Tunneling phenomena in solids

Lecture 1. Scattering and tunneling in quantum mechanics. Resonant tunneling. Exact solutions

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Outline of mini-course and requirements

Preliminary program:

- Lecture 1: Scattering and tunneling in quantum mechanics. Resonant tunneling. Exact solutions (July, 15)
- Lecture 2: Quantum-well states. Coupled potential wells. Exact solutions (July, 16)
- Lecture 3: Tunneling and quasiclassical approximation. Bardeen's approach. Quasistationary states (July, 16)
- Lecture 4: Tunneling in normal-metal junctions (July, 17)
- Lecture 5: Scanning tunneling microscopy and spectroscopy. Quasiparticle interference. Quantum-well states and tunneling interferometry (July, 18)
- Lecture 6: Tunneling in ferromagnet-insulator-ferromagnet junctions. Spin-polarized scanning tunneling microscopy (July, 19) → very close to the lectures of Irina Bobkova on magnetism and spintronics

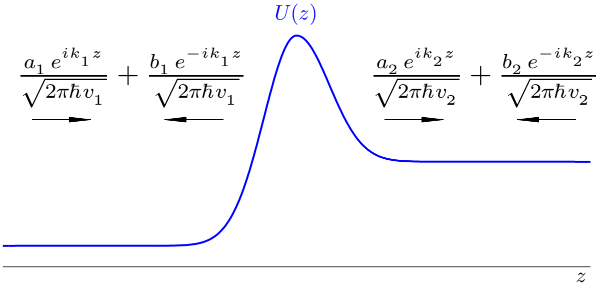
Requirements:

- Differential and integral calculus
- Basics of quantum mechanics and solid-state physics

Part 1: basic definitions

Scattering states in quantum mechanics

We consider one-dimensional (1D) movement a quantum particle with a full energy $E_\parallel$ in a system, where the potential energy depends only on the z coordinate. Hereafter we assume that the potential is localized in a certain region (see figure)



The stationary solution of time-dependent Schrödinger equation $i\hbar\,\partial\Psi(z,t)/\partial t = \hat{H}\Psi(z,t)$ has the following form $\Psi(z,t) = \psi(z)\cdot e^{-iE_\parallel t/\hbar}$, where time-independent function $\psi(z)$ meets the stationary Schrödinger equation

$$\hat{H}\psi(z) = E_\parallel \psi(z) \quad \text{or} \quad \left\{-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} + U(z)\right\}\psi(z) = E_\parallel \psi(z).$$

If the regions located at a large distance from the inhomogeneities of the potential energy are classically allowed ($E_{\|} > U(z)$ at $z \to \pm\infty$), then the states of the continuous spectrum will be double degenerate: nonuniform electronic waves can travel from left to right and from right to left.

Particular case: if the potential energy at a large distance is constant (*i.e.* $U(z) = U_0$ at $z \to \pm\infty$) and $E_{\|} > U_0$, then there are two possible solutions: plane electronic waves $e^{ik_0 z}$ и $e^{-ik_0 z}$, where $k_0 = \sqrt{2m^*(E_{\|} - U_0)}/\hbar$ is the wave number.

Provided that $U(z)$ is localized and tends to certain values far from the scattering center

$$U(z) = \begin{cases} U_1 & \text{at } z \to -\infty, \\ U_2 & \text{at } z \to +\infty, \end{cases}$$

and $E_{\|} > \max\{U_1, U_2\}$, then wave function of the particle far from the scatter can be considered as a combination of two plane waves

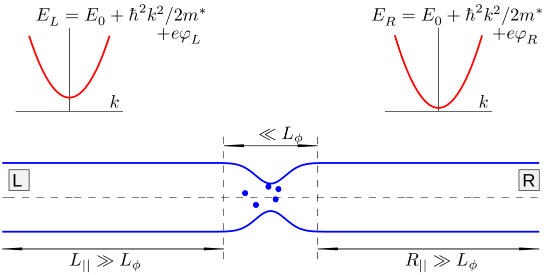
$$\psi(z) = \begin{cases} A_1\, e^{ik_1 z} + B_1\, e^{-ik_1 z} & \text{at } z \to -\infty, \\ A_2\, e^{ik_2 z} + B_2\, e^{-ik_2 z} & \text{at } z \to +\infty, \end{cases}$$

