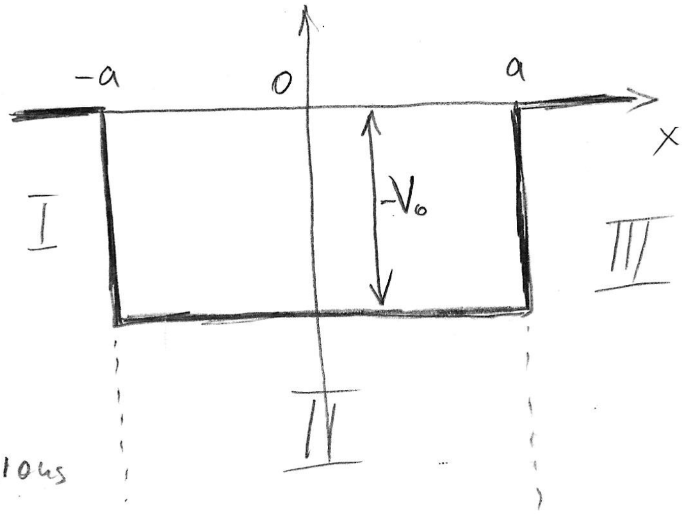
Finite square well

Let us consider the bound states $(E<0)$ of the potential:



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

where V_0 is some positive constant. We will solve the Schrödinger equation in regions I, II, III (as depicted) separately and then use the matching conditions.

In region I $V(x)=0$. Therefore, we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \text{or} \quad \psi'' - k^2\psi = 0 \quad \text{where} \quad k = \frac{\sqrt{-2mE}}{\hbar} = \frac{\sqrt{2m|E|}}{\hbar} > 0$$

The general solution of the above equation is

$$\psi = Ae^{-kx} + Be^{kx}$$

The requirement of the square integrability yields $A=0$

Thus,

$$\psi_I = Be^{kx}$$

Similarly, in region III we obtain $\psi_{III} = Fe^{-kx}$.

In region II, on the other hand, we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \quad \text{or} \quad \psi'' + \varkappa^2\psi \quad \text{with} \quad \varkappa \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar} > 0$$

The general solution is

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

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

As we showed it in a previous lecture, if $V(-x)=V(x)$ then $\psi(-x) = \pm\psi(x)$ [when each E corresponds to a single eigenfunction)

For even solutions then

$$\psi(x) = \begin{cases} F e^{-kx}, & x > a \\ D \cos \varkappa x, & -a < x < a \\ F e^{kx}, & x < -a \end{cases}$$

note $B = F$ in order to satisfy $\psi(-x) = \psi(x)$

The continuity of ψ at $x = a$ gives

$$F e^{-ka} = D \cos \varkappa a$$

ψ' must also be continuous (which can be shown easily by integrating the Schrödinger equation in the vicinity of $x = a$ or any other point). The continuity of ψ' results in the following matching condition

$$-k F e^{-ka} = -\varkappa D \sin \varkappa a$$

By dividing the last equation by the second last gives

$$k = \varkappa \tan \varkappa a$$

This is a trancendental equation with respect to E. We can solve it graphically (or numerically). For this purpose it is convenient to introduce the following notations:

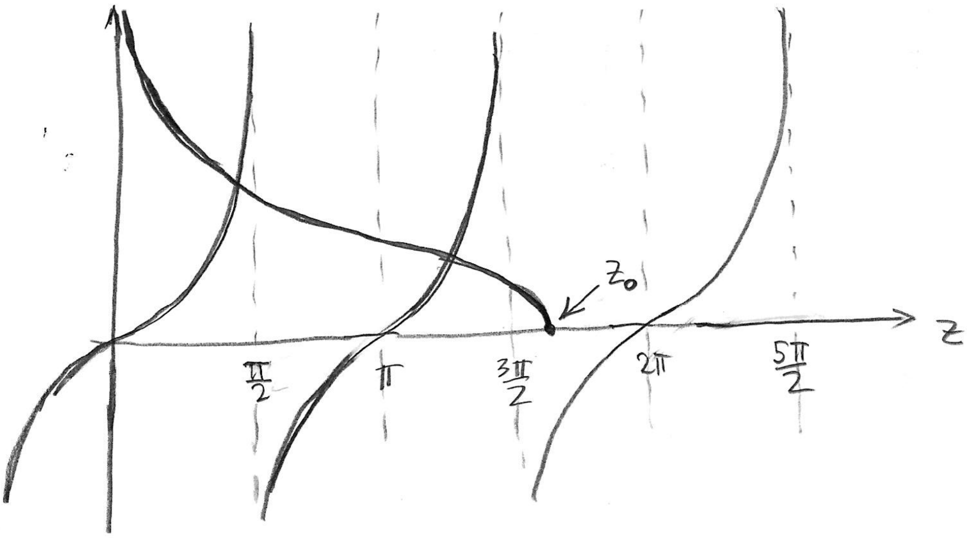
$$z = \varkappa a \qquad z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$$

