1.1 One-dimensional motion in a field of two «delta-wells»

Let us consider solution of Schrodinger equation in position representation for the quantum particle, which moves in a field of two delta-wells (fig. 1) $U(x) = -\alpha(\delta(x) + \delta(x-a))$

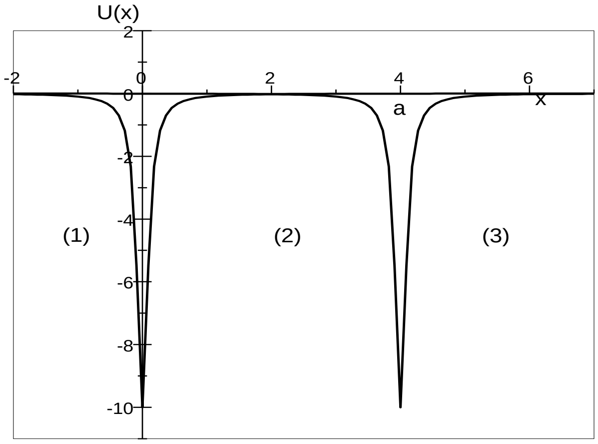

Fig.1. Schematic drawing of the potential energy $U(x) = -\alpha\left(\delta(x) + \delta(x-a)\right)$

Solution

Let us consider one-dimensional time-independent Schrodinger equation (SchE)

$$-\frac{\hbar^2}{2m}\psi''(x) + U(x)\psi(x) = E\psi \tag{1.1}$$

Depending on the energy sign E particle's motion can be finite when $E<0$, as well as infinite when $E>0$. When $E<0$, motion is finite and particle state is bound.

Let us consider firstly negative energies $E<0$. SchE in this case has the form:

$$-\frac{\hbar^2}{2m}\psi''(x) - \alpha\left(\delta(x) + \delta(x-a)\right)\psi(x) = -\varepsilon\psi, \quad \varepsilon = -|E|. \tag{1.2}$$

We insert the expression for the potential energy in the equation and took into the account that bound states should have negative energies.

Wave function will be defined by different analytic expressions in three areas: $1.\, x \le 0; \quad 2.\, 0 \le x \le a; \quad 3.\, x \ge a$.

Since delta-function $\delta(x)$ and $\delta(x-a)$ are non-zero just in points $x=0, x=a$, so SchE (1.2) at $x \ne 0, x \ne a$ has the form

$$\psi'' - k_0^2\psi(x) = 0, \quad k_0^2 = \frac{2m|E|}{\hbar^2}. \tag{1.3}$$

We will define boundary conditions of the equation (1.3). As is well known, wave function is always continuous. From the equation (1.2) follows that in singular points $x=0, x=a$ second derivative from wave function experiences infinite discontinuities.

This means, that first derivative has finite jumps in this points. Let us define them. Delta-function $\delta(x)$ and $\delta(x-a)$ contribute only in boundary conditions, which define jumps of the first derivative from the wave function in the points $x=0,\ x=a$.

Integrating (1.2) firstly near the point $x=0$ from $-\varepsilon$ to $+\varepsilon$

$$\int_{-\varepsilon}^{+\varepsilon} -\frac{\hbar^2}{2m}\psi''(x)dx - \alpha\int_{-\varepsilon}^{+\varepsilon}\delta(x)\psi(x)dx = -|E|\int_{-\varepsilon}^{+\varepsilon}\psi dx$$

$$-\frac{\hbar^2}{2m}\psi'(x)\Big|_{-\varepsilon}^{+\varepsilon} - \alpha\psi(0) = -|E|\int_{-\varepsilon}^{+\varepsilon}\psi dx$$

$$-\frac{\hbar^2}{2m}\left[\psi'(+\varepsilon)-\psi'(-\varepsilon)\right] - \alpha\psi(0) = -|E|\left[F(+\varepsilon)-F(-\varepsilon)\right]$$

Let's pass on to the limit $\varepsilon \to +0$. Then in consequence of persistence of the wave function $F(+0)=F(-0)=F(0)$, and the jump of the first derivative of the wave function equals to

$$\psi_2'(+0)-\psi_1'(-0) = -\frac{2m\alpha}{\hbar^2}\psi(0).$$

Similarly one finds the jump of the first derivative in the point $x=a$. Integrating the equation (1.2) near the point $x=a$.