where

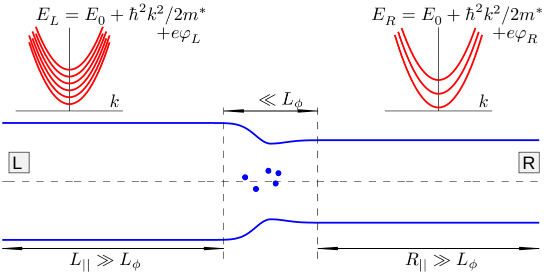
$$k_1 = \sqrt{2m^* \left(E_{\|} - U_1\right)}/\hbar \quad \text{and} \quad k_2 = \sqrt{2m^* \left(E_{\|} - U_2\right)}/\hbar.$$

This problem of the determination of the dimension constants A_1, A_2, B_1, and B_2 for given incoming flux and potential profile can be referred as a scattering problem.

Single-channel scattering:



Multi-channel scattering:



Normalization criteria in quantum mechanics

We assume that a quantum particle can be described by a plane wave $\psi_k(z) = Ce^{ikz}$.

1. If this particle is localized in a one-dimensional crystal of length L (particle-in-the-box), then one can apply the condition $\langle\psi_k|\psi_k\rangle = 1$ in order to find the coefficient C

$$\langle\psi_k|\psi_k\rangle = \int_{-L/2}^{L/2} \psi_k^*(z)\,\psi_k(z)\,dz = |C|^2 \int_{-L/2}^{L/2} dz = |C|^2\,L = 1 \quad\Longrightarrow\quad |C| = \frac{1}{\sqrt{L}}.$$

2. For freely travelling particle one can use the condition of orthogonality of the states with different k and k' in the form $\langle\psi_{k'}|\psi_k\rangle = \delta(k-k')$, then

$$\langle\psi_{k'}|\psi_k\rangle = |C|^2 \int_{-\infty}^{\infty} e^{i(k-k')z}\,dz = 2\pi|C|^2\,\delta(k-k') = \delta(k-k') \quad\Longrightarrow\quad |C| = \frac{1}{\sqrt{2\pi}}.$$

3. Alternatively, one can use the condition $\langle\psi_{E'}|\psi_E\rangle = \delta(E_{||}-E'_{||})$, then

$$\langle\psi_{E'}|\psi_E\rangle = 2\pi|C|^2\,\delta(k-k') = 2\pi|C|^2\,\frac{\delta(E_{||}-E'_{||})}{|dk/dE_{||}|} = \delta(E_{||}-E'_{||}) \quad\Longrightarrow\quad |C| = \frac{1}{\sqrt{2\pi\hbar v}},$$

$v = \hbar^{-1}\,|dE_{||}/dk|$ is a group velocity, $\hbar = 1.054\cdot 10^{-34}$ J·s is the reduced Planck constant.

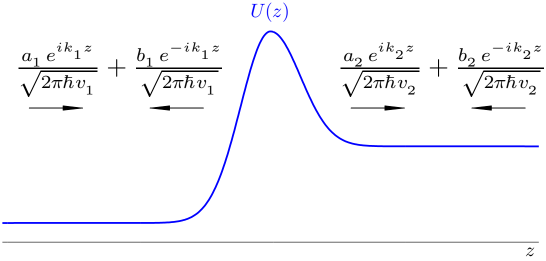
Thus, for the localized potential

$$U(z) = \begin{cases} U_1 & \text{at } z \to -\infty, \\ U_2 & \text{at } z \to +\infty, \end{cases}$$

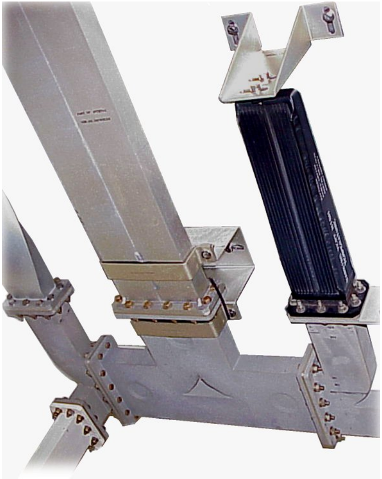
a single-particle wave function at large distances can be viewed as a linear combination of the normalized plain waves (now a_1, a_2, b_1, b_2 are dimensionless coefficients)