Note that $k^2 + \varkappa^2 = \frac{2mV_0}{\hbar^2}$ and $ka = \sqrt{z_0^2 - z^2}$

In the above notations our trancendental equation becomes

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

The solutions are such points z where $\tan z$ intersects with $\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$:



The actual number of solutions depends on the value z_0

If we consider the limiting case of a very deep or wide well then $z_0 = \frac{a}{\hbar}\sqrt{2mV_0} \to \infty$. It is easy to see that the number of solutions then is infinite and the are given by $z_n = \frac{n\pi}{2}$, $n = 1,3,5..$

and
$$E_n \approx -V_0 + \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

This expression reproduces the energy levels in an infinite square well (corresponding to even wave functions)

Now in the opposite case, when the well becomes very shallow (and narrow) we have a situation when only a single solution exists:

$$z = 0$$

Note, however, that there is always at least one solution (and thus a bound state), regardless of the magnitude of V_0 and a.

So far we discussed the even solutions $(\psi(-x) = \psi(x))$

Now let us turn our attention to the odd solutions

If $\psi(-x) = -\psi(x)$ then our wave function is

$$\psi(x) = \begin{cases} F e^{-\kappa x}, & x > a \\ C \sin \varkappa x, & 0 < x < a \\ -F e^{\kappa x}, & x < 0 \end{cases}$$

Again, the continuity of ψ and ψ' yields the matching conditions

$$F e^{-\kappa a} = C \sin \varkappa a$$

$$-\kappa F e^{-\kappa a} = \varkappa C \cos \varkappa a$$

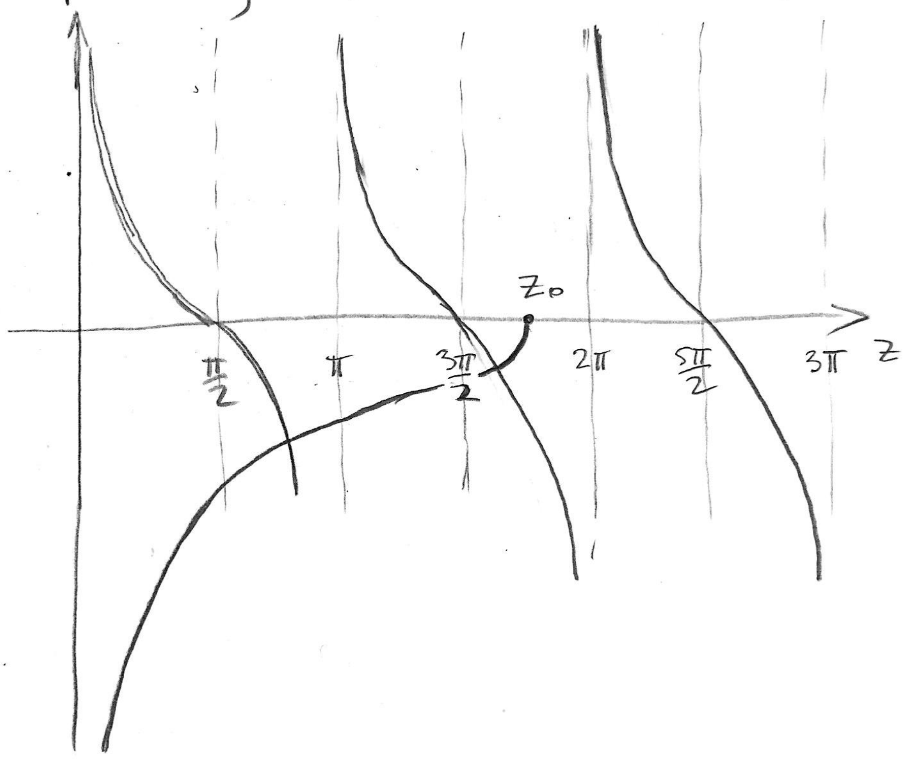
or, if we divide one equation by the other:

