace{\frac{\hbar^2 n^2 \pi^2}{2mL^2}}_{E_n} \delta_{mn}$

So $\quad u = \sum_{n=1}^{\infty} a_n |n\rangle$

$$\langle m|u\rangle = \sum_{n=1}^{\infty} a_n \langle m|n\rangle$$

$$= \sum_{n=1}^{\infty} a_n \delta_{mn}$$

$$= a_m$$

$$a_m = \langle m|u\rangle = \int_0^6 dx\, u_m^* u \qquad \text{(general)}$$

$$= \int_0^L dx \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \sqrt{\frac{30}{L^5}}\, x(L-x)$$

$$= \frac{\sqrt{60}}{L^3} \int_0^L dx \sin\frac{n\pi x}{L}\, x(L-x)$$

$$= \sqrt{60} \int_0^1 dz \sin n\pi z \; z(1-z)$$

$$= \sqrt{60} \left\{ \int_0^1 dz\, z \sin n\pi z - \int_0^1 dz\, z^2 \sin n\pi z \right\}$$

$$\frac{2\sqrt{60}\,(1-(-1)^n)}{n^3\pi^3}$$

Note: $\quad 1-(-1)^n = 0$ when n is even

$= 2$ when n is odd

$$a_n = \frac{4\sqrt{60}}{n^3\pi^3} \qquad n \text{ odd}$$

The power spectrum

$$a_1 = \frac{4\sqrt{60}}{\pi^3} = 0.999277$$

$a_n = a_1/n^3$

$a_1/a_1 = 1$
$a_2/a_1 = 0$
$a_3/a_1 = \frac{1}{27}$
$a_4/a_1 = 0$
$a_5/a_1 = \frac{1}{125}$

← mostly a_1

etc...

Kinetic energy?

$$K = \langle u|\hat{K}|u\rangle \qquad \left(\frac{5\hbar^2}{2mL^2}\right)$$

$$= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} \langle a_m u_m|\hat{K}|a_n u_n\rangle$$

$$= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} a_m^* a_n \langle u_m|K_n u_n\rangle$$

$$= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} a_m^* a_n \frac{\hbar^2\pi^2 n^2}{2mL^2} \underbrace{\langle u_m|u_n\rangle}_{=\delta_{mn}}$$

$$= \frac{\hbar^2\pi^2}{2mL^2}\sum_{n=1}^{\infty} |a_n|^2 n^2 \qquad a_n = \frac{4\sqrt{60}}{n^3\pi^3}$$

n odd

$$= \frac{\hbar^2\pi^2}{2mL^2}\sum_{n=1}^{\infty} \frac{16\cdot 60}{n^6\pi^6} n^2$$

$$= \frac{\hbar^2 480}{mL^2\pi^4}\sum_{\substack{n=1\\ n\,\text{odd}}}^{\infty} \frac{1}{n^4}$$

$$= \frac{\hbar^2 480}{mL^2\pi^4} \underbrace{\sum_{n=1}^{\infty} \frac{1}{(2n-1)^4}}_{\text{all } n} = \frac{\pi^4}{96}$$

See Gradshteyn & Ryzhik 0.234(5.)

$$= \frac{5\hbar^2}{mL^2}$$ as expected

Parity

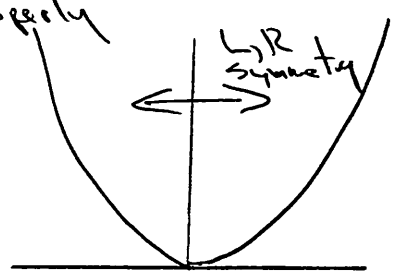
Fact Every symmetry in nature results in a conserved quantity, expressed by a quantum number.

"Parity" results from the exchange of spatial coordinate

$$x \rightleftharpoons -x$$

How does this work?

Consider a potential $V(x)$ that is arbitrary, except that it has the property



$$V(-x) = V(x)$$

e.g. $V(x) = \frac{1}{2}kx^2$

$$V(-x) = \frac{1}{2}k(-x)^2$$

$$= \frac{1}{2}kx^2$$

$$V(-x) = V(x)$$

The SE is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}u(x) + V(x)u(x) = Eu(x) \quad (1)$$

Let Π represent the parity operator.
It operates in a similar sense to the operation of complex conjugation, but instead of changing the sign of i, Π changes the sign of x.

e.g $\Pi u(x) = u(-x)$

$\Pi \left(\frac{d^2}{dx^2}\right) = \frac{d^2}{dx^2}$

So, Π on (1) $\Rightarrow$

$$\Pi \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) + V(x)u(x) \right) = E\Pi u(x)$$

$$-\frac{\hbar^2}{2m}u(-x) + V(x)u(-x) = Eu(-x) \quad (2)$$

($V(x)$ ↑ did not change, this is important!)

(2) $\Rightarrow$ if $u(x)$ is a soln to the SE
$u(-x)$ is a " " " <u>same</u> SE

Operate Twice with Π

Π^2(1) $\Rightarrow$

$$\frac{\hbar^2}{2m}u(x) + V(x)u(x) = E\Pi^2 u(x) = Eu(x)$$

$$\Rightarrow \Pi^2 u(x) = u(x) \quad (3)$$

So, assign a quantum # p to the operation of parity.

From (3) $\quad \Pi^2 u = p^2 u \quad (4)$

$\Rightarrow \quad p^2 = 1$

$\Rightarrow \quad \boxed{p = \pm 1} \quad (5)$

Parity, if it exists, can only have one of two values, $+1$ or -1.
(even parity) (odd parity)

Recall the infinite square well potential

$$V(x) = \begin{cases} 0 & 0 \le x \le L \\ \to \infty & \text{otherwise} \end{cases}$$

We did not see parity there, because $V(x) \neq V(-x)$ in this case.

So, re-analyze the problem making the parity evident.

"Hidden" parity

$V(x) = 0 \quad 0 \le x \le L, \to \infty$ else

$E_n = \dfrac{\hbar^2 n^2 \pi^2}{2mL^2} \quad n = 1,2,3,\ldots$

$u_n = \sqrt{\dfrac{2}{L}} \sin \dfrac{n\pi x}{L}$

"Explicit" parity

$V(x) = 0 \quad -\frac{L}{2} \le x \le \frac{L}{2}, \to \infty$ else

$E_n = \dfrac{\hbar^2 n^2 \pi^2}{2mL^2}$, $n = 1,2,3,\ldots$

(no change in physics)

$u_n = \sqrt{\dfrac{2}{L}} \sin\left(\dfrac{n\pi}{L}\left(x + \frac{L}{2}\right)\right)$

note:

examine

$$u_n = \sqrt{\frac{2}{L}} \sin\left[\frac{n\pi}{L}\left(x + \frac{L}{2}\right)\right]$$

$$= \sqrt{\frac{2}{L}} \sin\left[\frac{n\pi x}{L} + \frac{n\pi}{2}\right]$$

$$= \sqrt{\frac{2}{L}} \left[\sin\left(\frac{n\pi x}{L}\right)\cos\frac{n\pi}{2} + \cos\left(\frac{n\pi x}{L}\right)\sin\frac{n\pi}{2} \right]$$

$\cos\frac{n\pi}{2} = 0$ when n is odd $1,3,5\ldots$

$\sin\frac{n\pi}{2} = 0$ when n is even

odd parity solutions

$u(-x) = -u(x)$

n even

even parity solutions

$u(x) = u(-x)$

n odd

So right now we are in the awkward position where

$\sin \frac{n\pi x}{L}$ is the solution when n is even

$\cos \frac{n\pi x}{L}$ " " " " " " odd

So, let's make another change $n \to n+1$ and state the solution for.

$$V(x) = 0 \qquad -\tfrac{L}{2} \le x \le \tfrac{L}{2}$$

$$E_n = \frac{\hbar^2 (n+1)^2 \pi^2}{2mL^2} \qquad n = 0, 1, 2, \ldots$$

(note: $(n+1)^2$; note: $n = 0, 1, 2, \ldots$)

$$u_n = \begin{cases} \sqrt{\frac{2}{L}} \cos \frac{(n+1)\pi x}{L} & n = 0, 2, 4, \ldots \text{ (even)} \quad \text{even parity} \\ \sqrt{\frac{2}{L}} \sin \frac{(n+1)\pi x}{L} & n = 1, 3, 5 \text{ (odd)} \quad \text{odd parity} \end{cases}$$

Now the even n's are associated with even parity solutions, and odd n's with odd parity solutions.

