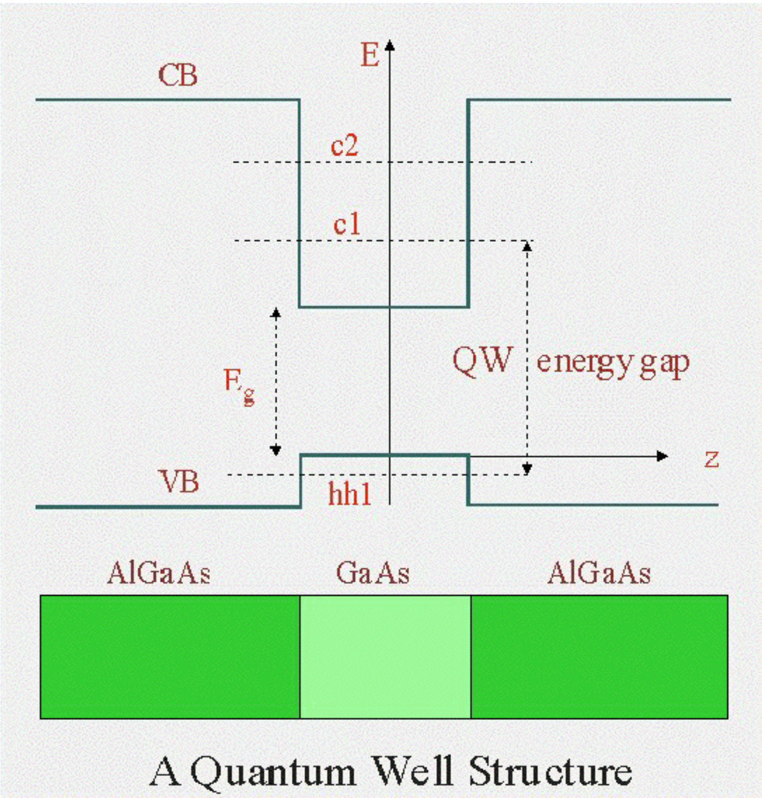
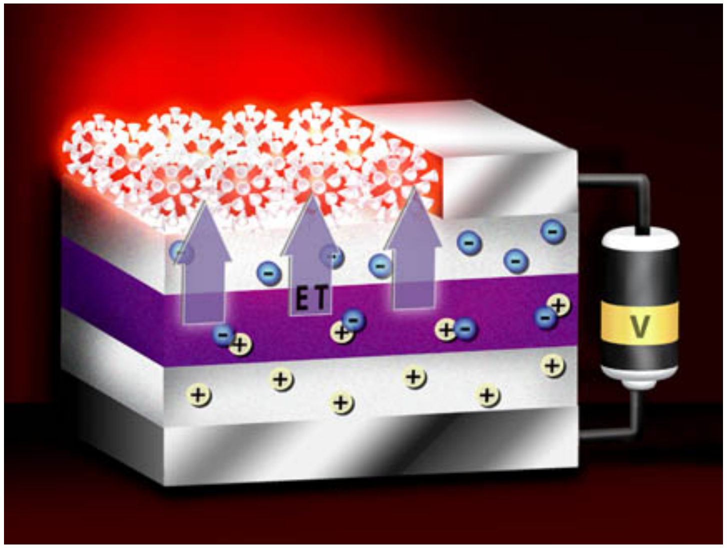
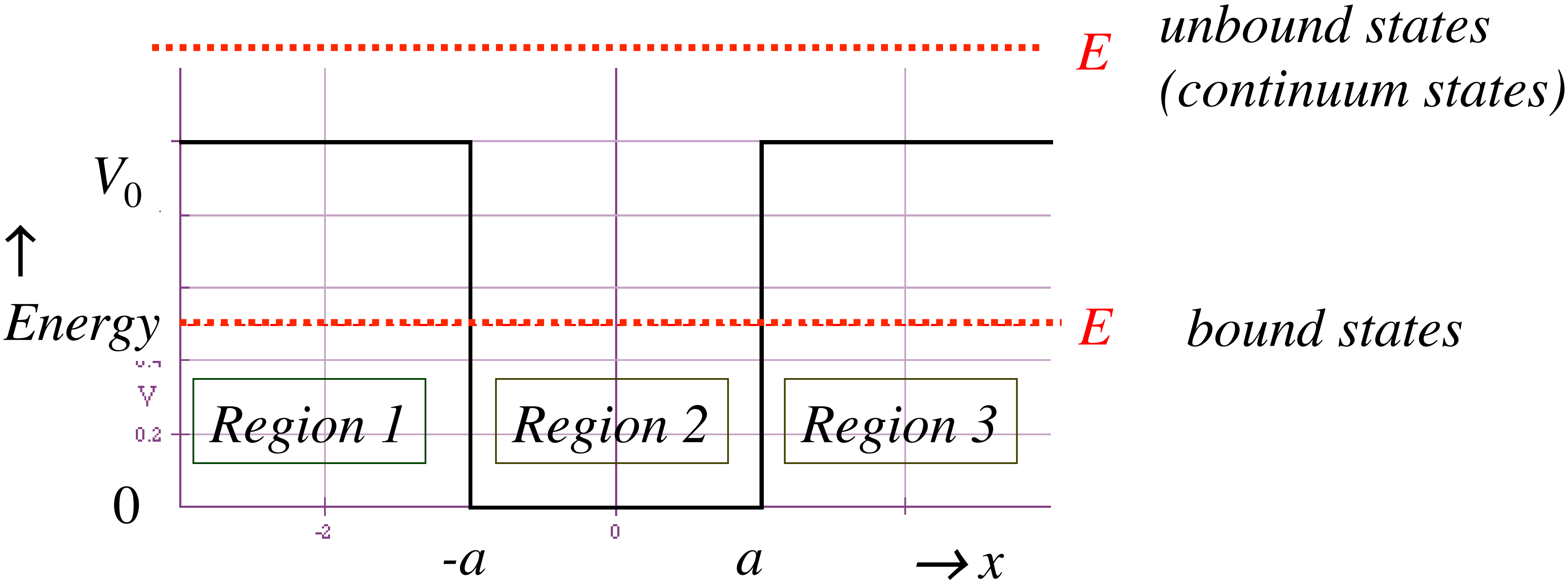
ENERGY EIGENFUNCTIONS & EIGENVALUES OF THE FINITE WELL