$$\psi_E(z) = \begin{cases} a_1\, e^{ik_1 z}/\sqrt{2\pi\hbar v_1} + b_1\, e^{-ik_1 z}/\sqrt{2\pi\hbar v_1} & \text{при } z \to -\infty, \\ a_2\, e^{ik_1 z}/\sqrt{2\pi\hbar v_2} + b_2\, e^{-ik_2 z}/\sqrt{2\pi\hbar v_2} & \text{при } z \to +\infty, \end{cases}$$

where $k_1 = \sqrt{2m^* \left(E_\parallel - U_1\right)}/\hbar$ and $v_1 = \hbar k_1/m^*$,
$k_2 = \sqrt{2m^* \left(E_\parallel - U_2\right)}/\hbar$ and $v_2 = \hbar k_2/m^*$.

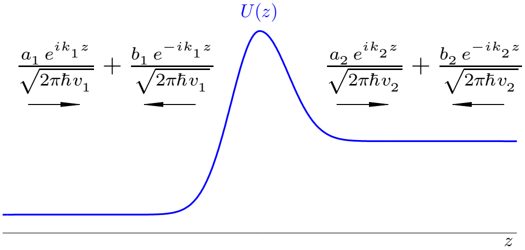


Travelling waves in radio-circuits, electrodynamics and optics



The developed approach based on plane wave decomposition is applicable for any linear systems with travelling and evanescent waves: for example, coax-based circuits, waveguides and (quasi-)optical schemes.

Definition: scattering matrix



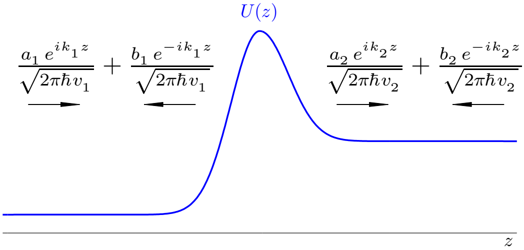
A general linear relationship between the amplitudes of outcoming normalized waves and the amplitudes of incoming normalized waves

$$|out\rangle = \begin{pmatrix} b_1 \\ a_2 \end{pmatrix} \quad \text{and} \quad |in\rangle = \begin{pmatrix} a_1 \\ b_2 \end{pmatrix}$$

can be written in the form of a matrix equation

$$|out\rangle = \hat{S}|in\rangle \qquad \text{or} \qquad \begin{pmatrix} b_1 \\ a_2 \end{pmatrix} = \hat{S} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix}.$$

Definition: transfer matrix



A general linear relationship between the amplitudes of the normalized waves on the left of the scatter and the amplitudes of the normalized waves on the right of the scatter

$$|left\rangle = \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \quad \text{and} \quad |right\rangle = \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}.$$

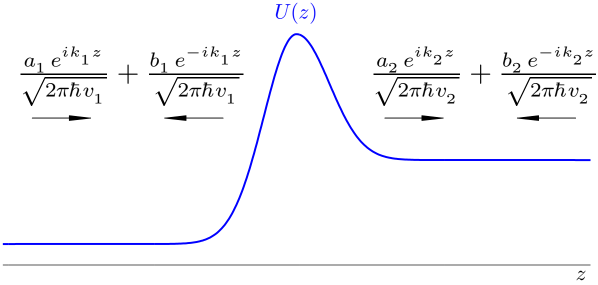
can be written in the form of a matrix equation

$$|left\rangle = \hat{T}|right\rangle \qquad \text{or} \qquad \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \hat{T} \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}.$$

Probability flux for the normalized wave functions

We can calculate the probability flux for the particle in the state describing by the sum of the normalized plane waves running from left to right and from right to left

$$\psi_E(z) = \frac{a\, e^{ikz}}{\sqrt{2\pi\hbar v}} + \frac{b\, e^{-ikz}}{\sqrt{2\pi\hbar v}}, \quad \text{where} \quad v = \frac{1}{\hbar}\frac{dE}{dk} = \frac{\hbar k}{m} \quad \text{is the group velocity.}$$



According to the standard quantum mechanics, the probability flux equals

$$j = \frac{i\hbar}{2m^*}\left\{\psi_E \frac{d\psi_E^*}{dz} - \psi_E^* \frac{d\psi_E}{dz}\right\}.$$