Why is parity important?

1) Parity is a conserved quantum number
2) Nature chooses its wavefunctions to be either even or odd.
3) Nuclei in their ground state are either even or odd parity (This will be seen to be important in NERS312
4) Making the symmetry evident can save a lot of calculation.

example. Recall $u = Nx(L-x)$ in the asymmetric infinite well.

In the symmetric well $x \rightarrow x + \frac{L}{2}$

$$u = N\left(x+\frac{L}{2}\right)\left(\frac{L}{2}-x\right)$$

$$= -N\left(x^2 - \frac{L^2}{4}\right)$$

As seen above u_1 is an even function. Therefore, as a conjecture, we can immediately write

$$u = \sum_{\substack{n=0 \\ n \text{ even}}}^{\infty} a_n u_n$$ } only even eigenfunctions contribute

5) Using parity, you can instantly tell if the expectation value of an operator (if it has a known parity) will be zero.

That is

$\langle m|\hat{O}|n\rangle = 0$ if $\hat{O}$ has even parity and m, n have different parities.

$\langle m|\hat{O}|n\rangle = 0$ if $\hat{O}$ has odd parity and m, n have the same parity

For the symmetric well

e.g. $\langle 5|x^3|3\rangle = 0$

$\langle 18|x^5|2\rangle = 0$

odd

same parities

$\langle 4|x^3|3\rangle = 0$

$\langle 1027|x^4|1026\rangle = 0$

even

different parities

Transition rates

The transition rate for initial state "i" to final state "f" is given by

$$\lambda_{i\to f} \propto |\langle f|\hat{O}|i\rangle|^2 \qquad (6)$$

($\hat{O}$: operator that causes the transition)

Thus, we can easily compare the relative transition rates from two different levels.

Example Assume that $\hat{O} = x$.
(This is very close to the γ-transition operator)

For the infinite potential well, what is

$$r = \frac{\lambda_{2\to 0}}{\lambda_{1\to 0}} ; \frac{\lambda_{3\to 0}}{\lambda_{1\to 0}} ; \frac{\lambda_{4\to 0}}{\lambda_{1\to 0}} ; \frac{\lambda_{5\to 0}}{\lambda_{1\to 0}}$$

i	1	2	3	4	5
$r_i = \frac{\lambda_{i\to 0}}{\lambda_{1\to 0}}$	r_i	1 :	0 :	0.0064 :	0 :	0.00049

(0: can exclude due to parity)

$$\frac{r_3}{r_5} \simeq 13$$

$$r_3' = \frac{\lambda_{3\to 0}}{\lambda_{1\to 0}} = \frac{|\langle 0|x|3\rangle|^2}{|\langle 0|x|1\rangle|^2}$$

$$= \frac{\left| \int_{-4/2}^{4/2} dx \sqrt{\frac{2}{L}} \cos \pi x/L \,(x) \sqrt{\frac{2}{L}} \sin 4\pi x/L \right|^2}{\left| \int_{-4/2}^{4/2} dx \sqrt{\frac{2}{L}} \cos \pi x/L \,(x) \sqrt{\frac{2}{L}} \sin 2\pi x/L \right|^2}$$

$z = \frac{\pi x}{L}$

$$= \left| \frac{\int_{-\pi/2}^{\pi/2} dz \; z \cos z \sin 4z}{\int_{-\pi/2}^{\pi/2} dz \; z \cos z \sin 2z} \right|^2$$

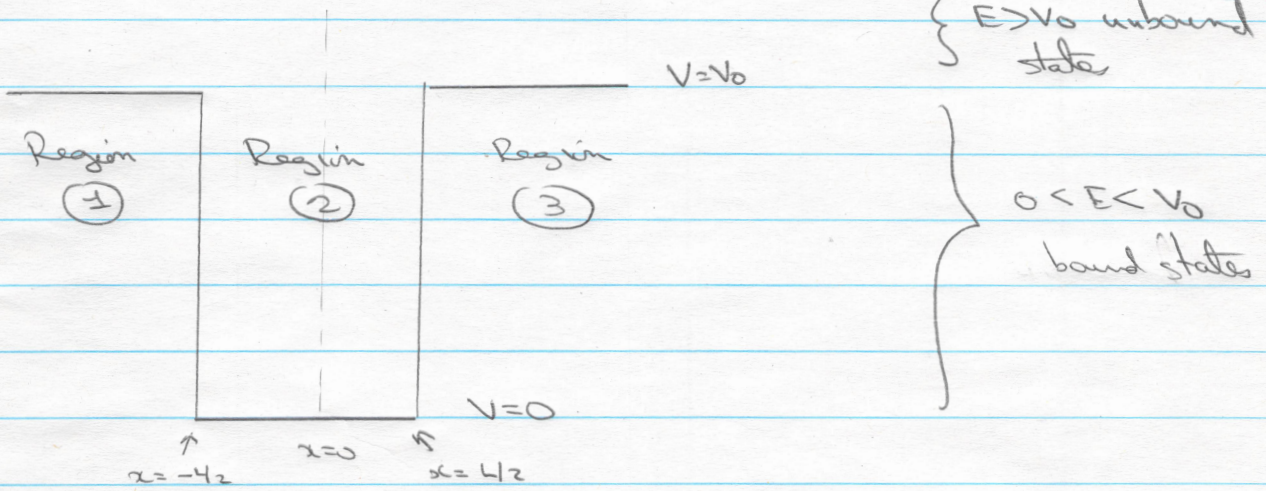
$$= 4/625 = 0.0064 \quad \text{mathematica}$$

$r_5 =$ (replace "4" above with "6")

$$= \frac{729}{1500625} = 0.00049$$

$$\frac{r_5}{r_3} = 0.076$$

Bound states of the 1D finite well potential



So far, we have only considered unbound states of this potential. ($E > V_0$). Now we consider <u>bound</u> states $E < V_0$.

The SE for this system:

$$-\frac{\hbar^2}{2m}u'' + Vu = Eu \qquad (1)$$

$(1) \times \left(\frac{-2m}{\hbar^2}\right) \Rightarrow$

$$u'' + k^2 u = 0 \qquad (2)$$

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

Tangential questions:
How does the particle get "bound"?
What is this a model for?

Two cases.

Outside the well, $k^2 = \frac{2m(E-V_0)}{\hbar^2} = -K^2$

$$K^2 = \frac{2m(V_0-E)}{\hbar^2} \quad (3)$$

$$u'' - K^2 u = 0 \quad (4)$$

Solutions are of the form:

$$u = A e^{-Kx} + C e^{Kx} \quad (5)$$

For $x < -L/2$ $C = 0$ for normalizability

$x > L/2$ $A = 0$ " "

Inside the well

$$k^2 = \frac{2mE}{\hbar^2}$$

$$u(x) = B \begin{pmatrix} \cos kx \\ \sin kx \end{pmatrix} \quad (6)$$

$\cos kx$: even parity

$\sin kx$: odd parity

So,

(7) $$u(x) = \begin{cases} u_1(x) = A e^{Kx} & x \le -L/2 \\ u_2(x) = B\begin{pmatrix}\cos kx \\ \sin kx\end{pmatrix} & -\frac{L}{2} \le x \le \frac{L}{2} \\ u_3(x) \quad C\ e^{-Kx} & x \ge \frac{L}{2} \end{cases}$$

(8) $$\begin{cases} k^2 = \dfrac{2mE}{\hbar^2} \\ K^2 = \dfrac{2m(V_0 - E)}{\hbar^2} \end{cases}$$

To complete the solution, we require

1) u, u' continuous
2) u normalised

Even states: Continuity at $x = -L/2 \Rightarrow$ from L

$$\frac{u_1'(-\frac{L}{2})}{u_1(-\frac{L}{2})} = \frac{u_2'(-\frac{L}{2})}{u_2(\frac{L}{2})} \quad ; \quad \frac{AK e^{-KL/2}}{A e^{-KL/2}} = \frac{Bk\sin(kL/2)}{B\cos(kL/2)}$$

note: used $\sin(-\Box) = -\sin(\Box)$

$\cos(-\Box) = \cos(\Box)$

Or $K = k\tan(kL/2)$ (9)

We will see the combinations $kL/2$, $KL/2$ frequently

So, define $\alpha \equiv \frac{kL}{2}$; $\beta = \frac{KL}{2}$ (10)

Going back to (8)

$$\alpha^2+\beta^2 = \frac{L^2}{4}\left\{\frac{2mE}{\hbar^2} + \frac{2m(V_0-E)}{\hbar^2}\right\} = \frac{2mV_0L^2}{4\hbar^2}$$

$$\alpha^2+\beta^2 = \frac{mV_0L^2}{2\hbar^2} \quad (11)$$

dimensions check

$$\frac{\left(M\right)\left(\frac{ML^2}{T^2}\right)L^2}{\left[\frac{ML^2}{T^2}\right]^2}$$

dimensionless

[we'll use this result later]

So, $\frac{L}{2} \times (9) \Rightarrow$

$$\boxed{\beta = \alpha\tan\alpha} \quad (12)$$

This is a transcendental equation for k in terms of m, V_0, L, the physical parameters of this application. Only certain values of k (and hence E) satisfy (12). Before showing this, let's derive the analogous relation for the odd parity states.