Reading:
McIntyre- ch 5.5
(also review 5.4)





Solve the energy eigenvalue equation for different potentials and for examples where there are many solutions with different energies.



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

$$\varphi(x) = \begin{cases} \varphi_1 & x < -a \\ \varphi_2 & -a < x < a \\ \varphi_3 & x > a \end{cases}$$

$$\hat{H}\varphi(x) = E\varphi(x)$$

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

defines k^2

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

V_0 if region 1,3

0 if region 2

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

$$k_2 = \sqrt{\frac{2m}{\hbar^2}E}$$

$$k_1 = k_3 = \sqrt{\frac{2m}{\hbar^2}(E-V_0)}$$

real if $E>V_0$;
imag if $E<V_0$

$$\varphi(x) = Ce^{-ikx} + C'e^{+ikx}$$

Focus first on the case $E < V_0$ ("bound states")

In regions 1 & 3, k is imaginary

$$\varphi_1(x) = Ce^{-ik_1x} + C'e^{+ik_1x}$$

$$\varphi_3(x) = D'e^{-ik_3x} + De^{+ik_3x}$$

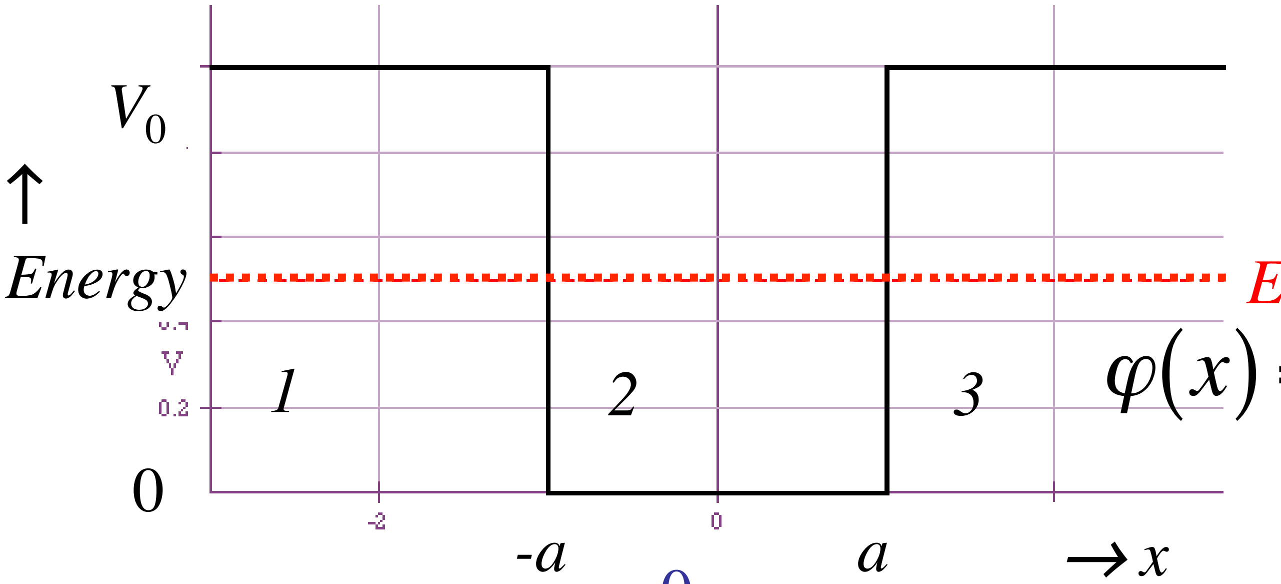
Imaginary k means exponential growth or exponential decay! (classically forbidden region)

