Finding Roots Numerically (Finite Square Well)

We solved for the allowed energies of the finite square well and we were left with two transcendental equations,

With $k = \sqrt{\frac{2mE}{\hbar^2}}$ and $q = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$,

ψ_{even}: $\quad k\tan(ka) = q$

ψ_{odd}: $\quad -k\cot(ka) = q$

McIntyre shows how to solve this problem graphically by finding the intersection of two functions.

We will discuss a different approach that will still yield the allowed energies "Root Finding."

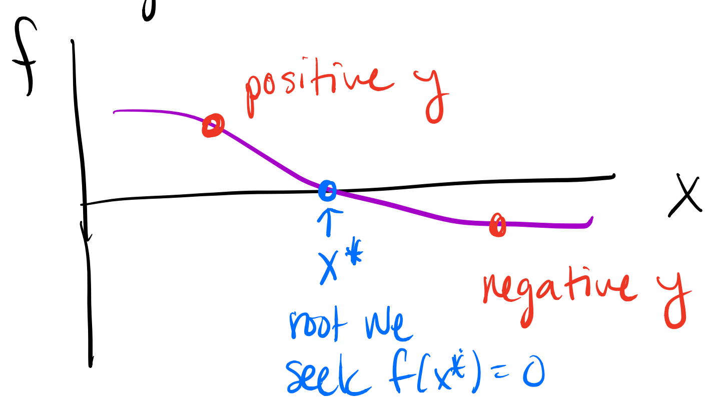
Conceptually, we produce a function $f(x)$ and we search for x^*

where $f(x^*) = 0$.

There are many root finding methods, but we will use simplest → the bisection method.

The Bisection Method

- The bisection method "brackets" a root by using the fact that function is continuous and thus admits positive and negative values near the root.



- the bisection method will work with any continuous function. But it can be slow.
- It can also have problems we the function is oscillating wildly or when initial guesses are bad.

Steps for Bisection Method. ③

① Pick two points near the root, a & b.

⇒ Make sure f(a) & f(b) have opposite signs!

② Calculate the midpoint between a & b ⇒ $c = \frac{a+b}{2}$

③ Calculate f(c).

⇒ check if f(c) is smaller than tolerance

eg. if Tolerance is 0.005 check if

$-0.005 < f(c) < 0.005$

if it is, stop!

if not, continue

④ Assuming $|f(c)| > \text{tolerance}$, check sign of f(c).

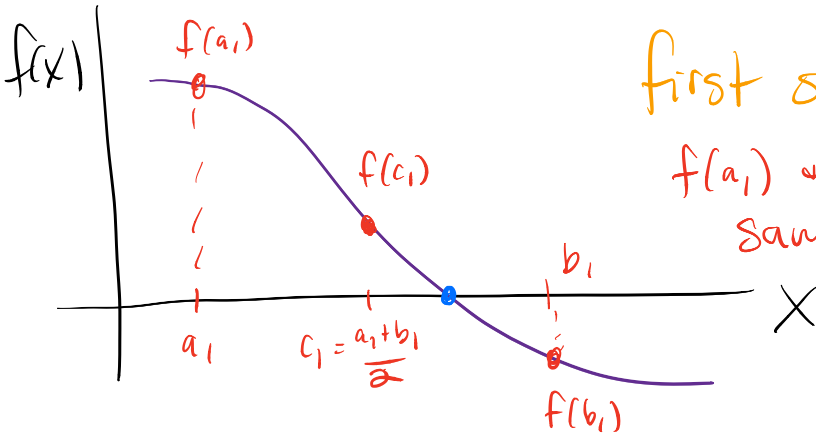
⑤ if f(c) same sign as f(a)?

replace a with c & f(a) with f(c)

if f(c) same sign as f(b)?