Odd states:

$$\frac{u_1'(-L/2)}{u_1(-L/2)} = \frac{u_2'(-\frac{L}{2})}{u_2(L/2)} \quad (13)$$

Using (7)

$$\frac{AKe^{-kL/2}}{Ae^{-kL/2}} = \frac{Bk\cos([-kL/2])}{B\sin([-kL/2])} \qquad (14)$$

or, using $\frac{L}{2} \times (9) \Rightarrow$

$$\boxed{\beta = -\alpha \cot\alpha} \qquad (15)$$

This is the quantization condition for k, in the case of odd states.

The quantized k's in graphical form

The intercepts of $\alpha\tan\alpha$, or $-\alpha\cot\alpha$ with the $\alpha^2+\beta^2$ circle determines $K(E,V_0)$ in terms of $k(E)$

(Show graph)

Strategy

1) Find α_0 knowing that $\alpha_0 < \frac{\pi}{2}$, and hence β_0

Do a zero find on

$$\beta_0 = \alpha_0 \tan\alpha_0$$

or $$0 = \alpha_0\tan\alpha_0 - \beta_0$$

$$= \alpha_0\tan\alpha_0 - \sqrt{\underbrace{(\alpha_0^2+\beta_0^2)}_{\frac{mV_0L^2}{2\hbar^2}} - \alpha_0^2}$$

$E_0 = 0.78491$

$E_1 = 3.1339$

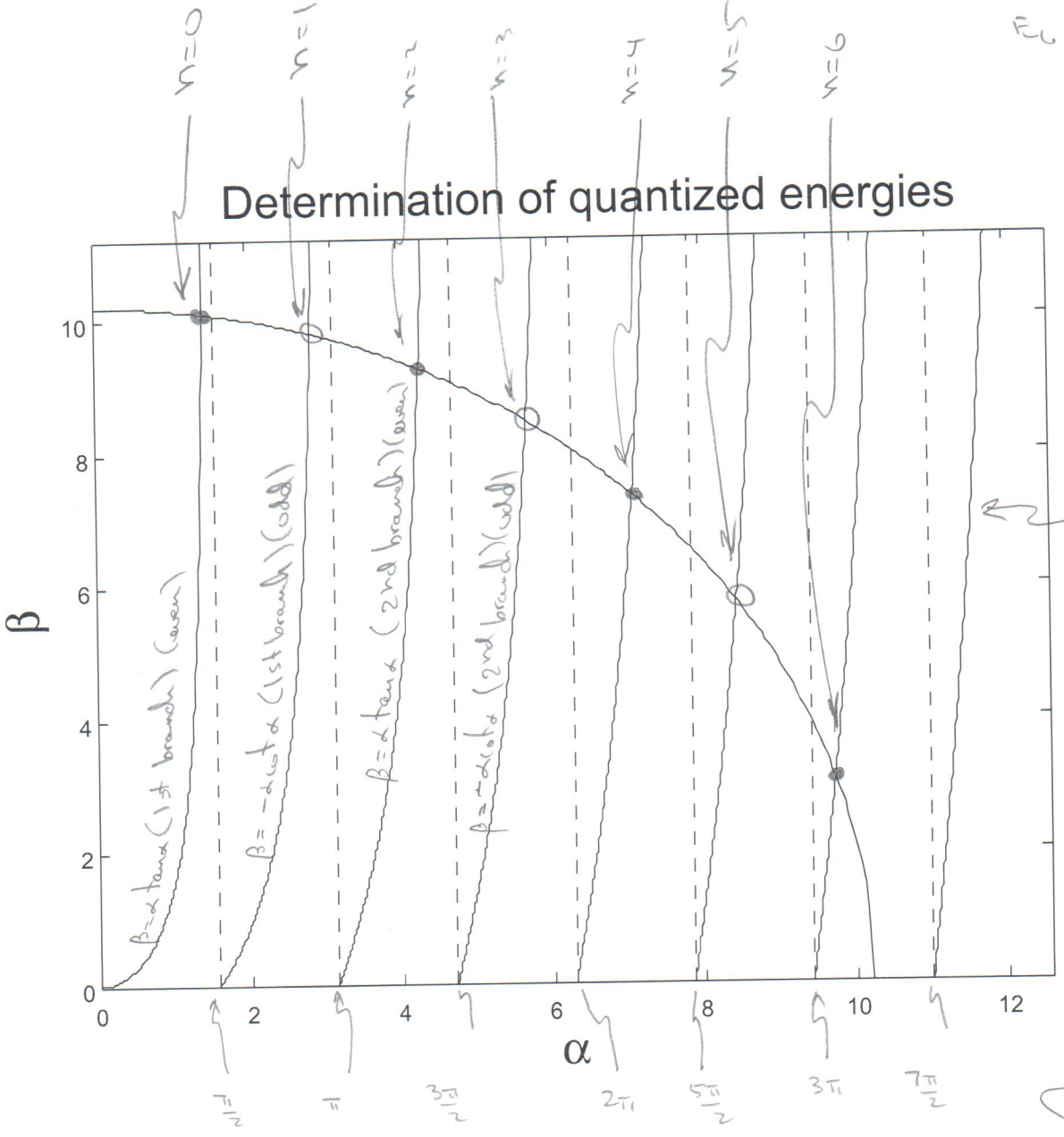
$E_2 = 7.0283$

$E_3 = 12.431$

$E_4 = 19.271$

$E_5 = 27.397$

$E_6 = 36.341$



e.g. ^{90}Zr

$V_0 = 40 MeV$

$L = 7.37909$ (fm)

$m_\alpha c^2 = 3727.379$ MeV

2) Find α_1 knowing $\frac{\pi}{2} < \alpha_1 < \pi$

Do a zero find on

$$\beta_1 = -\alpha_1 \cot \alpha_1$$

$$0 = \beta_1 + \alpha_1 \cot \alpha_1$$

$$0 = \sqrt{\underbrace{(\alpha_1^2 + \beta_1^2)}_{\frac{mV_0L^2}{2\hbar^2}} - \alpha_1^2} + \alpha_1 \cot \alpha_1$$

3) continue until exhausted all possibilities

The number of bound states

- There is at least one. ✓
- Calculate the constant

$$C^2 = \alpha^2 + \beta^2 = \frac{mV_0L^2}{2\hbar^2}$$

		Nmax
If $C \leq \pi/2$		1 state (even)
$\pi/2 < C \leq \pi$		2 states ($1_e, 1_o$)
$\pi < C \leq 3\pi/2$		3 states ($2_e, 1_o$)
⋮		
$\frac{(N-1)\pi}{2} < C \leq \frac{N\pi}{2}$		N states

