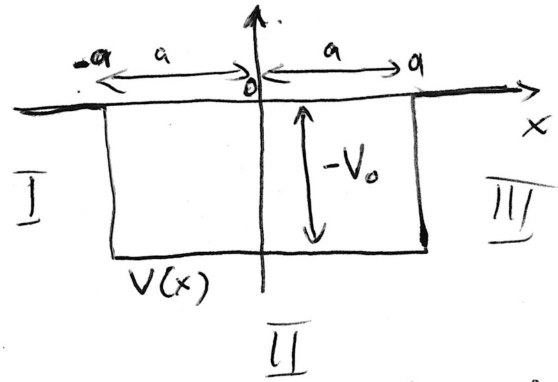
Finite square well

Let us consider the potential



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

with some positive constant V_0

In region I $V(x) = 0$ and the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad \text{or} \qquad \frac{d^2\psi}{dx^2} = k^2\psi \qquad \text{where} \quad k = \frac{\sqrt{-2mE}}{\hbar}$$ $E<$ $k>$

The general solution is $Ae^{-kx} + Be^{kx}$. The requirement of the square integrability yields $A = 0$. Thus

$$\psi_I(x) = Be^{kx}$$

In region III we obtain in the similar way

$$\psi_{III} = Fe^{-kx}$$

In region II we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \qquad \text{or} \qquad \frac{d^2\psi}{dx^2} = -\ell^2\psi$$

with $\ell \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar} > 0$

The general solution is

$$\psi_{II}(x) = C\sin(\ell x) + D\cos(\ell x)$$

Let us note that since $V(x)$ is symmetric then

$\psi(-x) = \pm\psi(x)$

For even solutions

$$\psi(x) = \begin{cases} Fe^{-kx} & x > a \\ D\cos(\ell x) & 0 < x < a \\ \psi(-x) & x < 0 \end{cases}$$

The continuity of ψ at $x = a$ gives:

$$Fe^{-ka} = D\cos(\ell a)$$

The continuity of ψ' says

$$-\kappa F e^{-\kappa a} = -\ell D \sin(\ell a)$$

Dividing the last equation by the previous one results in the following relation:

$$\kappa = \ell \tan(\ell a)$$

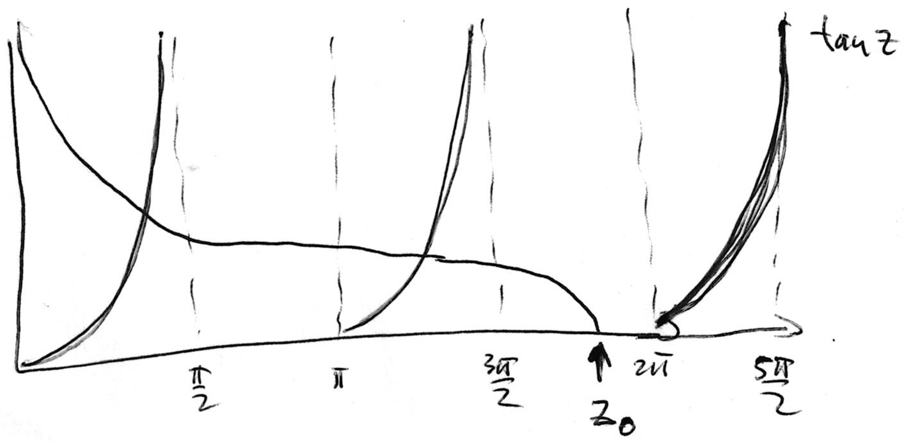
Let us now introduce notations: $z \equiv \ell a, \quad z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$

$$\kappa^2 + \ell^2 = \frac{2mV_0}{\hbar^2} \quad \text{and} \quad \kappa a = \sqrt{z_0^2 - z^2}$$

With that our equation becomes

$$\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

Its solution can be found graphically



The number of solutions depend on the value of z_0.

Limiting case of a deep wide well:

if $z_0 \to \infty$ $\quad z_n \approx \frac{n\pi}{2}$ with n odd

$$E_n \approx -V_0 + \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$ ⟵ energy levels of a infinite square well

Limiting case of a shallow, narrow well:

As z_0 decreases we get into a situation when only one solution is kept. Note that there is always a bound state, ~~no matter~~ regardless of the choice of V_0 and a.