In region 2, k is real

$$\varphi_2(x) = Ae^{-ik_2x} + Be^{+ik_2x}$$

Real k means oscillatory behavior
(classically allowed region)

It would not be physically reasonable to allow an infinite probability of finding a particle in a classically forbidden region.



$$\varphi(x) = \begin{cases} \varphi_1 & x < -a \\ \varphi_2 & -a < x < a \\ \varphi_3 & x > a \end{cases}$$

$$\varphi_1(x) = Ce^{-ik_1x} + C'e^{ik_1x}$$

$$\varphi_3(x) = D'e^{-ik_1x} + De^{ik_1x}$$

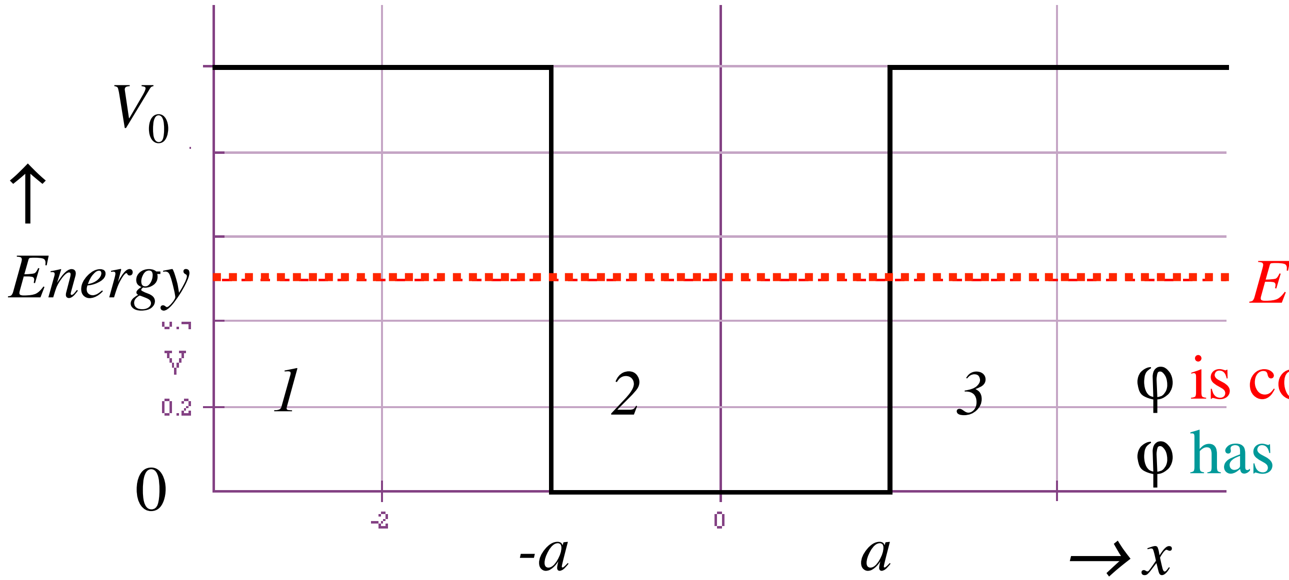
0 0

$$\varphi_2(x) = Ae^{ik_2x} + Be^{-ik_2x}$$

- φ is continuous everywhere
- φ has a continuous derivative
- φ goes to zero at ±∞
- φ is normalized

$$k_1 = i\sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$k_2 = \sqrt{\frac{2mE}{\hbar^2}}$$



φ is continuous everywhere

φ has a continuous derivative

$$\varphi_1(-a) = \varphi_2(-a) \qquad Ce^{ik_1 a} = Ae^{-ik_2 a} + Be^{ik_2 a}$$

$$\varphi_3(a) = \varphi_2(a) \qquad Ae^{ik_2 a} + Be^{-ik_2 a} = De^{ik_1 a}$$

$$\varphi_1'(-a) = \varphi_2'(-a) \qquad -ik_1 Ce^{ik_1 a} = ik_2 Ae^{-ik_2 a} - ik_2 Be^{ik_2 a}$$

$$\varphi_3'(a) = \varphi_2'(a) \qquad ik_2 Ae^{ik_2 a} - ik_2 Be^{-ik_2 a} = ik_1 De^{ik_1 a}$$