$\left(\frac{N+1}{2}\right)$ even ← integer division

$N - \left(\frac{N+1}{2}\right)$ odd states

The Complete solution

The solution is not complete until we have a normalized wave function

From (7)

$$1 = \int_{-\infty}^{\infty} dx\, u^* u =$$

$$= \int_{-\infty}^{-L/2} dx\, u_1^* u_1 + \int_{-L/2}^{L/2} dx\, u_2^* u_2 + \int_{L/2}^{\infty} dx\, u_3^* u_3 \qquad (16)$$

involves the 3 constants A, B, C
They are not independent

From $u_1(-\frac{L}{2}) = u_2(-\frac{L}{2})$ and (7)

$$A e^{-\beta} = B \begin{pmatrix} \cos\alpha \\ -\sin\alpha \end{pmatrix} \quad (17)$$

From $u_2(\frac{L}{2}) = u_3(\frac{L}{2})$

$$B \begin{pmatrix} \cos\alpha \\ \sin\alpha \end{pmatrix} = C e^{-\beta} \quad (18)$$

(12) & (13) $\Rightarrow$

$$C = B e^{\beta} \begin{pmatrix} \cos\alpha \\ \sin\alpha \end{pmatrix}$$
$$A = B e^{\beta} \begin{pmatrix} \cos\alpha \\ -\sin\alpha \end{pmatrix}$$

and

$$1 = B^* B \left\{ e^{2\beta} \begin{pmatrix} \cos^2\alpha \\ \sin^2\alpha \end{pmatrix} \int_{-\infty}^{-L/2} dx\, e^{2Kx} + \int_{-L/2}^{L/2} dx \begin{pmatrix} \cos^2 kx \\ \sin^2 kx \end{pmatrix} + e^{2\beta} \begin{pmatrix} \cos^2\alpha \\ -\sin^2\alpha \end{pmatrix} \int_{L/2}^{\infty} dx\, e^{-2Kx} \right\}$$

$\Rightarrow$ Lots of tedious work

$$B = \sqrt{\frac{2}{L}}\sqrt{\frac{\beta}{1+\beta}} \quad \Big\} \text{ same for even and odd}$$

So,

$$u(x) = \sqrt{\frac{2}{L}}\sqrt{\frac{\beta}{1+\beta}} \begin{cases} e^{Kx} & x < -\frac{L}{2} \\ \begin{pmatrix}\cos kx \\ \sin kx\end{pmatrix} & -\frac{L}{2} < x < \frac{L}{2} \\ e^{-Kx} & x > \frac{L}{2} \end{cases}$$

Recovering the ∞ well, $V_0 \to \infty$

$\beta \to \infty$ ⟩ exponentials drop off

$$u(x) \underset{V_0 \to \infty}{=} \sqrt{\frac{2}{L}} \begin{pmatrix}\cos k_n x \\ \sin k_n x\end{pmatrix}$$

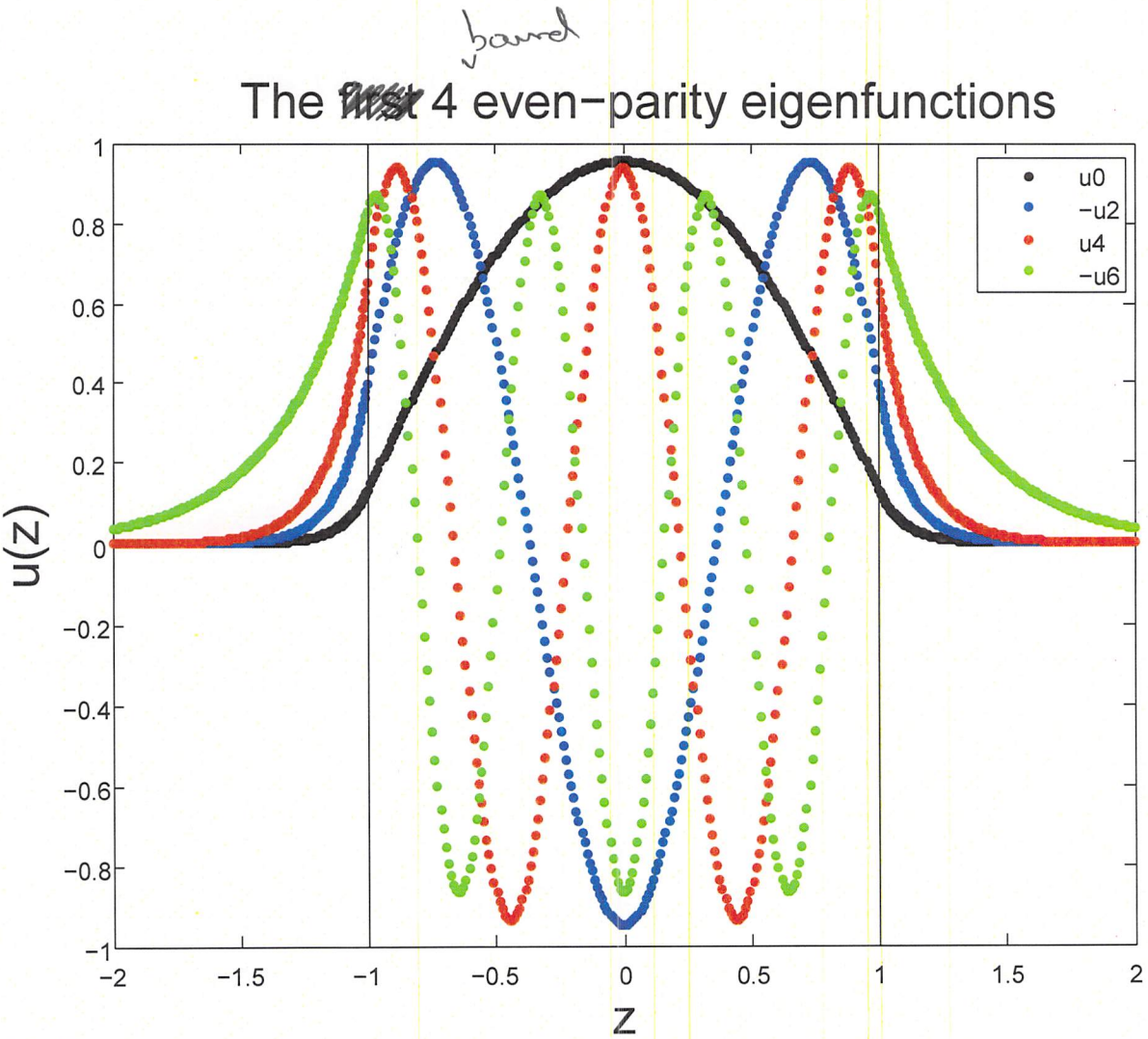
$$\alpha_n = \frac{(n+1)\pi}{2} \qquad n = 0, 1, 2, 3, \ldots \infty$$