$$\int_{a-\varepsilon}^{a+\varepsilon} -\frac{\hbar^2}{2m}\psi''(x)dx - \alpha\int_{a-\varepsilon}^{a+\varepsilon}\delta(x-a)\psi(x)dx = -|E|\int_{a-\varepsilon}^{a+\varepsilon}\psi dx$$

$$-\frac{\hbar^2}{2m}\psi'(x)\Big|_{a-\varepsilon}^{a+\varepsilon} - \alpha\psi(a) = -|E|\int_{a-\varepsilon}^{a+\varepsilon}\psi dx$$

$$-\frac{\hbar^2}{2m}\left[\psi'(a+\varepsilon)-\psi'(a-\varepsilon)\right] - \alpha\psi(a) = -|E|\left[F(a+\varepsilon)-F(a-\varepsilon)\right]$$

$$F(a+0)=F(a-0)=F(a)$$

Consequently, the jump of the first derivative in the point $x=a$ equals to

$$\psi_3'(a+0)-\psi_2'(a-0) = -\frac{2m\alpha}{\hbar^2}\psi(a).$$

To sum up all boundary conditions, receive four equations

$$\begin{aligned}
&\psi_2(+0)=\psi_1(-0);\\
&\psi_2'(+0)-\psi_1'(-0) = -\frac{2m\alpha}{\hbar^2}\psi(0);\\
&\psi_3(a+0)=\psi_2(a-0);\\
&\psi_3'(a+0)-\psi_2'(a-0) = -\frac{2m\alpha}{\hbar^2}\psi(a),
\end{aligned} \tag{1.4}$$

and $\psi(x\to\pm\infty)$ should be finite. For bound states in means, that $\psi(x\to\pm\infty)\to 0.$ As it was said before, wave function is defined by three different analytic expressions in three areas $1.\ x\le 0;\quad 2.\ 0\le x\le a;\quad 3.\ x\ge a$

$\psi_1(x) = A_1 e^{kx} + B_1 e^{-kx};\ B_1 = 0,$ as the result of the boundary condition $\psi(x \to -\infty) \to 0.$

$\psi_2(x) = A_2 e^{kx} + B_2 e^{-kx};$

$\psi_3(x) = A_3 e^{k(x-a)} + B_3 e^{-k(x-a)};\ A_3 = 0,$ as the result of the boundary condition $\psi(x \to -\infty) \to 0.$

Consequently, four coefficients A_1, A_2, B_2, B_3 of the wave function

$$\begin{aligned}\psi_1 &= A_1 e^{kx};\\ \psi_2 &= A_2 e^{kx} + B_2 e^{-kx};\\ \psi_3 &= B_3 e^{-k(x-a)}\end{aligned} \tag{1.5}$$

are connected with four boundary conditions (1.4)

When $x = 0$ $\begin{cases} A_2 + B_2 = A_1; \\ A_2 - B_2 = \left(1 - \dfrac{2m\alpha}{\hbar^2 k}\right) A_1; \end{cases}$. Hence: $\begin{cases} A_2 = \left(1 - \dfrac{m\alpha}{\hbar^2 k}\right) A_1; \\ B_2 = \dfrac{m\alpha}{\hbar^2 k} A_1. \end{cases}$

When $x = a$ $\begin{cases} A_2 e^{ka} + B_2 e^{-ka} = B_3; \\ A_2 e^{ka} - B_2 e^{-ka} = \left(-1 + \dfrac{2m\alpha}{\hbar^2 k}\right) B_3; \end{cases}$ Hence: $\begin{cases} A_2 = \dfrac{m\alpha}{\hbar^2 k} e^{-ka} B_3; \\ B_2 = \left(1 - \dfrac{m\alpha}{\hbar^2 k}\right) e^{ka} B_3. \end{cases}$

Consequently, we defined connections between coefficient A_1, B_3 in areas 1 and 3:

$$\begin{aligned} A_2 &= \left(1 - \frac{m\alpha}{\hbar^2 k}\right) A_1 = \frac{m\alpha}{\hbar^2 k} e^{-ka} B_3; \\ B_2 &= \frac{m\alpha}{\hbar^2 k} A_1 = \left(1 - \frac{m\alpha}{\hbar^2 k}\right) e^{ka} B_3. \end{aligned}.$$

This coefficients are defined by the system of two linear homogeneous algebraic equations with two unknown values A_1, B_3

$$\begin{cases} \left(1 - \dfrac{m\alpha}{\hbar^2 k}\right) A_1 - \dfrac{m\alpha}{\hbar^2 k} e^{-ka} B_3 = 0; \\ \dfrac{m\alpha}{\hbar^2 k} A_1 - \left(1 - \dfrac{m\alpha}{\hbar^2 k}\right) e^{ka} B_3 = 0; \end{cases} \tag{1.6}$$