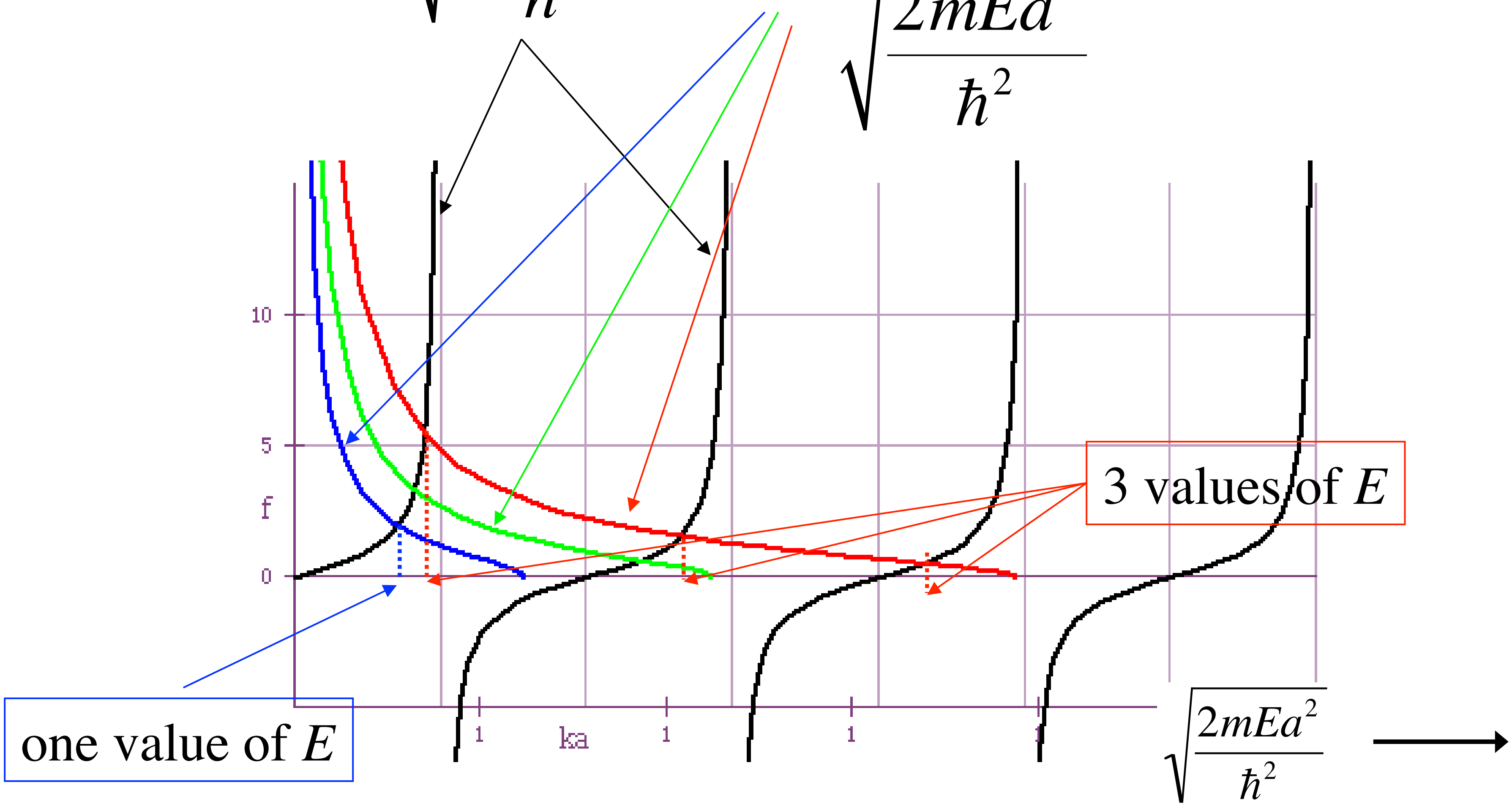
4 equations, 5 unknowns (A, B, C, D, E). (E is buried in k_1 and k_2)
Normalization gives fifth condition.

$$\begin{pmatrix} e^{-ik_2a} & e^{ik_2a} & -e^{ik_1a} & 0 \\ e^{ik_2a} & e^{-ik_2a} & 0 & e^{ik_1a} \\ ik_2e^{-ik_2a} & -ik_2e^{ik_2a} & -ik_1e^{ik_1a} & 0 \\ ik_2e^{ik_2a} & -ik_2e^{-ik_2a} & 0 & ik_1e^{ik_1a} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = 0$$

This set of equations has a solution when the determinant of the 4x4 matrix is zero. Tedious! See Liboff for details. When the determinant condition is set up, we get a condition on *E!* This condition can be satisfied in 2 sets of ways. One set has $A = B$ (even solutions) and the other set has $A = -B$ (odd solutions).