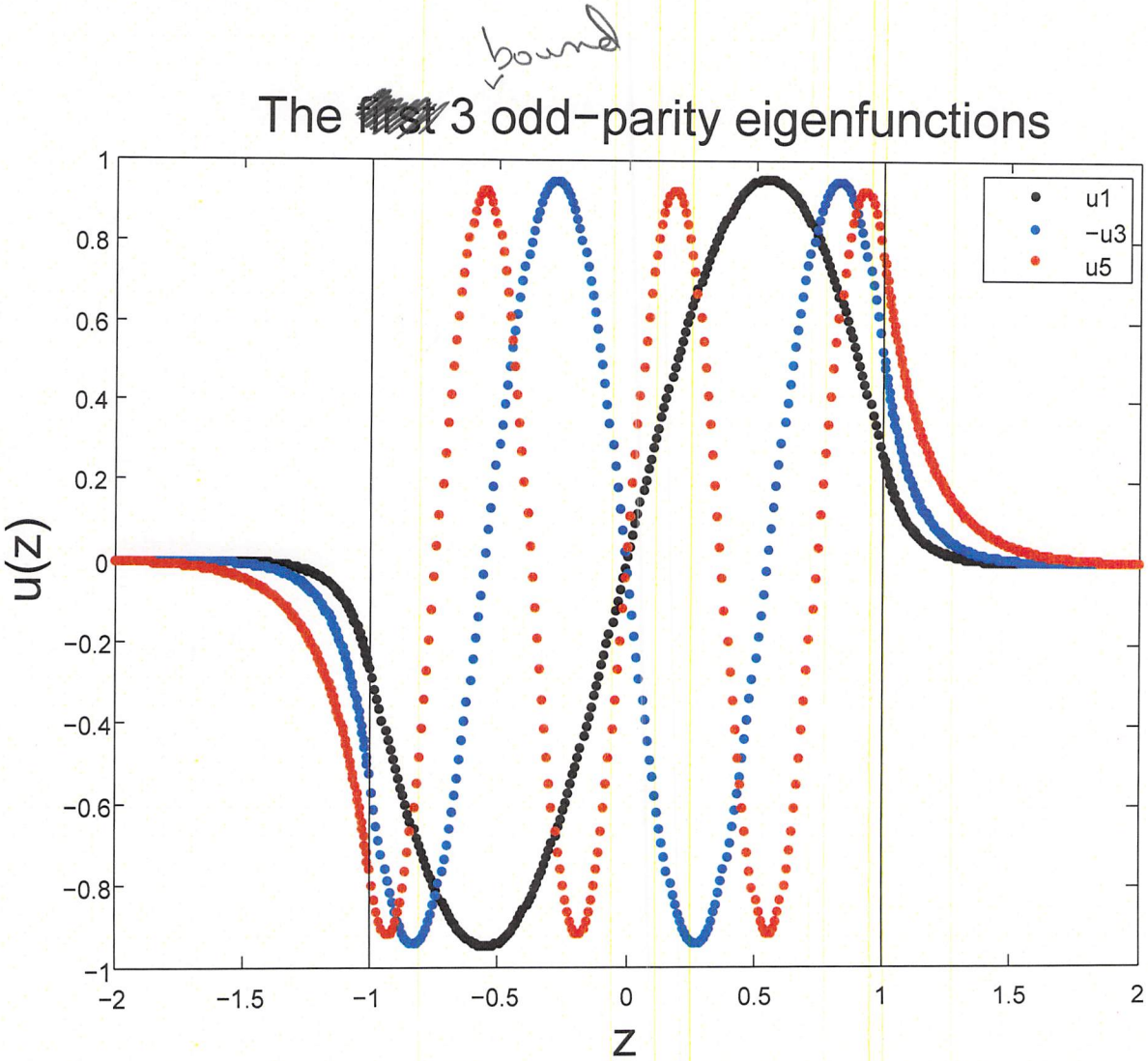
$$E_n \overset{V_0 \to \infty}{=} \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \left(\frac{k_n L}{2}\right)^2 \frac{4}{L^2}}{2m}$$

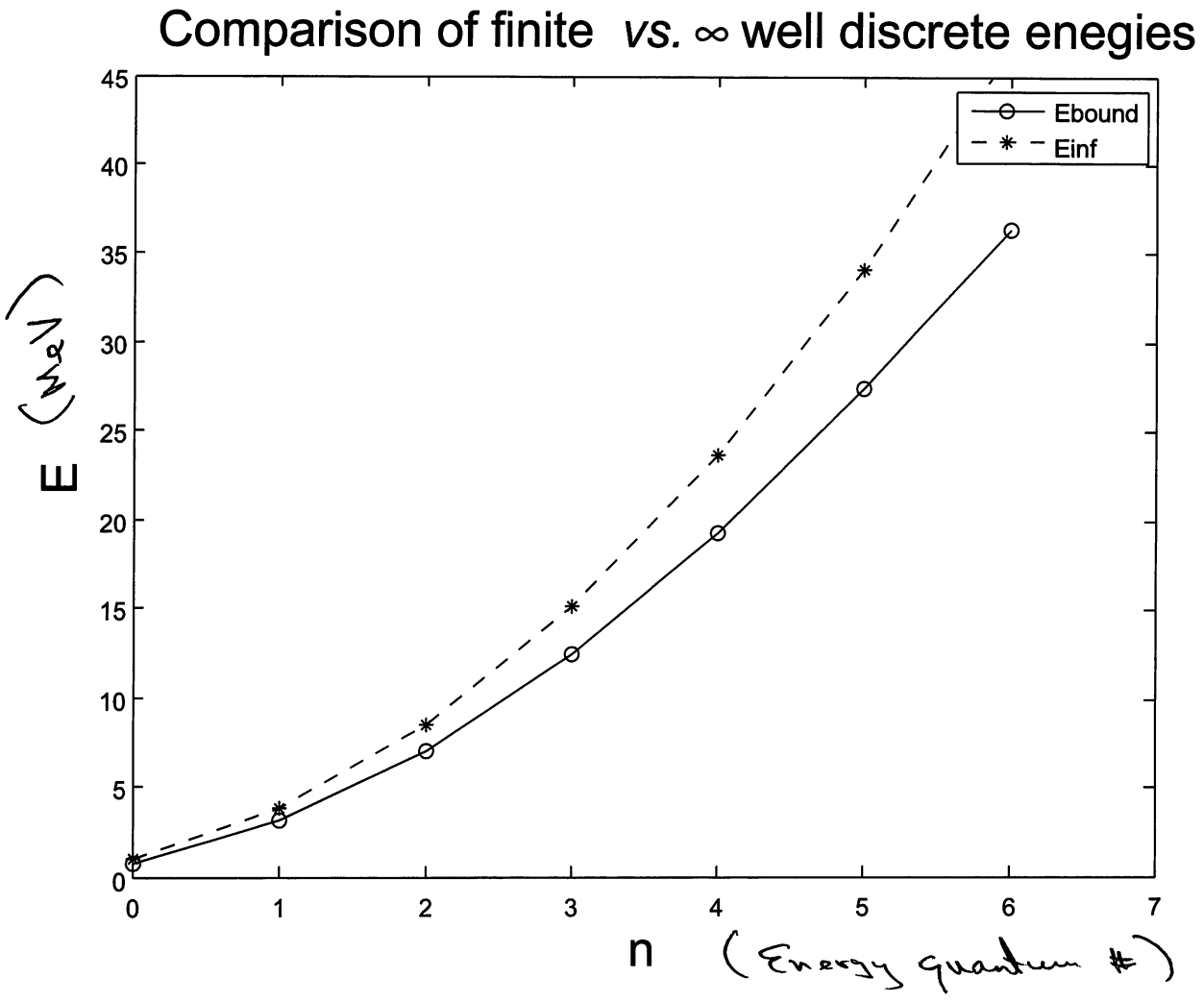
$$= \frac{2\hbar^2}{mL^2}\alpha_n^2$$

$$= \frac{2\hbar^2}{mL^2}(n+1)^2\frac{\pi^2}{4}$$

$$E_n \overset{V=\infty}{=} \frac{\hbar^2 \pi^2 (n+1)^2}{2mL^2}$$


The first 4 even−parity eigenfunctions
u0
−u2
u4
−u6
u(z)
z
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−2
−1.5
−1
−0.5
0
0.5
1
1.5
2


The bound 3 odd−parity eigenfunctions
u1
−u3
u5
u(z)
z
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−2
−1.5
−1
−0.5
0
0.5
1
1.5
2


Comparison of finite vs. ∞ well discrete enegies
Ebound
Einf
E (MeV)
n (Energy quantum #)
0
5
10
15
20
25
30
35
40
45
0
1
2
3
4
5
6
7