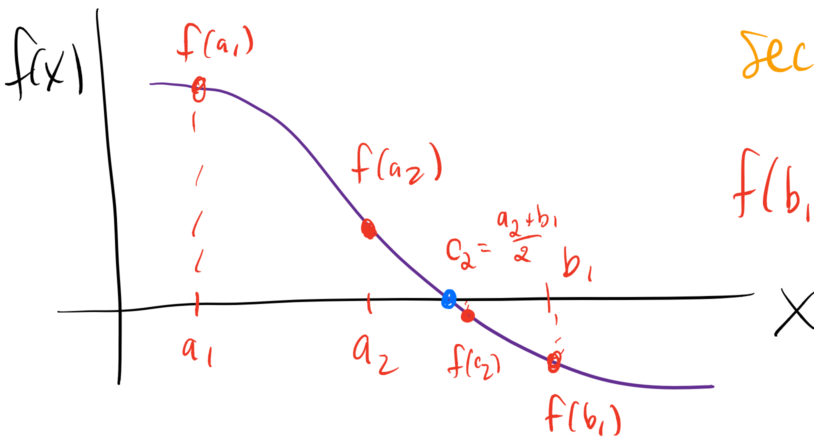
replace b with c & $f(b)$ with $f(c)$ ④

⑥ Continue 2–5 until $|f(c)| < \text{tolerance}$.



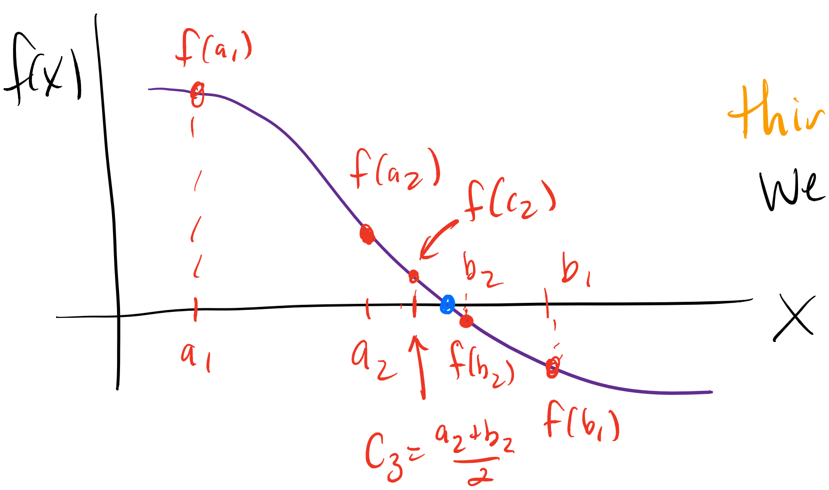
first step

$f(a_1)$ & $f(c_1)$ same sign



second step

$f(b_1)$ & $f(c_2)$ same sign



third step

We could continue but that's the idea.

Back to the finite Square Well

$$k\tan(ka) = q \qquad -k\cot(ka) = q$$

even solutions — odd solutions.

McIntyre argues we can transform these equations using,

$$z = ka = \sqrt{\frac{2mEa^2}{\hbar^2}} \qquad z_0 = \sqrt{\frac{2mV_0a^2}{\hbar^2}}$$

&

$$qa = \sqrt{\frac{2m(V_0-E)a^2}{\hbar^2}}$$

thus,

$$(qa)^2 + (ka)^2 = z_0^2$$

$$(qa)^2 = z_0^2 - (ka)^2$$

or,

$$(qa)^2 = z_0^2 - z^2$$

Given that $qa = (ka)\tan(ka)$ even

& $qa = -(ka)\cot(ka)$ odd

then,

$$qa = z\tan(z)$$

$$qa = -z\cot(z)$$

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or,

$$z\tan(z) = \sqrt{z_0^2 - z^2}$$

$$-z\cot(z) = \sqrt{z_0^2 - z^2}$$

We rewrite these as,

$$\boxed{\begin{aligned} z\tan(z) - \sqrt{z_0^2 - z^2} &= 0 \\ \sqrt{z_0^2 - z^2} - z\cot(z) &= 0 \end{aligned}}$$

This is our root finding problem,

$$f_1(z) = z\tan(z) - \sqrt{z_0^2 - z^2}$$

$$f_2(z) = \sqrt{z_0^2 - z^2} - z\cot(z)$$

Find z^*'s such that

$$f_1(z^*) = 0 \quad \text{or} \quad f_2(z^*) = 0$$

A jupyter notebook will walk through this with you on HW 3.