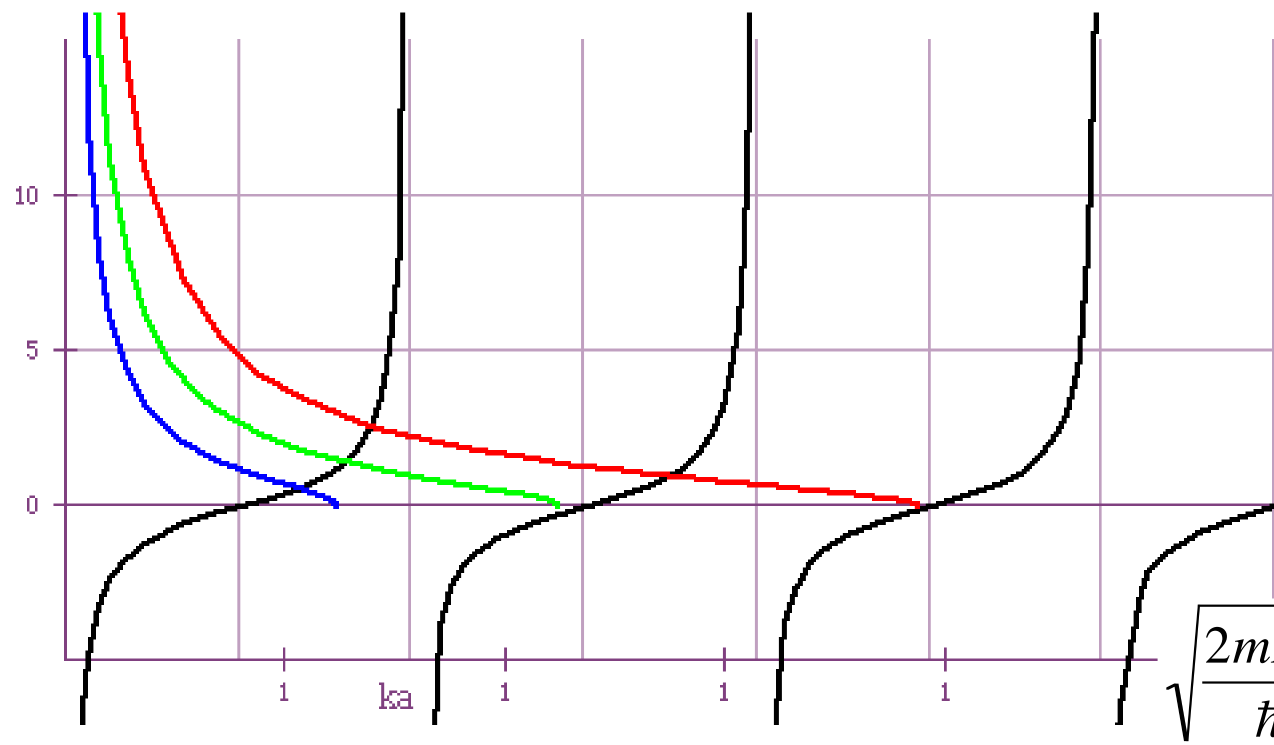
Here is one condition for the determinant to be zero (Eqn 5.83 in McIntyre):

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



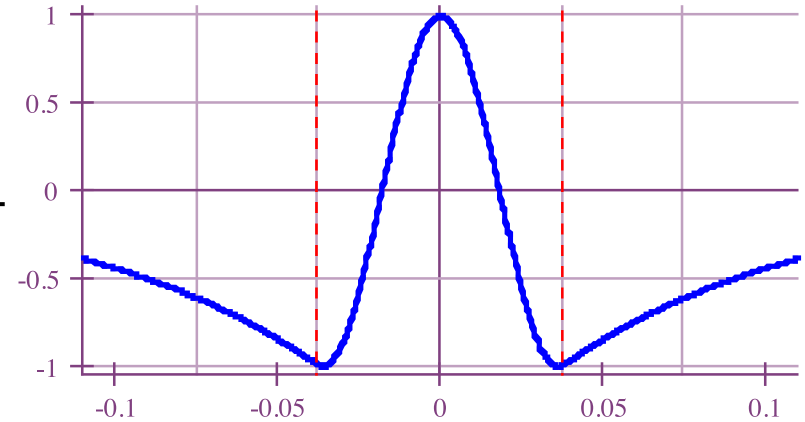
Here is the other condition for the determinant to be zero:
(Eqn 5.85 in McIntyre):

$$-\cot\sqrt{\frac{2mEa^2}{\hbar^2}} = \frac{\sqrt{\frac{2m\left(V_0 - E\right)a^2}{\hbar^2}}}{\sqrt{\frac{2mEa^2}{\hbar^2}}}$$

