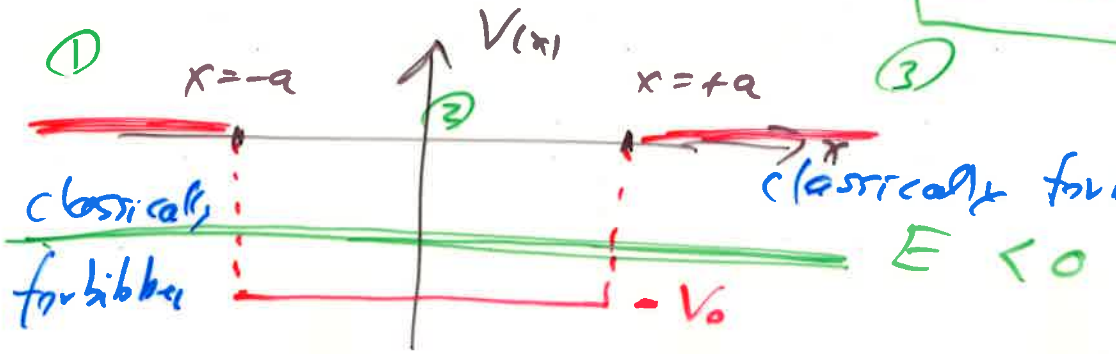
Finite Square Well

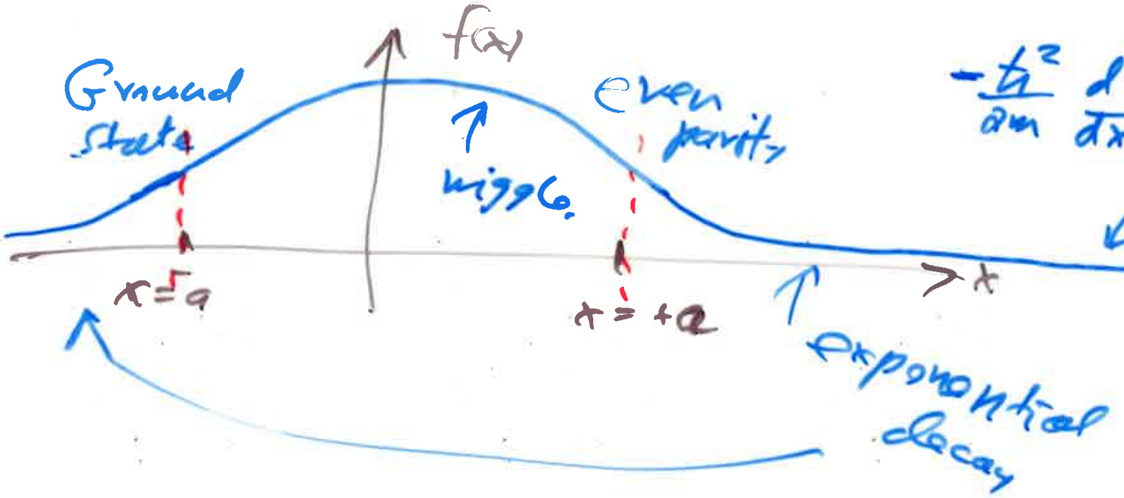
A) Bound States

① $x < -a$
② $-a < x < a$
③ $a < x$



kinetic energy
$K(x) = E - V(x) < 0$

Expectations? At least one solution (even).
Wave functions $f(x)$ have a definite parity (even or odd) because $V(x)$ even.

