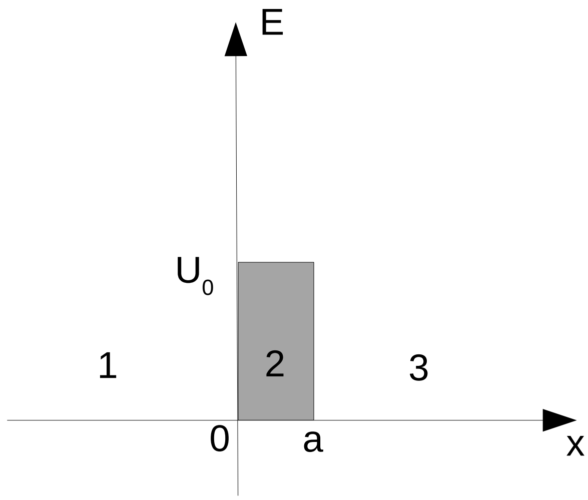
1. Propagation of particles over a rectangle barrier.

<u>We start with the option **E>U$_0$.**</u>

The flow of particles moves from left to right and falls on a rectangular barrier. The width of the barrier is



a and the height is U$_0$. The coordinate-area can be separated on three regions 1,2 and 3(see picture). The Schrodinger equations for different regions are:

First region / Second region / Thirth region

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi_1}{dx^2}=E\varphi_1 \qquad -\frac{\hbar^2}{2m}\frac{d^2\varphi_2}{dx^2}+U_0\varphi_2=E\varphi_2 \qquad -\frac{\hbar^2}{2m}\frac{d^2\varphi_3}{dx^2}=E\varphi_3$$

The solution is elementary and can be written directly:

$$\varphi_1=Ae^{ik_1x}+Be^{-ik_1x} \qquad \varphi_2=Ce^{ik_2x}+De^{-ik_2x} \qquad \varphi_3=Fe^{ik_1x}$$

here $k_1=\frac{\sqrt{2mE}}{\hbar}$, $k_2=\frac{\sqrt{2m(E-U_0)}}{\hbar}$ both parameters are real numbers. The unknown parameters A,B,C,D and F can be calculated from continuity property of wavefunction:

$$\varphi_1(0)=\varphi_2(0)\ ,\ \varphi_2(a)=\varphi_3(a)\ ,\ \left.\frac{d\varphi_1}{dx}\right|_{x=0}=\left.\frac{d\varphi_2}{dx}\right|_{x=0}\ ,\ \left.\frac{d\varphi_2}{dx}\right|_{x=a}=\left.\frac{d\varphi_3}{dx}\right|_{x=a}\ .$$

The corresponding system of linear equations are looks like as follows:

$$\begin{array}{l} 1+B=C+D \\ (1-B)\cdot k_1=(C-D)\cdot k_2 \\ Ce^{ik_2a}+De^{-ik_2a}=Fe^{ik_1a} \\ Ck_2e^{ik_2a}-Dk_2e^{-ik_2a}=k_1Fe^{ik_1a} \end{array} .$$

This system of equations (with complex coefficients) can be represented in the matrix form **My=b**, here **M** is the coefficient matrix for unknown parameters A,B,C and F, **y-** is the column matrix containing the these parameters and **b-** is the column matrix for free parameters. To simplify the further derivation, let's take parameter A=1. The expressions for the corresponding matrices look like this:

$$M=\begin{pmatrix} -1 & 1 & 1 & 0 \\ 1 & \frac{k_2}{k_1} & -\frac{k_2}{k_1} & 0 \\ 0 & e^{ik_2a} & e^{-ik_2a} & -e^{ik_1a} \\ 0 & k_2e^{ik_2a} & -k_2e^{-ik_2a} & -k_1e^{ik_1a} \end{pmatrix}\quad , \quad b=\begin{pmatrix}1\\1\\0\\0\end{pmatrix} \quad \text{and} \quad y=\begin{pmatrix}B\\C\\D\\F\end{pmatrix} \quad .$$

Transmission coefficient can be calculated as ratio of the probability current densities for particles passed into area 3 j_t and incident particles j_i. The easiest way to find a solution to this system is to use some kind of mathematical framework, such as ***Mathematica*** or ***Maple***. After applying equation for calculation of the probability current density $j=\frac{i\hbar}{2m}(\varphi\nabla\varphi^*-\varphi^*\nabla\varphi)$ the corresponding vectors are equal: $j_t=\frac{\hbar k_1}{m}F^2$ and $j_i=\frac{\hbar k_1}{m}$ for **T** coefficient we have:

$$T=\frac{4k_1^2k_2^2}{4k_1^2k_2^2\cos^2(k_2a)+(k_1^2+k_2^2)^2\sin^2(k_2a)} \quad \text{for } \mathbf{E>U_0}.$$

for aim of visualization it is make sense use dimensionless parameters $x=\frac{E}{U_0}$ and effective dimension-less width of barrier $a^*=\frac{a\sqrt{2mU_0}}{\hbar}$, then transmission coefficient can be represented as follows:

$$T=\frac{4x(x-1)}{4x(x-1)\cos^2(a^*\cdot\sqrt{x-1})+(2x-1)^2\sin^2(a^*\cdot\sqrt{x-1})} \quad \text{for } x>1$$

2. Propagation of particles under a rectangle barrier.

<u>For case **E<U₀.**</u>

The Schrodinger equations for different regions are the same as in the previous case.