Such a system has non-trivial solutions under the condition of it's determinant to equal to zero

$$\begin{vmatrix} \left(1-\dfrac{m\alpha}{\hbar^2 k}\right) & -\dfrac{m\alpha}{\hbar^2 k}e^{-ka} \\ \dfrac{m\alpha}{\hbar^2 k} & -\left(1-\dfrac{m\alpha}{\hbar^2 k}\right)e^{ka} \end{vmatrix} = 0. \qquad (1.7)$$

From the equation (2.7) one finds dispersion relations for the levels of energy to define

$$\frac{\hbar^2 k}{m\alpha} - 1 = \pm e^{-ka}, \qquad (1.8)$$

And from the equations (1.7) and (1.8) – connection between A_1, B_3

$$B_3 = \pm A_1 e^{-ka}.$$

Let's introduce notations: $y = ka, \quad y_0 = \dfrac{m\alpha a}{\hbar^2}$. In the new variables equations (1.8) takes the form

$$\frac{y}{y_0} - 1 = \pm e^{-y}. \qquad (1.9)$$

Graphic solution of the equation (1.9) is represented in the fig.2.

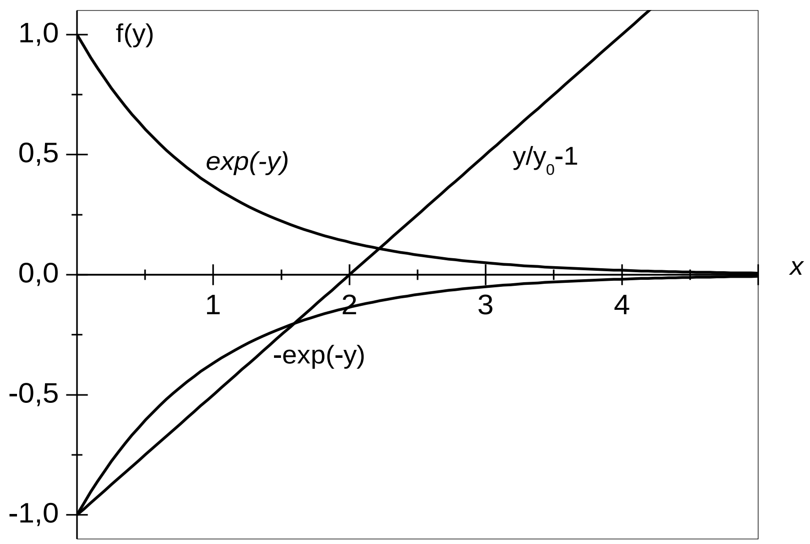

Fig.2. Graphic solution of the equation (1.9) when $a = 5, m = 1, \alpha = 10, \hbar = 1$.

As one sees from the fig. 2, equation $\frac{y}{y_0}-1=+e^{-y}$ always has only one solution, when equation $\frac{y}{y_0}-1=-e^{-y}$ has solution $y\neq 0$ only in the fulfilling of the condition $y_0>1$ which means, that $m\alpha a>\hbar^2$.

Normalized wave functions are listed below (2.5) (see fig.3)

$$\begin{cases} \psi_1=\sqrt{\frac{k}{2}}\frac{1}{\sqrt{1\pm e^{-ka}(1+ka)}}\left(e^{kx}\pm e^{k(x-a)}\right), x\leq 0 \\ \psi_2=\sqrt{\frac{k}{2}}\frac{1}{\sqrt{1\pm e^{-kx}(1+ka)}}\left(\pm e^{k(x-a)}+e^{-kx}\right), 0\leq x\leq a \\ \psi_3=\pm\sqrt{\frac{k}{2}}\frac{1}{\sqrt{1\pm e^{-kx}(1+ka)}}\left(e^{-k(x-a)}\pm e^{-kx}\right), x\geq a \end{cases} \tag{1.10}$$