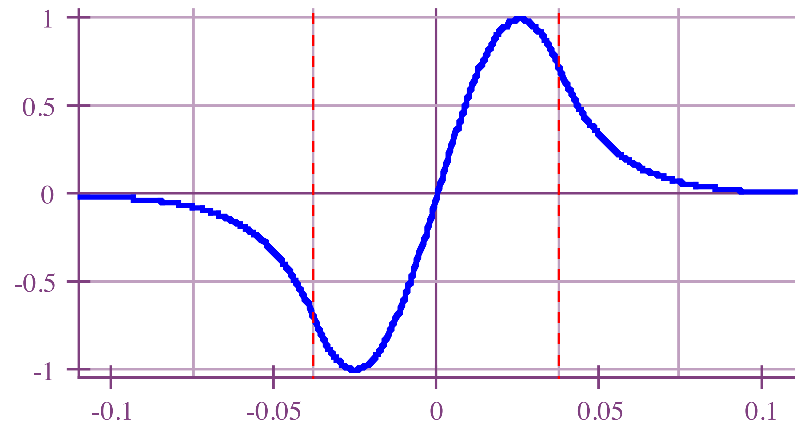


$$\sqrt{\frac{2mEa^2}{\hbar^2}} \longrightarrow$$

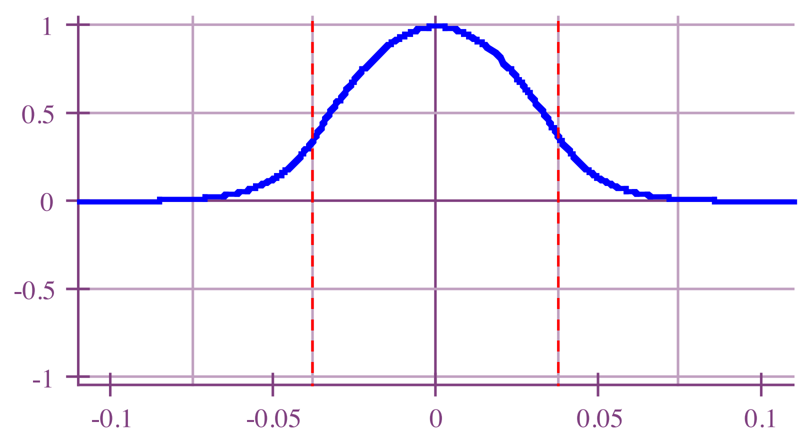
$$\tan\sqrt{\frac{2mE_3a^2}{\hbar^2}} = \frac{\sqrt{\dfrac{2m\left(V_0 - E_3\right)a^2}{\hbar^2}}}{\sqrt{\dfrac{2mE_3a^2}{\hbar^2}}}$$



$$-\cot\sqrt{\frac{2mE_2a^2}{\hbar^2}} = \frac{\sqrt{\dfrac{2m\left(V_0 - E_2\right)a^2}{\hbar^2}}}{\sqrt{\dfrac{2mE_2a^2}{\hbar^2}}}$$