After substituting $\psi_E(z)$ and rearranging, one can get

$$j = \frac{i\hbar}{2m^*}\left\{\psi_E\,\frac{d\psi_E^*}{dz} - \psi_E^*\,\frac{d\psi_E}{dz}\right\} =$$

$$= \frac{i\hbar}{2m^*}\left(\frac{a}{\sqrt{2\pi\hbar v}}\,e^{ikz} + \frac{b}{\sqrt{2\pi\hbar v}}\,e^{-ikz}\right)\left(\frac{(-ik)a^*}{\sqrt{2\pi\hbar v}}\,e^{-ikz} + \frac{(+ik)b^*}{\sqrt{2\pi\hbar v}}\,e^{ikz}\right)$$

$$- \frac{i\hbar}{2m^*}\left(\frac{a^*}{\sqrt{2\pi\hbar v}}\,e^{-ikz} + \frac{b^*}{\sqrt{2\pi\hbar v}}\,e^{ikz}\right)\left(\frac{(+ik)a}{\sqrt{2\pi\hbar v}}\,e^{ikz} + \frac{(-ik)b}{\sqrt{2\pi\hbar v}}\,e^{-ikz}\right) =$$

$$= \frac{|a|^2 - |b|^2}{2\pi\hbar}.$$

Taking into account the conservation of the probability flux at large distances from the scatters in one-dimension geometry, we come to the following contrain

$$\frac{|a_1|^2 - |b_1|^2}{2\pi\hbar} = \frac{|a_2|^2 - |b_2|^2}{2\pi\hbar} \quad\Longrightarrow\quad |a_1|^2 + |b_2|^2 = |a_2|^2 + |b_1|^2.$$

We demonstrate later that the relationship $|a_1|^2 + |b_2|^2 = |a_2|^2 + |b_1|^2$ ensures the unitarity of the scattering matrix: $\hat{S}^+\hat{S} = 1$.

Relationship between components of $\hat{S}$-matrix and $\hat{T}$-matrix

Two matrix relationships

$$\begin{pmatrix} b_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}$$

are equivalent to four algebraic equations

$$b_1 = S_{11} a_1 + S_{12} b_2 \qquad\qquad a_1 = T_{11} a_2 + T_{12} b_2$$

$$a_2 = S_{21} a_1 + S_{22} b_2 \qquad\qquad b_1 = T_{21} a_2 + T_{22} b_2$$

One can see that the elements of the T-matrix can be expressed via the components of the S-matrix as follows

$$T_{11} = \frac{1}{S_{21}}, \quad T_{12} = -\frac{S_{22}}{S_{21}}, \quad T_{21} = \frac{S_{11}}{S_{21}}, \quad T_{22} = S_{12} - \frac{S_{11}\, S_{22}}{S_{21}}.$$

The elements of the S-matrix can be also expressed via the components of the T-matrix

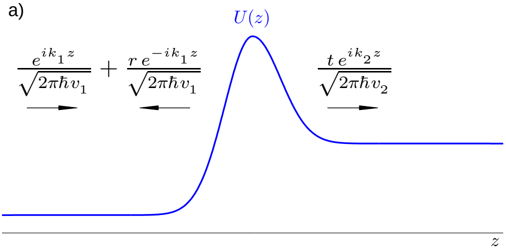
$$S_{11} = \frac{T_{21}}{T_{11}}, \quad S_{12} = T_{22} - \frac{T_{21}\, T_{12}}{T_{11}}, \quad S_{21} = \frac{1}{T_{11}}, \quad S_{22} = -\frac{T_{12}}{T_{11}}.$$

Components of $\hat{S}$-matrix for left scattering problem

Assume that the incoming wave of unit amplitude is running from left to right.

Let r and t be the amplitudes of reflection and transmission, respectively; therefore the wave function can be written in the form

$$\psi(z) = \begin{cases} 1 \cdot e^{ik_1 z}/\sqrt{2\pi\hbar v_1} + r \cdot e^{-ik_1 z}/\sqrt{2\pi\hbar v_1} & \text{at } z \to -\infty; \\ t \cdot e^{ik_2 z}/\sqrt{2\pi\hbar v_2} & \text{at } z \to +\infty. \end{cases}$$



$$\begin{pmatrix} r \\ t \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\Longrightarrow \quad S_{11} = r \text{ and } S_{21} = t.$$

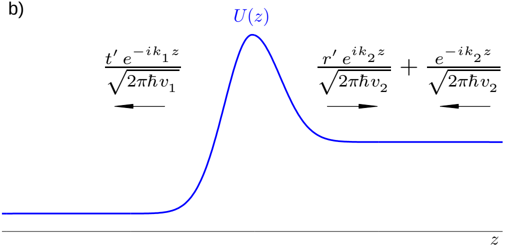
Components of $\hat{S}$-matrix for right scattering problem

Assume that the incoming wave of unit amplitude is running from right to left.