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi_1}{dx^2}=E\varphi_1 \qquad -\frac{\hbar^2}{2m}\frac{d^2\varphi_2}{dx^2}+U_0\varphi_2=E\varphi_2 \qquad -\frac{\hbar^2}{2m}\frac{d^2\varphi_3}{dx^2}=E\varphi_3$$

The solution is elementary and can be written directly:

$$\varphi_1=Ae^{ik_1x}+Be^{-ik_1x} \qquad \varphi_2=Ce^{k_2x}+De^{-k_2x} \qquad \varphi_3=Fe^{ik_1x}$$

here $k_1=\frac{\sqrt{2mE}}{\hbar}$, $k_2=\frac{\sqrt{2m(U_0-E)}}{\hbar}$. The unknown parameters A,B,C,D and F can be calculated from continuity property for wavefunction.

$$\varphi_1(0)=\varphi_2(0) \quad , \quad \varphi_2(a)=\varphi_3(a) \quad , \quad \left.\frac{d\varphi_1}{dx}\right|_{x=0}=\left.\frac{d\varphi_2}{dx}\right|_{x=0} \quad , \quad \left.\frac{d\varphi_2}{dx}\right|_{x=a}=\left.\frac{d\varphi_3}{dx}\right|_{x=a} \quad .$$

The corresponding equations are looks like as follows:

$$\begin{array}{l} 1+B=C+D \\ (1-B)\cdot i\,k_1=(C-D)\cdot k_2 \\ Ce^{k_2 a}+De^{-k_2 a}=Fe^{ik_1 a} \\ C\,k_2 e^{k_2 a}-D\,k_2 e^{-k_2 a}=ik_1\,Fe^{ik_1 a} \end{array} .$$

The corresponding matrices **M,y** and **b** are:

$$M=\begin{pmatrix} -1 & 1 & 1 & 0 \\ 1 & -i\dfrac{k_2}{k_1} & i\dfrac{k_2}{k_1} & 0 \\ 0 & e^{k_2 a} & e^{-k_2 a} & -e^{ik_1 a} \\ 0 & k_2 e^{k_2 a} & -k_2 e^{-k_2 a} & -ik_1 e^{ik_1 a} \end{pmatrix} ,\quad b=\begin{pmatrix}1\\1\\0\\0\end{pmatrix} \quad \text{and} \quad y=\begin{pmatrix}B\\C\\D\\F\end{pmatrix} .$$

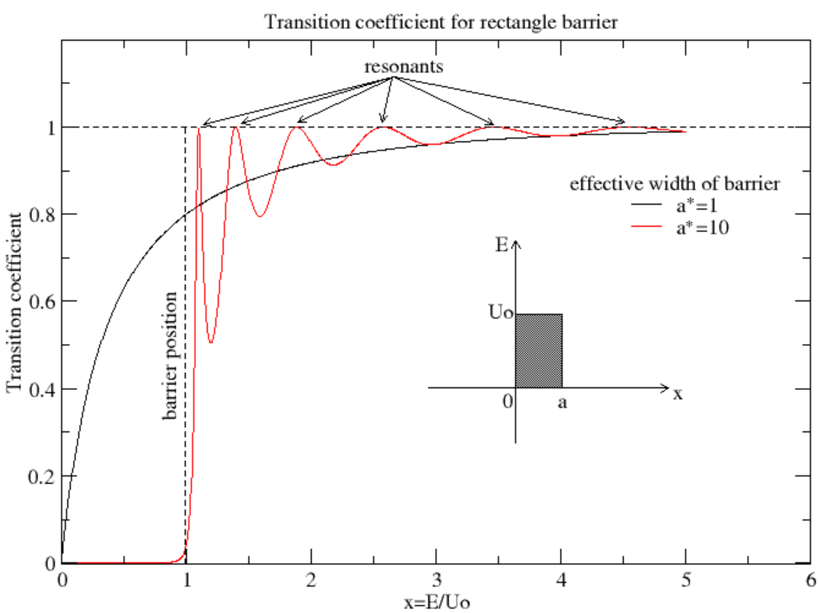
For transmission coefficient in this case we have:

$$T=\frac{4k_1^2k_2^2}{4k_1^2k_2^2\cosh^2(k_2 a)+(k_1^2-k_2^2)^2\sinh^2(k_2 a)}$$ for **E<U₀.**

The using of dimensionless parameters $x=\dfrac{E}{U_0}$ and effective dimensionless width of barrier

$a^*=\dfrac{a\sqrt{2mU_0}}{\hbar}$ gives for transmission coefficient :

$$T=\frac{4x(1-x)}{4x(1-x)\cosh^2(a^*\cdot\sqrt{1-x})+(2x-1)^2\sinh^2(a^*\cdot\sqrt{1-x})}$$ for x<1.



The result of calculating the transmission coefficient is shown in the figure. As you can see, there are windows of transparency (resonances) for the flow of incident particles for energies that satisfy the condition $k_2 a=\pi n$. Particles in this case pass through the barrier without reflection because for the corresponding energies the transmission coefficient is equal to 1. Resonances are takes place for the energies equal to:

$$E=\frac{\pi^2\hbar^2 n^2}{2ma^2}+U_0, n>0\in Z$$

and for dimensionless parameters

$$\frac{E}{U_0}=x=1+\left(\frac{\pi n}{a^*}\right)^2 .$$

These results can be compared with the classical behavior of the transmission coefficient. For classical physics we have:

$$T_{classic}(E)=\begin{cases}0, if\ E\leqslant U_0\\1, if\ E>U_0\end{cases}\ .$$

Can be shown that: $\lim_{a^* \to \infty} T_{quantum} \to T_{classic}$