The Harmonic potential $V(x) = \frac{1}{2}kx^2$ in Quantum Mechanics

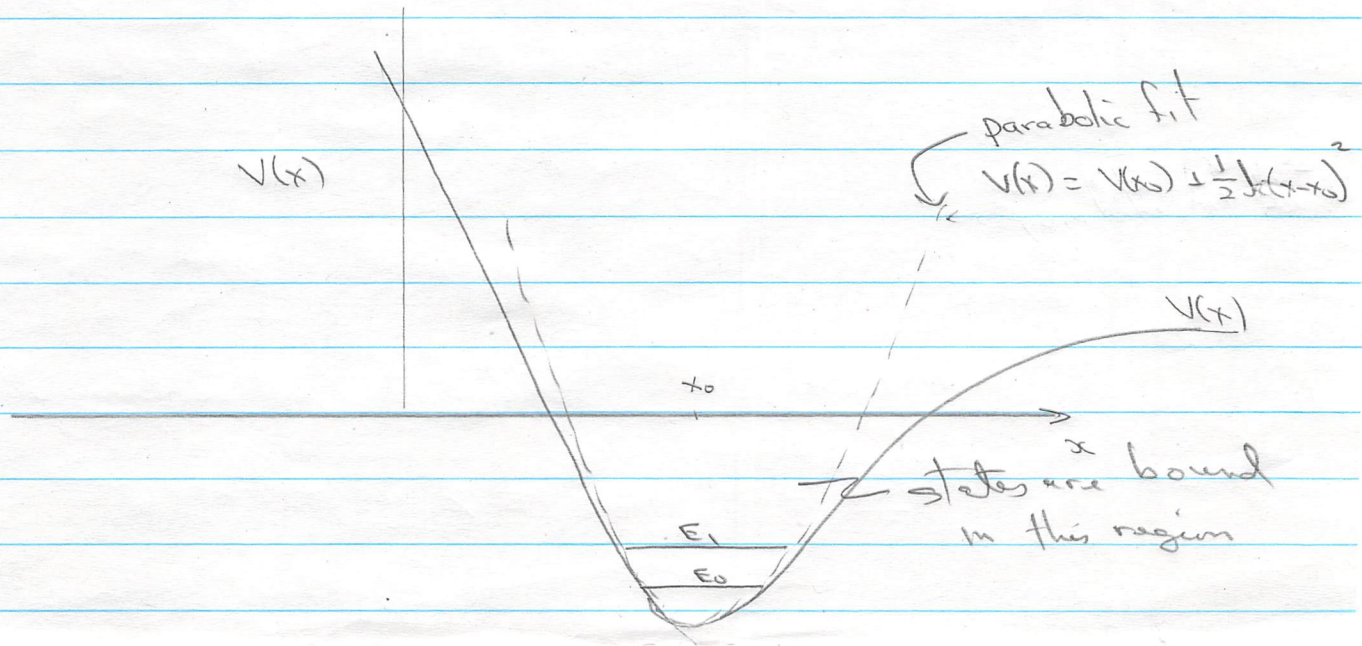
Why is the harmonic potential important?

The general solution to the Time Independent (TI) SE, namely

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) + V(x)u(x) = Eu(x) \qquad (1)$$

is only known analytically in a few special cases. In general, the solutions must be worked out numerically. However, often it is the low lying states, E_0 (ground state), E_1 (first excited) and so on, are of the most interest.

A general $V(x)$ that binds quantum particles has the general form



How is this done?

Let x_0 be that x where $V(x)$ is minimized. Expanding in a Taylor series expansion about x_0, we have

$$V(x) = V(x_0) + \underbrace{V'(x_0)}_{0,\text{ since } V(x) \text{ is minimized at } x_0}(x-x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2 + O((x-x_0)^3) \quad (2)$$

the smaller this is, the better the fit.

Thus, (2) $\Rightarrow$ (1) $\Rightarrow$

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + \left(\frac{1}{2}k(x-x_0)^2\right)u(x) = (E - V(x_0))u(x) \quad (3)$$

or, with $x \to x - x_0$, $E \to E - V(x_0)$

$$-\frac{\hbar^2}{2m}u'' + \left(\frac{1}{2}kx^2\right)u = Eu \quad (4)$$

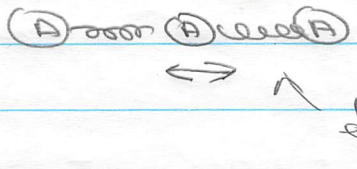
where u are the eigenfunctions about $x = x_0$

$k = V''(x_0)$

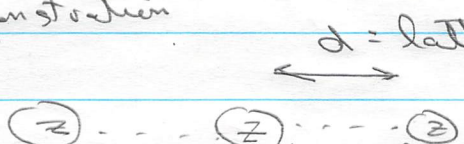
and E is relative to the potential minimum

most important application

GM of atoms in a crystal



demonstration



the potential on the middle atom is (Z is its effective charge)

$$V(x) = \frac{Z^2 e^2}{4\pi\varepsilon_0}\left\{\underbrace{\frac{1}{d-x}}_{\substack{\text{repulsion}\\ \text{from atom}\\ \text{at right}}} + \underbrace{\frac{1}{d+x}}_{\substack{\text{repulsion}\\ \text{from atom}\\ \text{at left}}}\right\}$$

$$V(0) = \frac{Z^2 e^2}{8\pi\varepsilon_0 d}$$

$$V'(0) = \frac{Z^2 e^2}{4\pi\varepsilon_0}\left\{\frac{1}{(d-x)^2} - \frac{1}{(d+x)^2}\right\}\Big|_{x=0} = 0$$

(as expected)

$$V''(0) = \frac{Z^2 e^2}{4\pi\varepsilon_0}\left\{\frac{2}{(d-x)^3} + \frac{2}{(d+x)^3}\right\}\Big|_{x=0} = \underbrace{\frac{Z^2 e^2}{\pi\varepsilon_0 d^3}}_{=k}$$

So $V(x) = \underbrace{\frac{Z^2e^2}{8\pi\varepsilon_0 d}}_{V(0)} + \frac{1}{2}\underbrace{\left(\frac{Z^2e^2}{\pi\varepsilon_0 d^3}\right)}_{k} x^2$

And

$$-\frac{\hbar^2}{2m}u'' + \left(\frac{1}{2}kx^2\right)u = Eu \quad (4) \text{ again}$$

E ↑ energy above $V(0)$

So, ... harmonic potential are important and can be applied to many situations

So! Let's investigate the complete solution to (4).

The QM solution to the Harmonic Oscillator

$$-\frac{\hbar^2}{2m}u'' + \frac{1}{2}kx^2 u = Eu \qquad (4)$$

after about 3 hours of mathematical development (nothing beyond your skill set)

$$E_n = \hbar\omega\left(n+\tfrac{1}{2}\right)$$

$n = 0, 1, 2, \ldots$ (0 ↑ ground state)

$$\omega^2 = \frac{k}{m}$$

eigenfunctions (orthonormal)

$$u_n(x) = \underbrace{\left(\frac{\alpha}{2^n n!\sqrt{\pi}}\right)^{1/2}}_{\text{normalization factor}} \underbrace{\exp\left[-(\alpha x)^2/2\right]}_{\text{Gaussian envelope}} \underbrace{H_n(\alpha x)}_{\text{Hermite polynomial}} \qquad (5)$$

$$\alpha = \left[\frac{mk}{\hbar^2}\right]^{1/4} = \left[\frac{m\omega}{\hbar}\right]^{1/2}$$

$$\underbrace{\langle V\rangle_n = \langle K\rangle_n}_{\text{share equally}} = \frac{E_n}{2}$$

(also the classical result)

info on this?

supplemental notes (online) "Hermite Polynomials.pdf"

Wikipedia searches: "Hermite Polynomials"

"Charles Hermite" 1822–1901

"Frobenius method"

"Ferdinand Georg Frobenius" 1849–1917

⋮

Properties $\langle m|n\rangle = \delta_{mn}$ (orthonormality)

$|n\rangle = u_n$ $\quad \langle m|n\rangle = \int_{-\infty}^{\infty} dx\, u_m^* u_n$

$\langle m| = u_m^*$

Properties of $H_n(z)$

Explicit forms:

$H_0(z) = 1$

$H_1(z) = 2z$

$H_2(z) = 4z^2 - 2$

$H_3(z) = 8z^3 - 12z$

$H_4(z) = 16z^4 - 48z^2 + 12$

⋮

Parity $(-1)^n$

Recursion relationship

(6) $H_{n+1}(z) = 2zH_n(z) - 2nH_{n-1}(z)$ $\quad n \geq 1$

Demonstration of normalization

$$\langle 0|0\rangle = \int_{-\infty}^{\infty} dx\, u_0^* u_0$$

$$= \int_{-\infty}^{\infty} dx\, |u_0|^2$$

$$= \int_{-\infty}^{\infty} dx \left(\frac{\alpha}{\sqrt{\pi}}\right) e^{-(\alpha x)^2}$$

$$= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dz\, e^{-z^2} = 1 \checkmark$$

$$\langle 2|0\rangle = \int_{-\infty}^{\infty} dx\, u_2^* u_0$$

$$= \int_{-\infty}^{\infty} dx \left(\frac{\alpha}{8\sqrt{\pi}}\right)^{1/2} \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-(\alpha x)^2} \left[4(\alpha x)^2 - 2\right]$$

$$= \frac{1}{2\sqrt{2\pi}} \int_{-\infty}^{\infty} dz\, e^{-z^2} \left(4z^2 - 2\right)$$