Let r' and t' be the amplitudes of reflection and transmission, respectively; therefore the wave function can be written in the form

$$\psi(z) = \begin{cases} t' \cdot e^{-ik_1 z} \sqrt{2\pi\hbar v_1} & \text{at } z \to -\infty; \\ r' \cdot e^{ik_2 z} \sqrt{2\pi\hbar v_2} + 1 \cdot e^{-ik_2 z} / \sqrt{2\pi\hbar v_2} & \text{at } z \to +\infty. \end{cases}$$

b)



$$\begin{pmatrix} t' \\ r' \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\Longrightarrow \quad S_{12} = t' \text{ and } S_{22} = r'.$$

$\hat{S}$- and $\hat{T}$-matrices for single-channel scattering: general case

Let r and t be the amplitudes of reflection and transmission for the left scattering problem.

Let r' and t' be the amplitudes of reflection and transmission for the right scattering problem.

We conclude that

$$\hat{S} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \quad \text{and} \quad \hat{T} = \begin{pmatrix} 1/t & -r'/t \\ r/t & t' - r\,r'/t \end{pmatrix}.$$

Important to note that all coefficients of the scattering matrix have physical meaning; while the only coefficient of the transfer-matrix $T_{11} = 1/t$ has physical meaning.

Structure of $\hat{S}$-matrix for multi-channel scattering*

Scattering in a system with magnetic impurities and spin-dependent tunneling

$$\begin{pmatrix} b_{1,\uparrow} \\ b_{1,\downarrow} \\ a_{2,\uparrow} \\ a_{2,\downarrow} \end{pmatrix} = \hat{S} \begin{pmatrix} a_{1,\uparrow} \\ a_{1,\downarrow} \\ b_{2,\uparrow} \\ b_{2,\downarrow} \end{pmatrix}, \quad \text{where} \quad \hat{S} = \begin{pmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{pmatrix} = \left(\begin{array}{cc|cc} r_{\uparrow\uparrow} & r_{\uparrow\downarrow} & t'_{\uparrow\uparrow} & t'_{\uparrow\downarrow} \\ r_{\downarrow\uparrow} & r_{\downarrow\downarrow} & t'_{\downarrow\uparrow} & t'_{\downarrow\downarrow} \\ \hline t_{\uparrow\uparrow} & t_{\uparrow\downarrow} & r'_{\uparrow\uparrow} & r'_{\uparrow\downarrow} \\ t_{\downarrow\uparrow} & t_{\downarrow\downarrow} & r'_{\uparrow\uparrow} & r'_{\downarrow\downarrow} \end{array}\right).$$

Scattering in a system with different types of travelling waves (N and M are the numbers of travelling waves in left and right parts)

$$\begin{pmatrix} b_{1,1} \\ \vdots \\ b_{1,N} \\ a_{2,1} \\ \vdots \\ a_{2,M} \end{pmatrix} = \hat{S} \begin{pmatrix} a_{1,1} \\ \vdots \\ a_{1,N} \\ b_{2,1} \\ \vdots \\ b_{2,M} \end{pmatrix}, \quad \hat{S} = \begin{pmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{pmatrix} = \left(\begin{array}{ccc|ccc} r_{11} & \cdots & r_{1N} & t'_{11} & \cdots & t'_{1M} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ r_{N1} & \cdots & r_{NN} & t'_{N1} & \cdots & t'_{NM} \\ \hline t_{11} & \cdots & t_{1N} & r'_{11} & \cdots & r'_{1M} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ t_{M1} & \cdots & t_{MN} & r'_{M1} & \cdots & r'_{MM} \end{array}\right)$$

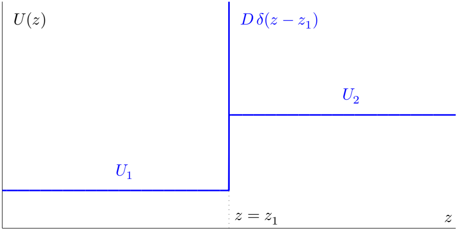
The scattering matrix has block-like structure similar to the single-channel case.