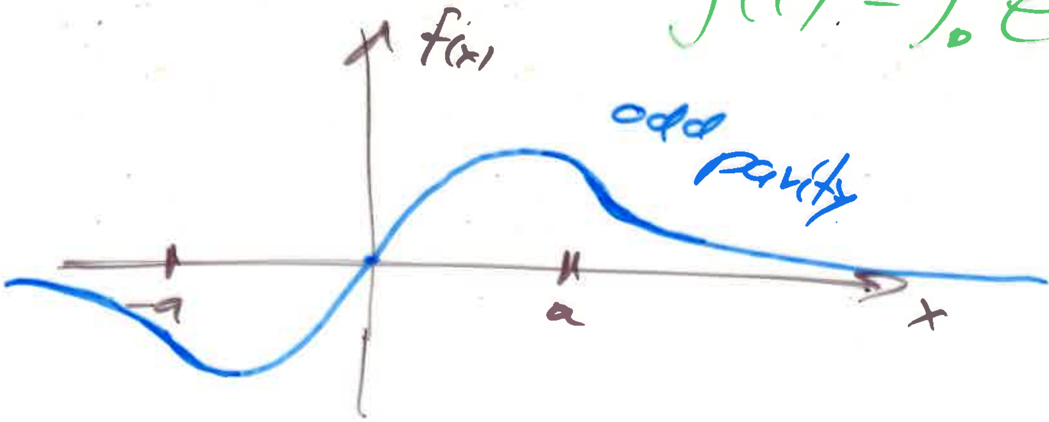


$$-\frac{\hbar^2}{2m}\frac{d^2 f(x)}{dx^2} + 0 = E f(x)$$

$V(x)=0$ here

$f(x)$ is continuous
$f'(x)$ also continuous

time function $g(t) = g_0 e^{-\frac{itE}{\hbar}}$



Plan: Solve the S.E. in the 3 regions
- match $f(x)$ at boundaries ($x = \pm a$)
- match $f'(x)$ at boundaries

S.E. $$-\frac{\hbar^2}{2m}\frac{d^2 f(x)}{dx^2} + V(x) f(x) = E f(x)$$

regime ① $x < -a$: $$\frac{-\hbar^2}{2m} f_1''(x) + 0 = E f_1(x)$$

$$f_1''(x) = \left(-\frac{2mE}{\hbar^2}\right) f(x) \qquad \gamma \equiv \sqrt{\frac{-2mE}{\hbar^2}} \in \mathbb{R}e$$

positive ($E<0$)

Solutions

$$f_1(x) = \cancel{A}^{0} e^{-\gamma x} + B e^{\gamma x}$$

set $A=0$ because $e^{-\gamma x}$ blows up as $x \to -\infty$

regime ③ $a < x$ same S.E.

$$f_3''(x) = \gamma^2 f_3(x) \Rightarrow f_3(x) = F e^{-\gamma x} + \cancel{G}^{0} e^{\gamma x}$$

set $G=0$ because $e^{\gamma x}$ blows up as $x \to \infty$

regime ②

S.E. $$-\frac{\hbar^2}{2m} f_2''(x) - V_0 f_2(x) = E f_2(x)$$

$$f_2''(x) = -\left[\frac{2m(E+V_0)}{\hbar^2}\right] f_2(x) \qquad k = \sqrt{\frac{2m(E+V_0)}{\hbar^2}} \in \mathbb{R}e$$

$$f_2''(x) = -k^2 f_2(x)$$

or $f_2(x) = C' e^{ikx} + D' e^{-ikx}$

$$f_2(x) = C \sin(kx) + D \cos(kx)$$

odd — even

Aside

$$\frac{e^{ikx} + e^{-ikx}}{2} = \frac{[\cos(kx) + \cancel{i\sin(kx)} + \cos(kx) - \cancel{i\sin(kx)}]}{2}$$

$$= \cos(kx)$$

$$\frac{e^{ikx} - e^{-ikx}}{2i} = \sin(kx)$$

① $f(x)$ is continuous across the boundaries

Look for even solutions $f(x)$ first (set $C=0$)

$$f_2(x) = D\cos(kx)$$

$x=-a$

I $f_1(-a) = f_2(-a) \Rightarrow Be^{-\gamma a} = D\cos(ka)$

$x=+a$

I $f_2(a) = f_3(a) = D\cos(ka) = Fe^{-\gamma a}$

② $f'(x)$ is also continuous across the boundaries (if $V(x) \neq \infty$ anywhere)

$$f_1(x) = Be^{\gamma x}$$
$$f_2(x) = D\cos(kx)$$
$$f_3(x) = Fe^{-\gamma x}$$

$$f_1'(x) = B\gamma e^{\gamma x}$$
$$f_2'(x) = -kD\sin(kx)$$
$$f_3'(x) = -\gamma F e^{-\gamma x}$$

$\underline{x=-a}$

III $f_1'(-a) = f_2'(-a) \Rightarrow B\gamma e^{-\gamma a} = +kD\sin(ka)$

$\underline{x=+a}$

IV $f_2'(a) = f_3'(a) \Rightarrow +kD\sin(ka) = +\gamma F e^{-\gamma a}$

4 equations $\longleftrightarrow$ B, D, F, E ← energy

eqs I+II $\longrightarrow$ $B=F$

eqs III+IV $\longrightarrow$ $B=F$

I $\Rightarrow$ $Be^{-\gamma a} = D\cos(ka)$ V

IV $\longrightarrow$ $\gamma B e^{-\gamma a} = kD\sin(ka)$ VI

$$\frac{\text{VI}}{\text{V}} = \gamma = k\frac{\sin(ka)}{\cos(ka)} = k\tan(ka)$$

$$\gamma \equiv \sqrt{\frac{-2mE}{\hbar^2}} \qquad k \equiv \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

Numerical Methods of Solution

$\gamma = k \tan(ka)$ transcendental equation

(as opposed to algebraic equation)

<u>Define</u> $u = ka$, u is dimensionless (pure number)