$$= \frac{1}{2\sqrt{2\pi}} \left\{ 4 \underbrace{\int_{-\infty}^{\infty} dz\, z^2 e^{-z^2}}_{\frac{\sqrt{\pi}}{2}} - 2 \underbrace{\int_{-\infty}^{\infty} dz\, e^{-z^2}}_{\sqrt{\pi}} \right\}$$

$$= 0 \checkmark$$

Aside: Some neat mathematical tricks

$$\int_{-\infty}^{\infty} dx\, e^{-x^2} = \left[\left(\int_{-\infty}^{\infty} dx\, e^{-x^2} \right) \left(\int_{-\infty}^{\infty} dy\, e^{-y^2} \right) \right]^{1/2}$$

$$= \left[\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\, e^{-(x^2+y^2)} \right]^{1/2}$$

$$= \left[\int_0^{2\pi} d\phi \int_0^{\infty} \rho\, d\rho\, e^{-\rho^2} \right]^{1/2}$$ switch to cylindrical coordinate

$$= \left[2\pi \int_0^{\infty} \rho\, d\rho\, e^{-\rho^2} \right]^{1/2}$$

$$= \left[\pi \underbrace{\int_0^{\infty} dz\, e^{-z}}_{=1} \right]^{1/2} \qquad z = \rho^2$$

$$\int_{-\infty}^{\infty} dx\, e^{-x^2} = \sqrt{\pi} \quad \checkmark$$

Aside

let $x^2 = kz^2$

$$\int_{-\infty}^{\infty} \sqrt{k}\, dz\, e^{-kz^2} = \sqrt{\pi} \qquad k > 0$$

$$\int_{-\infty}^{\infty} dz\, e^{-kz^2} = \sqrt{\pi}\, k^{-1/2}$$

$\frac{d}{dk}$ ⇒

$$-\int_{-\infty}^{\infty} dz\, z^2 e^{-kz^2} = -\frac{1}{2} k^{-3/2} \sqrt{\pi}$$

let $k = 1$

$$\int_{-\infty}^{\infty} dz\, z^2 e^{-z^2} = \frac{\sqrt{\pi}}{2} \quad \checkmark$$

Generating the Hermites

From (6) with $n=1$

$$H_2 = 2zH_1 - 2H_0$$

$$= 2z(2z) - 2(1)$$

$$= 4z^2 - 2 \quad \checkmark$$

From (6) with $n=2$ $\quad H_3 = 2zH_2 - 4H_1$

$$= 2z(4z^2 - 2) - 4(2z)$$

$$= 8z^3 - 12z \quad \checkmark$$

From (6) with $n=3$ $\quad H_4 = 2zH_3 - 6H_2$

$$= 2z(8z^3 - 12z) - 6(4z^2 - 2)$$

$$= 16z^4 - 48z^2 + 12 \quad \checkmark$$

$H_0 = 1$ no "nodes"

$H_1 = 2z$ $H(0) = 0$ one node

$H_2 = 4z^2 - 2$ $H(\pm \frac{1}{\sqrt{2}}) = 0$ two nodes

$H_3 = 8z^3 - 12z = 4z(2z^2 - 3)$ zeros at $x = 0, \pm\sqrt{\frac{3}{2}}$ 3 nodes

$H_4 = 16z^4 - 48z^2 + 12$; zeros at $z = \pm\left(\frac{3}{2} \pm \sqrt{\frac{3}{2}}\right)$

independent 4 nodes

Properties of the sol'n

$$\underbrace{\langle V \rangle_n = \langle K \rangle_n}_{\text{same as classical}} = \frac{1}{2} E_n = \frac{\hbar\omega}{2}(n+1)$$

ground state $E_0 = \frac{\hbar\omega}{2}$ } zero point energy

The lowest energy is > 0

$\Rightarrow$ In crystals at $T = 0$, the atoms are still vibrating!

This is a consequence of the

Heisenberg Uncertainty Relationship

$\Delta x = 0 \Rightarrow \Delta p \to \infty$!

3 dimensional solutions to the Schrodinger equation

Examples in Cartesian systems, time independent

In 3-dimensions, the time-independent SE is

$$-\frac{\hbar^2}{2m}\nabla^2 u(\vec{x}) + V(\vec{x})\,u(\vec{x}) = E\,u(\vec{x}) \qquad (1)$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad \text{(Laplacian)} \qquad (2)$$

$$-i\hbar\vec{\nabla} = \vec{p} \quad \text{(momentum operator)} \qquad (3)$$

$$\vec{\nabla} = \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z} \qquad (4)$$

(gradient)

$\hat{x}, \hat{y}, \hat{z}$ are unit vectors in the $\vec{x}, \vec{y}, \vec{z}$ directions

$$\frac{\vec{p}\cdot\vec{p}}{2m} = -\frac{\hbar^2}{2m}\nabla^2 \quad \text{(Kinetic energy operator)} \qquad (5)$$

$$P(\vec{x}) = u^*(\vec{x})\,u(\vec{x}) \quad \text{(probability density)} \qquad (6)$$

$$\vec{S}(\vec{x}) = -\frac{\hbar}{m}\,u(\vec{x})\,\vec{\nabla}\,u^*(\vec{x}) \qquad (7)$$

(probability current density)

When time is considered

$$i\hbar\frac{\partial}{\partial t} \quad \text{(energy operator)} \quad (8)$$

$$\frac{\partial P(\vec{x},t)}{\partial t} + \vec{\nabla}\cdot\vec{S}(\vec{x},t) = \frac{2}{\hbar}\psi^*(\vec{x},t)\left(\mathrm{Im}\,V(\vec{x})\right)\psi(\vec{x},t)$$

$=0$ when the potential is real

(continuity equation) (9)

We will study several 3D systems

(do this now)

1) The 3D ∞ box potential
   - simplest to solve
   - demonstrates the important concepts of a) parity b) degeneracy → later

2) The 3D harmonic operator
   - applications in materials

Ch 7

3) The 3D spherical box
   - application in nuclear physics

4) The Coulomb potential
   - applications in atomic & nuclear physics

new topics: quantized angular momentum

proceeding on to the solution ...

(11) becomes

(14) $$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)u(x,y,z)+k^2u(x,y,z)=0$$

Intuition suggests that we should treat each coordinate separately, and propose a solution of the form

(15) $$u(x,y,z)=X(x)\,Y(y)\,Z(z)$$

(15) $\Rightarrow$ (11) $\Rightarrow$

(16) $$YZX''+XZY''+XYZ''+k^2XYZ=0$$

(16) / XYZ $\Rightarrow$

(17) $$\frac{X''}{X}+\frac{Y''}{Y}+\frac{Z''}{Z}+k^2=0$$

We already know the solns of X, Y, Z

$$X=\sqrt{\frac{2}{L}}\begin{pmatrix}\cos k_x x\\ \sin k_x x\end{pmatrix} \qquad k_x=\frac{(n_x+1)\pi}{L}$$

$n_x=0,1,2,3,\ldots$

$$X/X''=-k_x^2$$

with similar expressions for Y & Z

The 3D ∞-box potential

(8) $V(\vec{x}) = 0$ for $-\frac{L}{2} \le x \le \frac{L}{2}$
and $-\frac{L}{2} \le y \le \frac{L}{2}$
and $-\frac{L}{2} \le z \le \frac{L}{2}$

$\rightarrow \infty$ otherwise

note: $V(\vec{x})$ is symmetric in a 3 coordinate variables

(9) i.e. $V(-\vec{x}) = V(\vec{x})$ $V(\vec{x})$ has even parity
⇒ expect parity to be important

The solution $u(\vec{x}) = 0$ outside the box (boundary condition)

SE is $-\frac{\hbar^2}{2m}\nabla^2 u - Eu = 0$ (10)

or, $\nabla^2 u + k^2 u = 0$ (11)

$k^2 = \frac{2mE}{\hbar^2}$ (12)

$k^2 > 0$ for a solution (13)