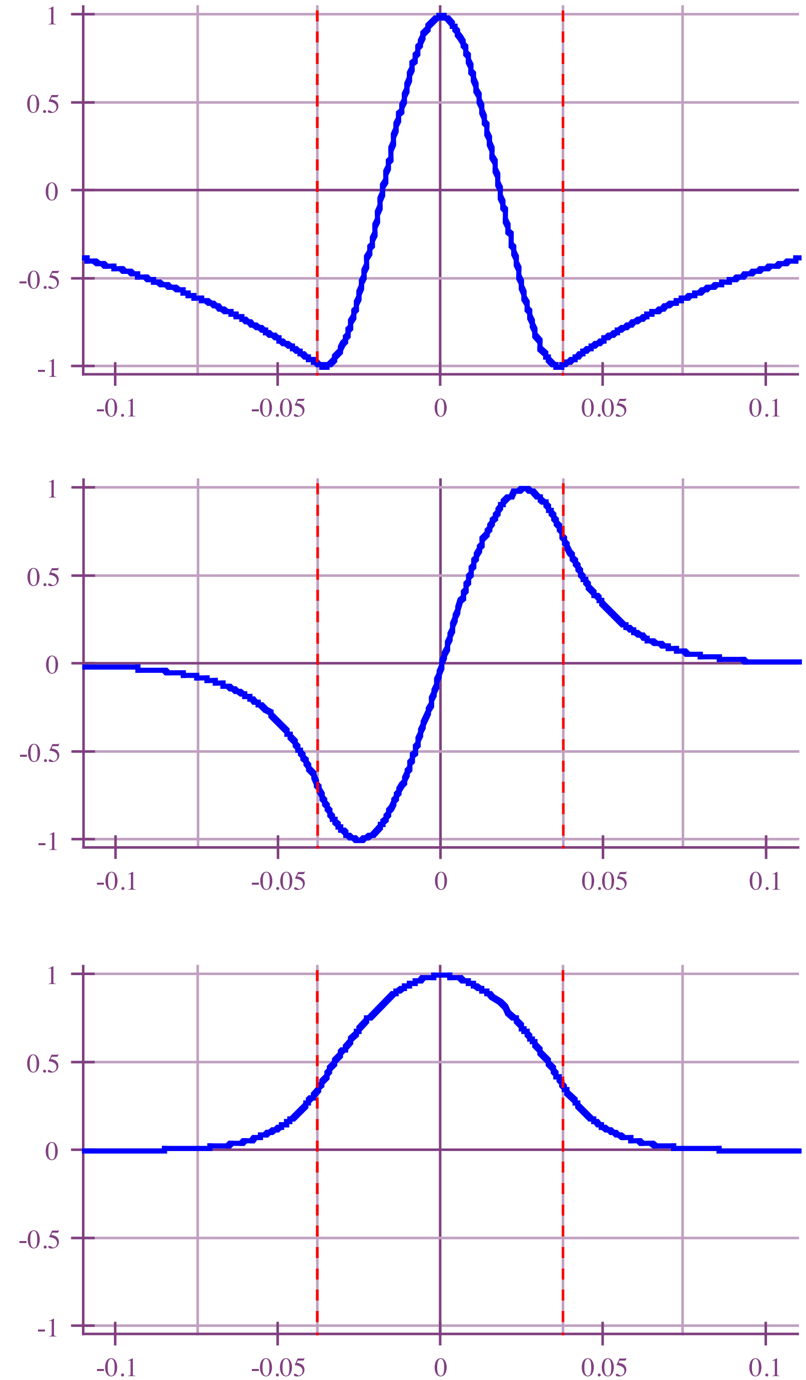


$$\tan\sqrt{\frac{2mE_1a^2}{\hbar^2}} = \frac{\sqrt{\dfrac{2m\left(V_0 - E_1\right)a^2}{\hbar^2}}}{\sqrt{\dfrac{2mE_1a^2}{\hbar^2}}}$$



This set corresponds to the green curves on the previous graphs - the value of V_0 that yields 3 solutions (2 even and 1 odd).

Note the size of the decay length for the state corresponding to each energy. Wave function "leaks" into forbidden region. We call this an evanescent wave.

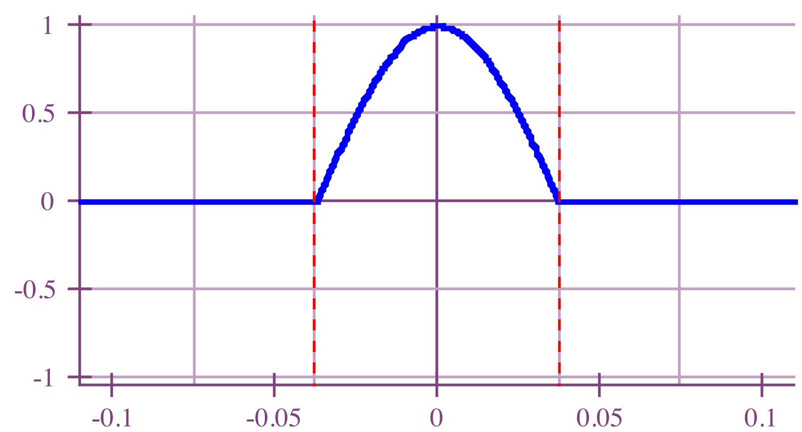


Limiting Case: $V_0 \rightarrow \infty$

$$\tan\sqrt{\frac{2mEa^2}{\hbar^2}} = \infty \Rightarrow \sqrt{\frac{2mEa^2}{\hbar^2}} = \frac{\pi}{2}$$

Decay length $\sqrt{\frac{\hbar^2}{2m\left(V_0 - E\right)}} \rightarrow 0$

$$E_1 = \frac{\hbar^2\pi^2}{2m\left(2a\right)^2}$$



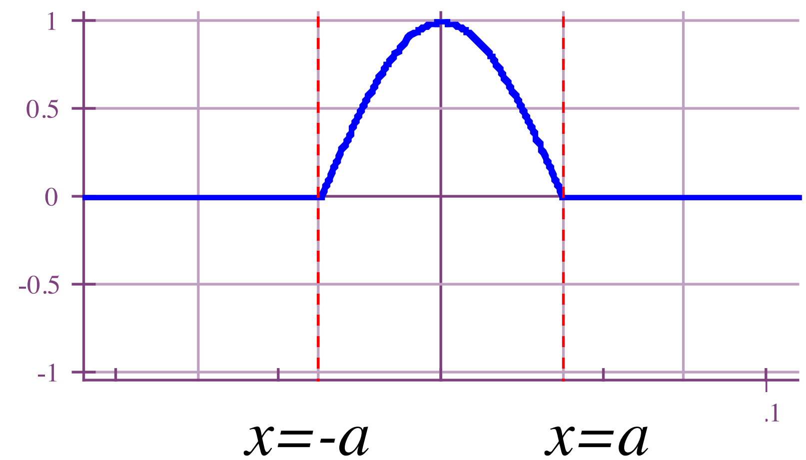
Infinite square well recovered!