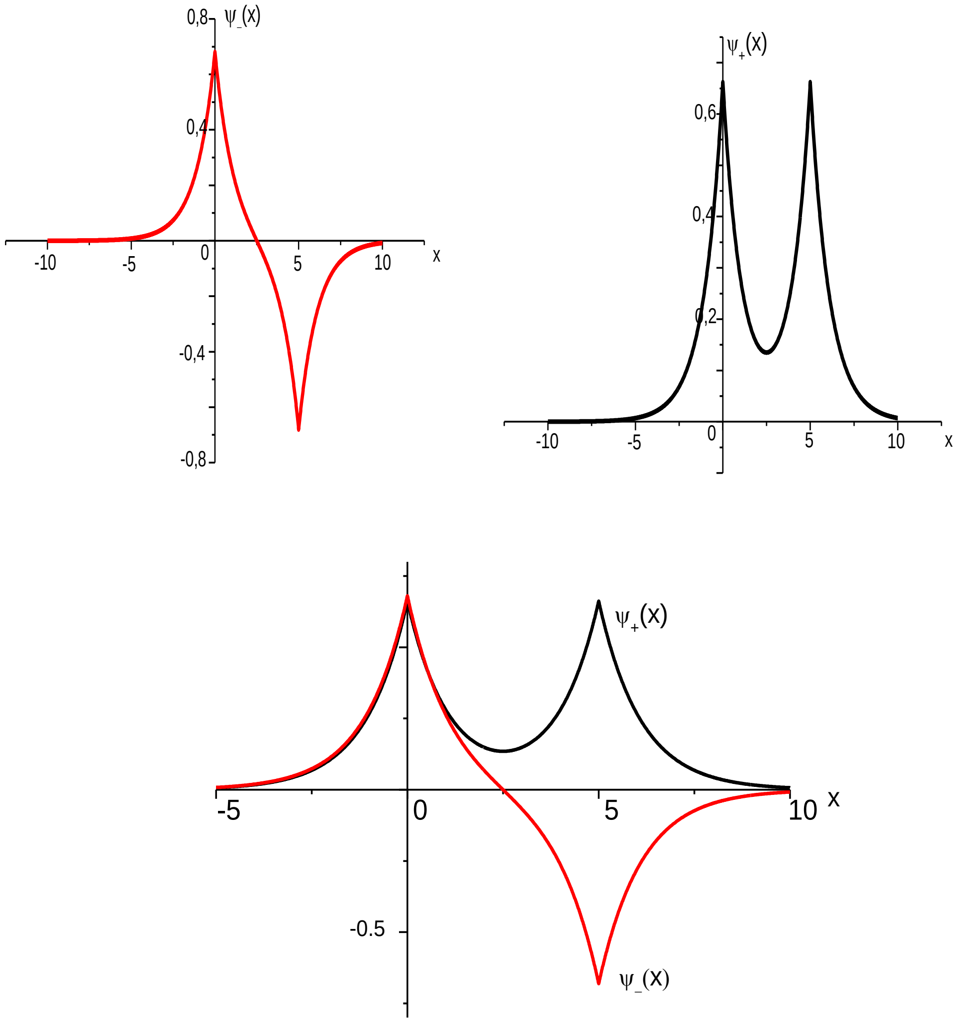

Fig.3. Wave functions (1.10) for $a=5, m=1, \alpha=10, \hbar=1$

Let's consider a case of $E>0$, which corresponds to above-the-barrier reflection. For the positive energies SchE (1.1) at $x \neq 0, x \neq a$ takes the form

$$\psi'' + k^2\psi(x) = 0, \quad \frac{2mE}{\hbar^2} = k^2. \tag{1.11}$$

with boundary conditions (1.4) for the wave function

$$\begin{cases} \psi_1 = A_1 e^{ikx} + B_1 e^{-ikx}; \\ \psi_2 = A_2 e^{ikx} + B_2 e^{-ikx}; \\ \psi_3 = A_3 e^{ik(x-a)}. \end{cases} \tag{1.12}$$

In equations (2.12) we supposed, that there is no particle's flow on the right, thus in third area there is only a transmitted wave. Coefficients A_3, B_1 are expressed through A_1 as follows

$$A_3 = \frac{A_1}{\gamma^2 e^{ika} + (1-i\gamma)^2 e^{-ika}}; \quad B_1 = \frac{2i\gamma(\cos ka - \gamma \sin ka)A_1}{\gamma^2 e^{ika} + (1-i\gamma)^2 e^{-ika}}; \quad \gamma = \frac{m\alpha}{k\hbar^2}. \tag{1.13}$$

Using usual definitions for the transmission and reflection coefficients

$$D = \frac{|j_{transmitted}|}{|j_{incidental}|} = \frac{|A_3|^2}{|A_1|^2}; \quad R = \frac{|j_{reflected}|}{|j_{incidental}|} = \frac{|B_1|^2}{|A_1|^2} \tag{1.14}$$

we have

$$\begin{cases} D = \dfrac{1}{1+4\gamma^2(\cos ka - \gamma \sin ka)^2}; \\ R = \dfrac{4\gamma^2(\cos ka - \gamma \sin ka)^2}{1+4\gamma^2(\cos ka - \gamma \sin ka)^2}. \end{cases} \tag{1.15}$$