Therefore, our 3D solution is

$$\psi(x,y,z) = X(x)Y(y)Z(z)$$

$$= \left(\frac{2}{L}\right)^{3/2} \begin{pmatrix} \cos k_x x \\ \sin k_x x \end{pmatrix} \begin{pmatrix} \cos k_y y \\ \sin k_y y \end{pmatrix} \begin{pmatrix} \cos k_z z \\ \sin k_z z \end{pmatrix}.$$

$$k_x = \frac{(n_x+1)\pi}{L} \qquad k_y = \frac{(n_y+1)\pi}{L} \qquad k_z = \frac{(n_z+1)\pi}{L}$$

$$n_x = 0,1,2,\ldots \qquad n_y = 0,1,2,\ldots \qquad n_z = 0,1,2,\ldots$$

$$k^2 = k_x^2 + k_y^2 + k_z^2 = \frac{\pi^2}{L^2}\left((n_x+1)^2 + (n_y+1)^2 + (n_z+1)^2\right)$$

$$E(n_x, n_y, n_z) = \frac{\hbar^2\pi^2}{2mL^2}\left((n_x+1)^2 + (n_y+1)^2 + (n_z+1)^2\right)$$

depends on 3 quantum numbers

$$E(0,0,0) = 3\frac{\hbar^2\pi^2}{2mL^2}$$ ground state energy

$$\Pi = (-1)^{n_x}(-1)^{n_y}(-1)^{n_z}$$

parity is multiplicative

(18)

degeneracy

Degeneracy ; Parity

$3*\frac{E(n_x,n_y,n_z)}{E(0,0,0)}$			D	Π
	⋮			
14	———	(2,2,0) (2,0,2) (0,2,2)	3	+1
18	———	(3,0,0), (0,3,0), (0,0,3)	3	−1
17	———	(1,1,2) (1,2,1) (2,1,1)	3	+1
14	———	(3,1,0), (3,0,1), (1,3,0), (0,3,1) (1,0,2) (0,1,2)	6	−1
12	———	(1,1,1)	1	−1
11	———	(2,0,0) or (0,2,0) or (0,0,2)	3	+1
9	———	(1,1,0) or (1,0,1) or (0,1,1)	3	+1
6	———	(1,0,0) or (0,1,0) or (0,0,1)	3	−1
3	———	(0,0,0)	1	+1

What is ...

... Degeneracy ... # of ways an energy level can get filled (by different solutions)

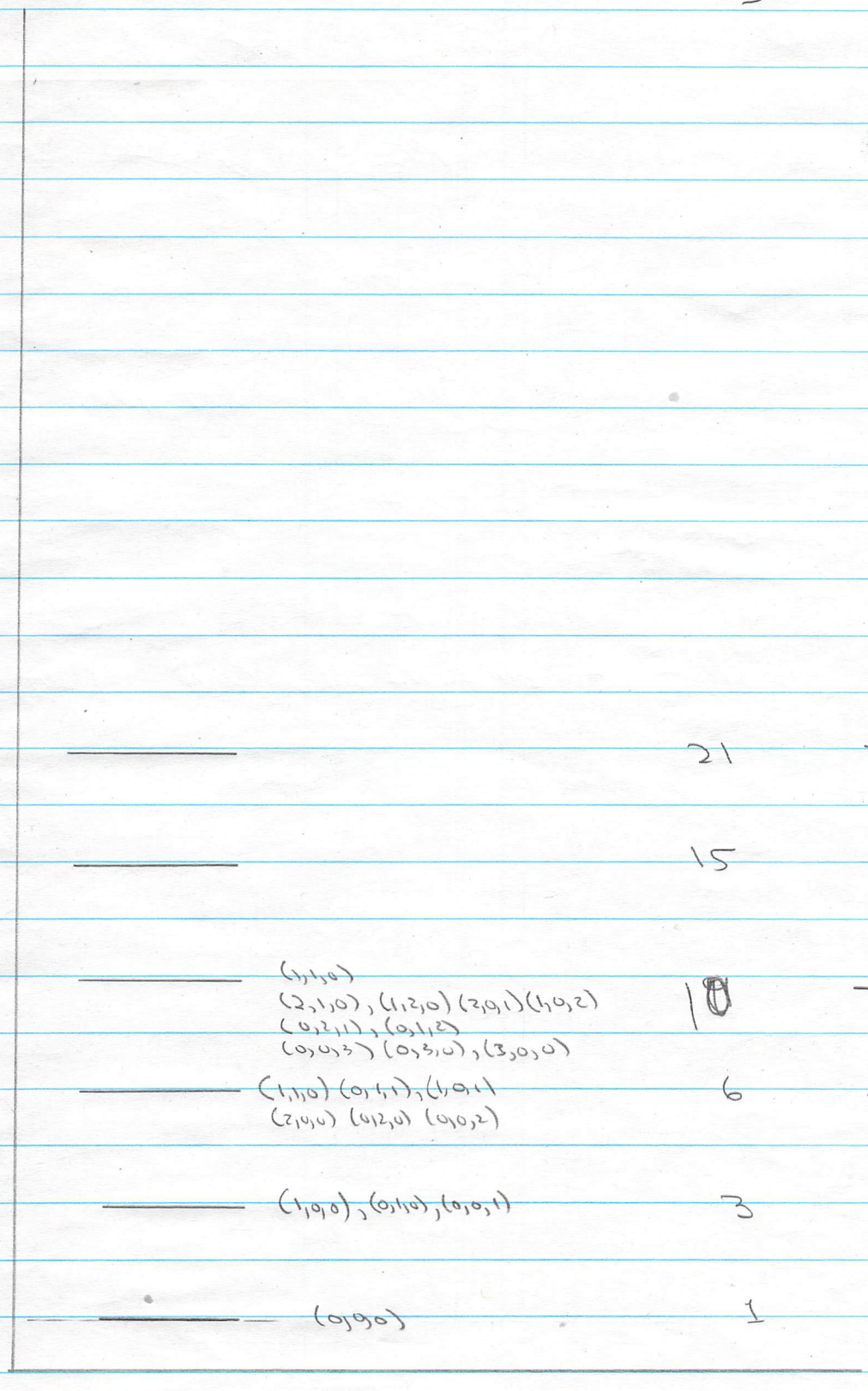
The Harmonics Oscillator

$$V(\vec{x}) = \frac{1}{2}k(x^2+y^2+z^2)$$

Using the same considerations

$$\begin{cases} \psi(\vec{x}) = \psi_{n_x}(x)\,\psi_{n_y}(y)\,\underbrace{\psi_{n_z}(z)}_{\text{1D harmonic oscillator solutions}} \\ E(n_x,n_y,n_z) = \hbar\omega\left(n_x+n_y+n_z+\frac{3}{2}\right) \end{cases}$$

$\uparrow$ note


D
Π
$\frac{E(n_x,n_y,n_z)}{\hbar\omega} - \frac{3}{2}$
5
21
−1
4
15
+1
3
(1,1,0)
(2,1,0), (1,2,0) (2,0,1) (1,0,2)
(0,2,1), (0,1,2)
(0,0,3) (0,3,0), (3,0,0)
10
−1
2
(1,1,0) (0,1,1), (1,0,1
(2,0,0) (0,2,0) (0,0,2)
6
+1
1
(1,0,0), (0,1,0), (0,0,1)
3
−1
0
(0,0,0)
1
+1

Aside In the box potential, prove that each level, regardless of level of degeneracy, has a unique parity

Let $\vec{n} = 2\vec{a} + \vec{b}$

$\vec{n} = (n_x, n_y, n_z)$

$\vec{a} = (a_x, a_y, a_z)$

$\vec{b} = (b_x, b_y, b_z)$

n's $0, 1, 2, \ldots \infty$

a's $0, 1, 2, \ldots \infty$

b's 0 or 1 only

$$|\vec{n}|^2 = 4(|\vec{a}|^2 + \vec{a}\cdot\vec{b}) + |\vec{b}|^2$$

So $\{|\vec{n}|^2\}_{\text{mod } 4} = \{|\vec{b}|^2\}_{\text{mod } 4}$ since

For a different combination at the same energy level

$$\{|\vec{b}|^2\}_{\text{mod } 4} = \{|\vec{b}'|^2\}_{\text{mod } 4}$$

i.e. $b_x + b_y + b_z = b_x' + b_y' + b_z'$

$0 = 0$

$1 = 1$

$2 = 2$

$3 = 3$

parity is preserved

Note $b_i^2 = b_i$

Proof by Yi Yi Lin (UCLA EE09 student)