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2}$$

$\varphi_n(x) = 0$ *n =1,2,3,4,5…for x<-a and x>a*

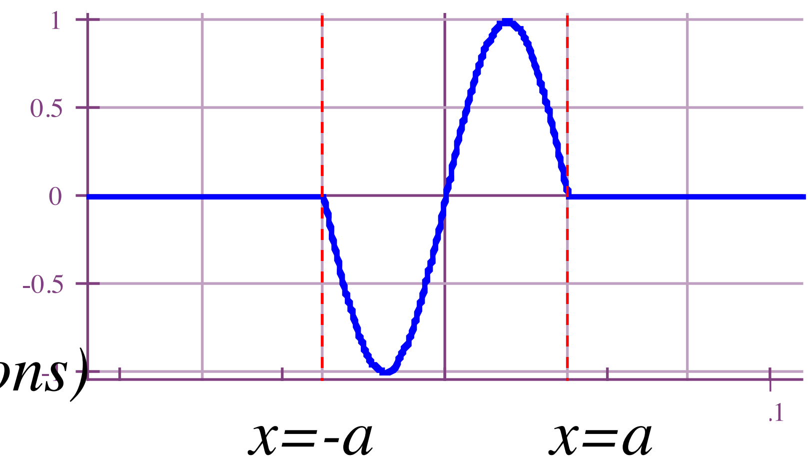
$$\varphi_n(x) = \sqrt{\frac{2}{2a}} \cos \frac{n\pi x}{2a}$$

n =1,3,5 (symmetric or even solutions)



$$\varphi_n(x) = \sqrt{\frac{2}{2a}} \sin \frac{n\pi x}{2a}$$

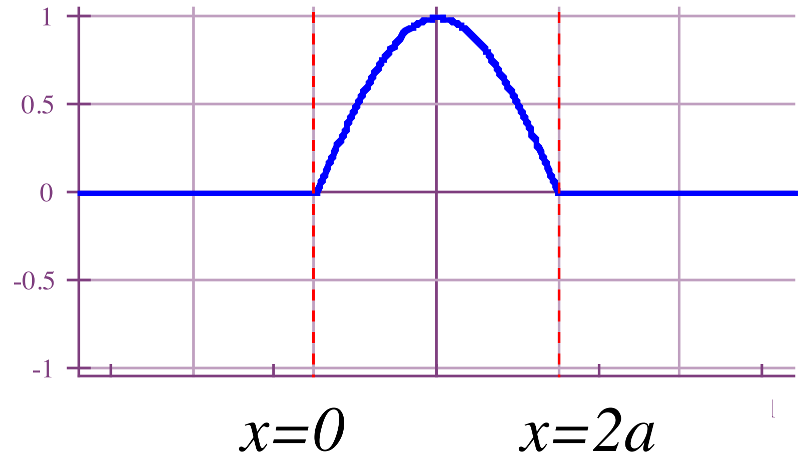
n =2,4,6 (antisymmetric or odd solutions)

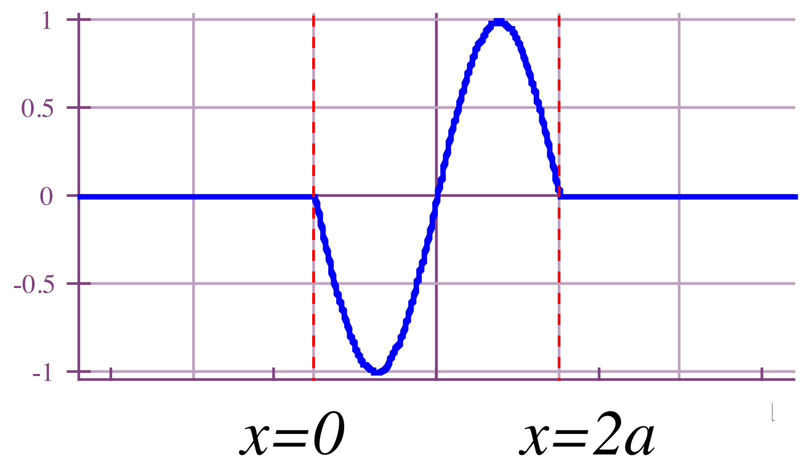


$$E_n = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

$$\varphi_n(x) = 0$$ *n =1,2,3,4,5…for x < 0 and x > 2a*

$$\varphi_n(x) = \sqrt{\frac{2}{2a}}\sin\frac{n\pi x}{2a}$$





n =1,2,3,4,5… and 0 < x < 2a (neither symmetric nor antisymmetric solutions - about x=0)

Important features of (**symmetric**) finite square well:

- Non-trivial solutions to energy eigenvalue equation
- application of boundary conditions
- Quantized energy
- Symmetric (even) and antisymmetric (odd) solutions
- Always one solution regardless of width or depth of well
- Wave function finite in classically forbidden region
- Recover infinite well solutions

- lots of manipulation to get it exactly right, but in the end we have sine- and cosine-like oscillations in the allowed region, decaying exponentially in the forbidden region. The decay length is longer the closer the particle's energy to the top of the well.

ENERGY EIGENFUNCTIONS & EIGENVALUES OF THE FINITE WELL REVIEW

- *Hamiltonian - set up with piecewise potential*
- *Solve energy eigenvalue equation*
- *Matching boundary conditions - continuity of ϕ and ϕ'*
- *Graphical solutions will suffice for now*
- *Discrete energies for bound states*
- *Limiting case is well-known infinite square well problem*

- *Mathematical representations of the above*