At $\tan ka = \dfrac{k\hbar^2}{m\alpha}$ there is no reflection (fig. 4), and the potential is transparent $T=1, \quad R=0.$

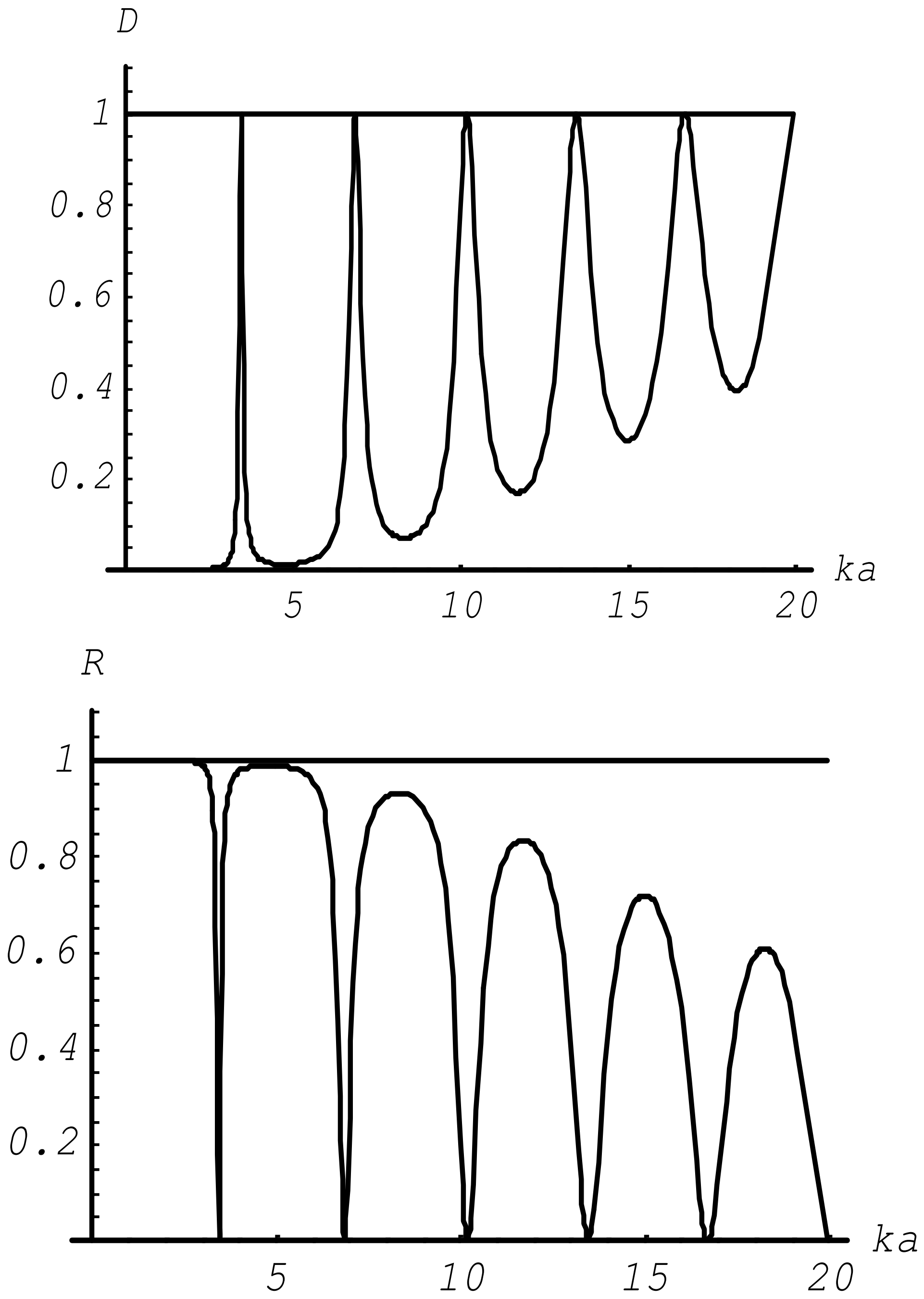

Fig.4. Transmission and reflection coefficients $a=5, m=1, \alpha=10, \hbar=1.$