$$\kappa = -\varkappa \cot \varkappa a$$

In our notations it becomes

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

Graphically it looks as follows. It can be seen that if z_0 is sufficiently small (shallow and narrow well) then there may be no odd solutions at all.



We have considered the bound states of the potential. Now let us discuss the continuum states, i.e. the states with $E > 0$.

For the continuum states there is no normalization requirement. The solution of the Schrödinger equation in region I is

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

Inside the well, in region II we have exactly what we had before (as there is no sign change in $\varkappa = \frac{\sqrt{2m(E+V_0)}}{\hbar}$ when E becomes positive). Thus,

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

For region III the general solution has a form similar to $\psi_I(x)$:

$$\psi_{III} = Fe^{ikx} + Ge^{-ikx}$$

If we are to compute the transmission and reflection coefficient then we must assume that there is no incoming wave from the right and, thus, $G = 0$. With that our entire wave function becomes

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < -a \\ C\sin\varkappa x + D\cos\varkappa x, & -a < x < a \\ Fe^{ikx}, & x > a \end{cases}$$

There are five undetermined coefficients here. We also have four continuity conditions – both the wave function and its derivative must be continuous at $x = a$ and $x = -a$. This allows to determine the ratios $\frac{B}{A}$ and $\frac{F}{A}$ and their squares:

$$\psi'(x) = \begin{cases} ik\left[Ae^{ikx} - Be^{-ikx}\right] & , \quad x < -a \\ \varkappa\left[C\cos\varkappa x - D\sin\varkappa x\right] & , \quad -a < x < a \\ ikFe^{ikx} & , \quad x > a \end{cases}$$

$\psi(-a)$: $$Ae^{-ika} + Be^{ika} = -C\sin\varkappa a + D\cos\varkappa a \qquad (1)$$

$\psi(a)$: $$C\sin\varkappa a + D\cos\varkappa a = Fe^{ika} \qquad (2)$$

$\psi'(-a)$: $$ik\left[Ae^{-ika} - Be^{ika}\right] = \varkappa\left[C\cos\varkappa a + D\sin\varkappa a\right] \qquad (3)$$

$\psi'(a)$: $$\varkappa\left[C\cos\varkappa a - D\sin\varkappa a\right] = ikFe^{ika} \qquad (4)$$

Let us multiply (2) by $\sin\varkappa a$ and add it to (4) multiplied by $\frac{1}{\varkappa}\cos\varkappa a$. We get

$$C = Fe^{ika}\left[\sin\varkappa a + \frac{ik}{\varkappa}\cos\varkappa a\right]$$

Let us also multiply (2) by $\cos\varkappa a$ and subtract from it (4) multiplied by $\frac{1}{\varkappa}\sin\varkappa a$. This gives

$$D = Fe^{ika}\left[\cos\varkappa a - \frac{ik}{\varkappa}\sin\varkappa a\right]$$

If we now plug these expressions for C and D into (1) we obtain

$$Ae^{-ika} + Be^{ika} = -Fe^{ika}\left[\sin\varkappa a + \frac{ik}{\varkappa}\cos\varkappa a\right]\sin\varkappa a +$$
$$+ Fe^{ika}\left[\cos\varkappa a - \frac{ik}{\varkappa}\sin\varkappa a\right]\cos\varkappa a =$$
$$= Fe^{ika}\left[\cos^2\varkappa a - \frac{ik}{\varkappa}\sin\varkappa a\cos\varkappa a - \sin^2\varkappa a - \frac{ik}{\varkappa}\sin\varkappa a\cos\varkappa a\right] =$$
$$= Fe^{ika}\left[\cos 2\varkappa a - \frac{ik}{\varkappa}\sin 2\varkappa a\right] \qquad (*)$$