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

$$\left(\gamma^2 + k^2 = \frac{2mV_0}{\hbar^2}\right)$$ multiply by a^2

$$\gamma^2 a^2 + \underbrace{k^2 a^2}_{u^2} = \frac{2mV_0 a^2}{\hbar^2} \equiv w^2$$

w ← dimensionless

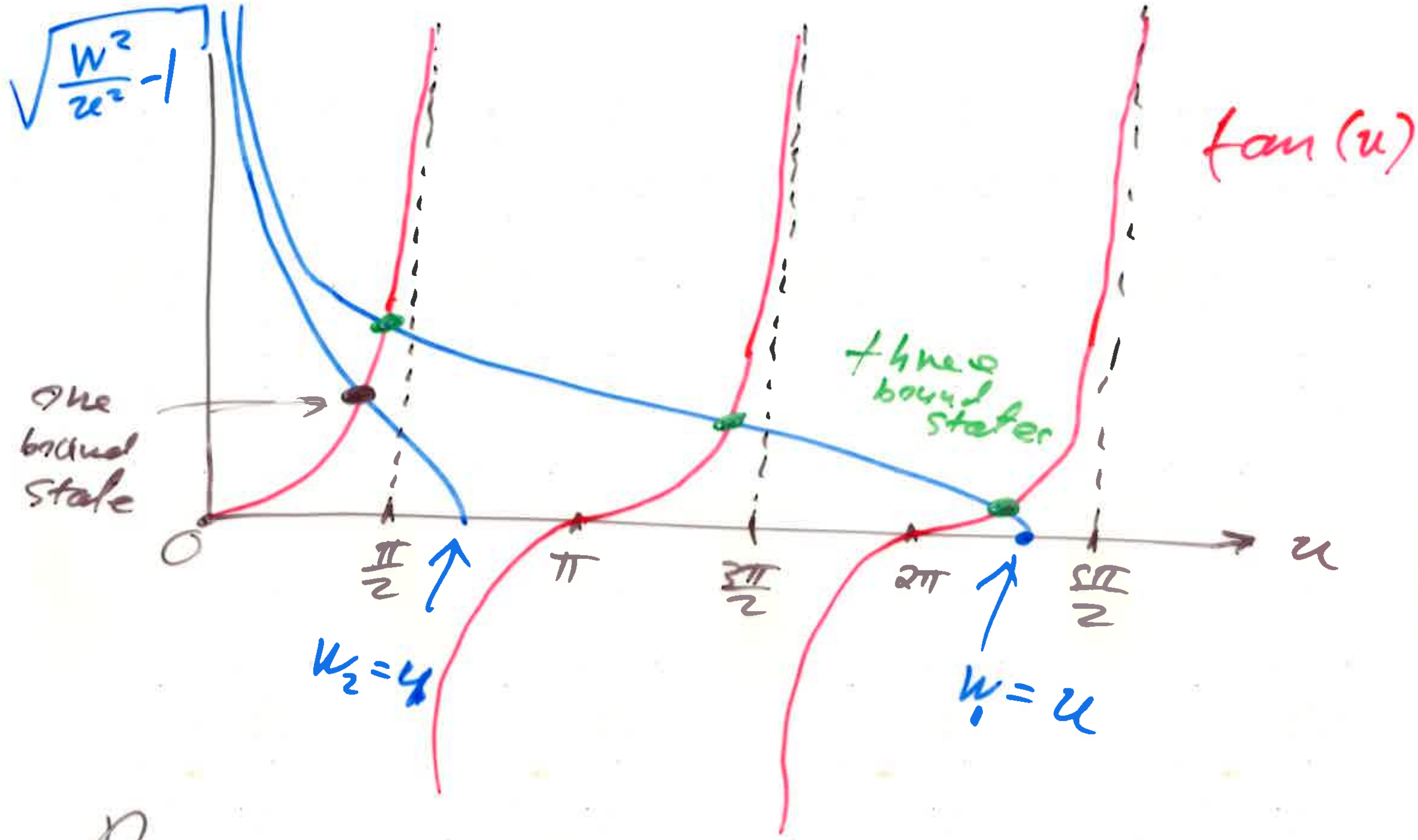
$$\gamma^2 a^2 = w^2 - u^2$$

$$\gamma a = \sqrt{w^2 - u^2} \quad ; \quad \gamma a = u \tan(u)$$

$$\sqrt{w^2 - u^2} = u \tan(u)$$

$$\sqrt{\left(\frac{w^2}{u^2}\right) - 1} = \tan(u)$$

u



Remember — those are for <u>even</u> solutions

$\Rightarrow$ there is always at least one even solution.

Next time $\Rightarrow$ <u>odd</u> <u>solutions</u>