For odd solutions

$$\psi(x) = \begin{cases} Fe^{-kx} & x > a \\ C\sin(\ell x) & 0 < x < a \\ \psi(-x) & x < 0 \end{cases}$$

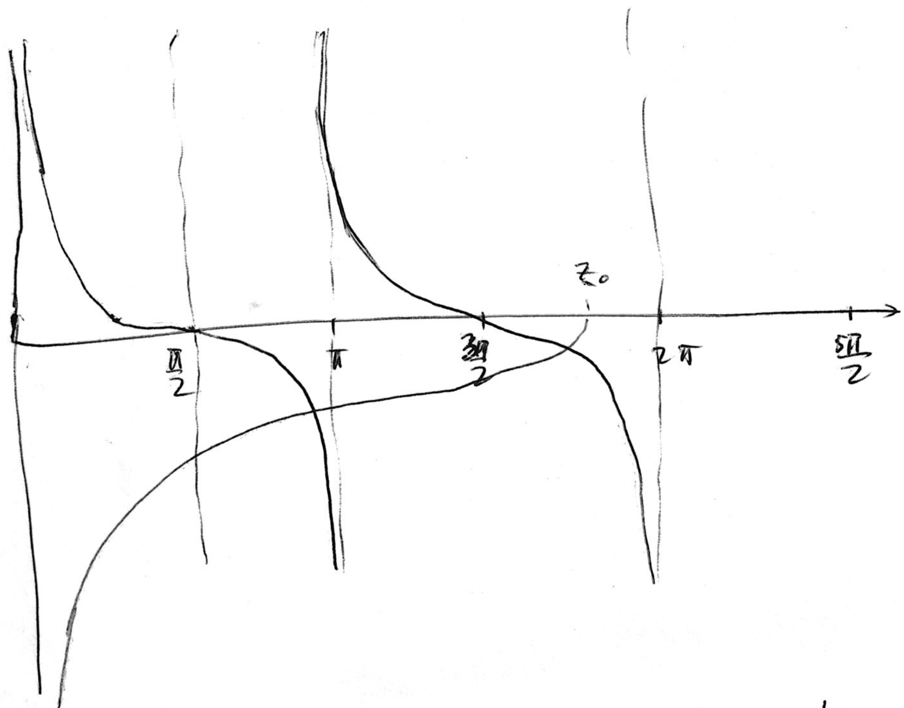
Again the continuity of ψ and ψ' yields

$$Fe^{-ka} = C\sin(\ell x)$$

$$-kFe^{-ka} = \ell C\cos(\ell x)$$

or

$$k = -\ell\cot(\ell a) \qquad \text{or} \qquad \cot z = -\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$



If z_0 is small enough there may be no odd solutions at all

Now let us consider the case of positive energies $(E>0)$. The solution in this case is:

$$\psi = Ae^{ikx} + Be^{-ikx} \quad (x<-a) \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi = C\sin(lx) + D\cos(lx) \quad (-a<x<0) \qquad l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

If no incoming wave on the right then $\psi = Fe^{ikx}$

Continuity of ψ at $x=-a$: $Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la)$

Continuity of ψ' at $x=-a$: $ik\left[Ae^{-ika} - Be^{ika}\right] = l\left[C\cos(la) + D\sin(la)\right]$

Continuity of ψ at $x=+a$: $C\sin(la) + D\cos(la) = Fe^{ika}$

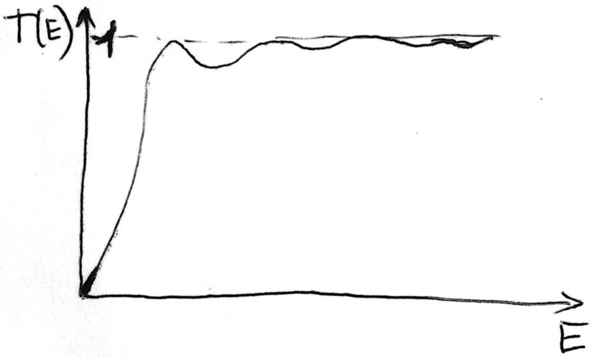
Continuity of ψ' at $x=+a$: $l\left[\cos(la) - D\sin(la)\right] = ikFe^{ika}$

Solving for B and F gives:

$$B = i\frac{\sin(2la)}{2kl}(l^2-k^2)F \qquad F = \frac{e^{-2ika}A}{\cos(2la) - i\frac{(k^2+l^2)}{2kl}\sin(2kl)}$$

The transmission probability is:

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)}$$



at $\frac{2a}{\hbar}\sqrt{2m(E+V_0)} = n\pi$ T becomes 1 (100% transparancy)

This perfect transmission occurs when

$$\underbrace{E + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}}_{\text{energy levels of infinite square well}}$$