We can also substitute C and D in (3):

$$Ae^{-ika} - Be^{ika} = -\frac{i\varkappa}{k} F e^{ika}\left[\left(\sin\varkappa a + \frac{ik}{\varkappa}\cos\varkappa a\right)\cos\varkappa a + \left(\cos\varkappa a - \frac{ik}{\varkappa}\sin\varkappa a\right)\sin\varkappa a\right] =$$

$$= -\frac{i\varkappa}{k} F e^{ika}\left[\sin\varkappa a\cos\varkappa a + \frac{ik}{\varkappa}\cos^2\varkappa a + \sin\varkappa a\cos\varkappa a - \frac{ik}{\varkappa}\sin\varkappa a\right]$$

$$= -\frac{i\varkappa}{k} F e^{ika}\left[\sin 2\varkappa a + \frac{ik}{\varkappa}\cos 2\varkappa a\right] = Fe^{ika}\left[\cos 2\varkappa a - \frac{i\varkappa}{k}\sin 2\varkappa a\right] \quad (**)$$

If we add (*) and (**) we get

$$2Ae^{-ika} = Fe^{ika}\left[2\cos 2\varkappa a - i\left(\frac{k}{\varkappa} + \frac{\varkappa}{k}\right)\sin 2\varkappa a\right]$$

or

$$\frac{F}{A} = \frac{e^{-2ika}}{\cos 2\varkappa a - i\frac{\sin 2\varkappa a}{2\varkappa k}(k^2+\varkappa^2)}$$

The transmission coefficient is given by the absolute square of $\frac{F}{A}$ ration:

$$T = \left|\frac{F}{A}\right|^2 = \frac{1}{\left|\cos 2\varkappa a - i\frac{\sin 2\varkappa a}{2\varkappa k}(k^2+\varkappa^2)\right|^2} = \frac{1}{\cos^2 2\varkappa a + \frac{\sin^2 2\varkappa a}{(2\varkappa k)^2}(k^2+\varkappa^2)^2}$$

This can be further simplified to

$$T = \frac{1}{1 + \frac{(k^2-\varkappa^2)^2}{(2k\varkappa)^2}\sin^2 2\varkappa a}$$

Inserting the expressions for k and $\varkappa$ yields the final expression for the transmission coefficient:

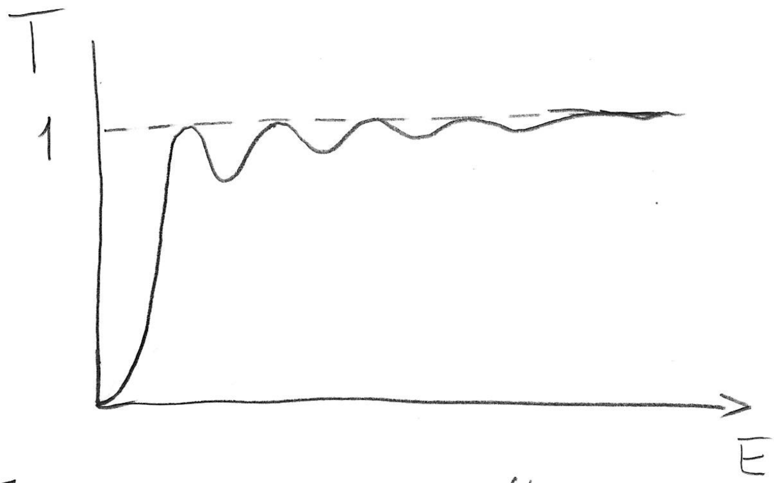
$$2\varkappa a = \frac{2a}{\hbar}\sqrt{2m(E+V_0)} \qquad k^2 - \varkappa^2 = -\frac{2mV_0}{\hbar^2}$$

$$\frac{(k^2-\varkappa^2)^2}{(2k\varkappa)^2} = \frac{\left(\frac{2m}{\hbar^2}\right)^2 V_0^2}{4\left(\frac{2m}{\hbar^2}\right)^2 E(E+V_0)} = \frac{V_0^2}{4E(E+V_0)}$$

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

The reflection coefficient is obviously given by

$$R = 1 - T$$



T becomes exactly 1 (full transparency) when

$$\frac{2a}{\hbar}\sqrt{2m(E+V_0)} = n\pi \qquad n = 0, 1, 2, \ldots$$

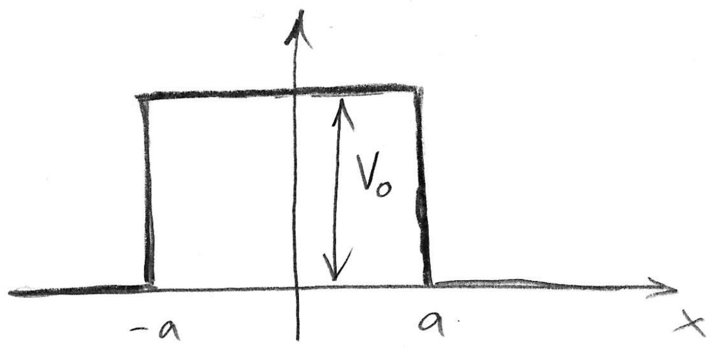
The energies for the perfect transmission

$$E_n = -V_0 + \frac{n^2\pi^2\hbar^2}{2m(2a)^2} \qquad (\text{but such that } E_n > 0)$$

Transmission through a rectangular barrier

Let us now consider the potential in the form of a rectangular barrier

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



This problem is, in fact, very similar to the potentia well $(E>0)$. When $E > V_0$ we essentially have exactly the same equations.

The only minor difference is the sign before V_0. However, if $E > V_0$ this sign does not make anything different. Therefore we can just copy the formula for T while replacing $V_0 \to -V_0$

$$T = \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E-V_0)}\right)} \quad , \quad E > V_0$$

When $0 < E < V_0$ we can still use the formula

$$\frac{F}{A} = \frac{e^{-2ika}}{\cos 2\varkappa a - i \frac{\sin 2\varkappa a}{2\varkappa k}(k^2+\varkappa^2)}$$

but with complex $\varkappa = \frac{\sqrt{2m(E-V_0)}}{\hbar} = i\frac{\sqrt{2m(V_0-E)}}{\hbar} = i\gamma \quad , \quad \gamma > 0$

Then we can also use the fact that

$$\sin ix = \frac{e^{i(ix)} - e^{-i(ix)}}{2i} = i \sinh x$$

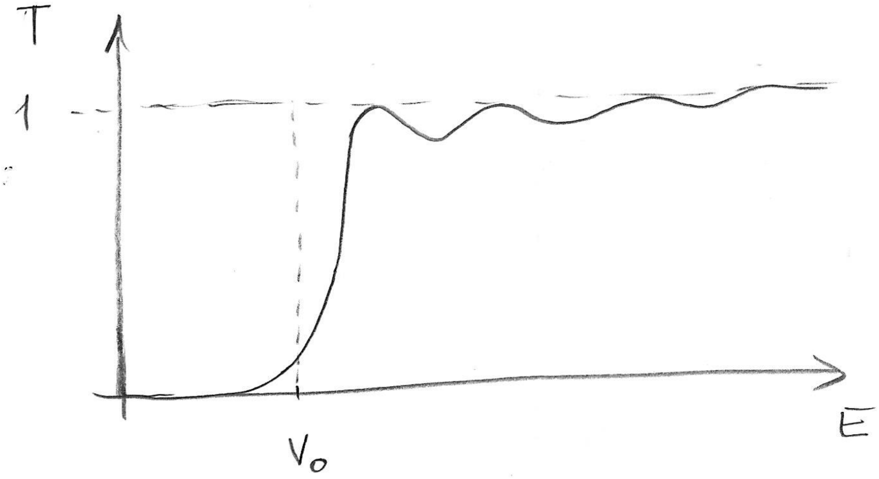
$$\cos ix = \frac{e^{i(ix)} + e^{-i(ix)}}{2} = \cosh x$$

With that

$$\frac{F}{A} = \frac{e^{-2ika}}{\cosh(2\gamma a) + i\frac{\sinh(2\gamma a)}{2\gamma k}(k^2-\gamma^2)}$$

After some manipulations we can obtain the expression for T:

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)} \sinh^2\left(\frac{2a}{\hbar}\sqrt{2m(V_0-E)}\right)} \qquad E < V_0$$


T
1
E
V_0