Part 2: scattering at delta-step potential

Model problem: scattering at delta-step-potential

The model potential is the combination of a delta-potential and a step-potential

$$U_\delta(z) = D\,\delta(z - z_1) + \begin{cases} U_1 \text{ at } z < z_1, \\ U_2 \text{ at } z > z_1. \end{cases}$$



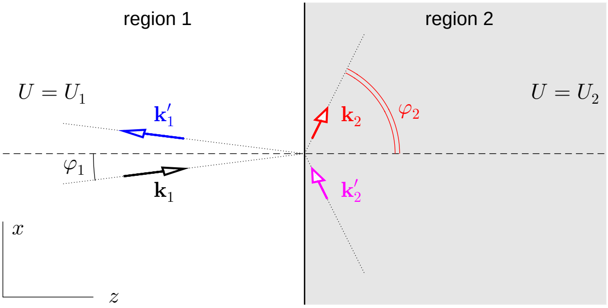
We assume that the incident plane coincides with the (x, z) plane, what allows us to consider 2D problem

$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right)\Psi(x, z) + U_\delta(z)\,\Psi(x, z) = E\,\Psi(x, z).$$

This equation can be solved by separation of variables $\Psi(x, z) = F(x) \cdot \psi(z)$, therefore we can analyze the motion along x- and z-axes independently

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2}F(x) = E_\perp\,F(x), \quad \text{where} \quad E_\perp = \frac{\hbar^2 k_x^2}{2m^*},$$

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}\psi(z) + U_\delta(z)\,\psi(z) = E_\parallel\,\psi(z), \quad \text{where} \quad E_\parallel = E - E_\perp.$$



◇ Solution for x-problem: $F(x) = e^{\pm i k_{1,x} x}$ at $z < z_1$ and $F(x) = e^{\pm i k_{2,x} x}$ at $z > z_1$, where $k_{1,2} = \sqrt{2m^*(E - U_{1,2})}/\hbar$ is the absolute values of the wave vector in the regions 1 and 2.

Boundary conditions for the x-problem: $(\varepsilon \to 0)$:

$$F(x, z_1 + \varepsilon) = F(x, z_1 - \varepsilon) \quad \text{and} \quad \left(\frac{dF}{dx}\right)_{x, z_1 + \varepsilon} = \left(\frac{dF}{dx}\right)_{x, z_1 - \varepsilon} .$$

Consequence of the boundary conditions for the x-problem:
$k_{1,x} = k_{2,x}$ and $k_1 \sin\varphi_1 = k_1 \sin\varphi_2$ (analog of the Snell's law in optics).

◇ Boundary conditions for the z-problem: ($\varepsilon \to 0$):

$$\psi(z_1 + \varepsilon) = \psi(z_1 - \varepsilon) \quad \text{and} \quad \left(\frac{d\psi}{dz}\right)_{z=z_1+\varepsilon} - \left(\frac{d\psi}{dz}\right)_{z=z_1-\varepsilon} = \frac{2m^* D}{\hbar^2}\,\psi(z_1).$$

◇ General solution for the 'left' scattering problem

$$\psi_L(z) = \begin{cases} e^{ik_1 z}/\sqrt{2\pi\hbar v_1} + r\,e^{-ik_1 z}/\sqrt{2\pi\hbar v_1} & \text{at } z < z_1; \\ t\,e^{ik_2 z}/\sqrt{2\pi\hbar v_2} & \text{at } z > z_1. \end{cases}$$

Consequence of the boundary conditions for the z-problem:

$$\frac{1}{\sqrt{2\pi\hbar v_1}}\left\{e^{ik_1 z_1} + r\,e^{-ik_1 z_1}\right\} = \frac{1}{\sqrt{2\pi\hbar v_2}}\,t\,e^{ik_2 z_1}.$$

$$\frac{1}{\sqrt{2\pi\hbar v_2}}\,ik_2 t\,e^{ik_2 z_1} - \frac{1}{\sqrt{2\pi\hbar v_1}}\left\{ik_1\,e^{ik_1 z_1} - ik_1 r\,e^{-ik_1 z_1}\right\} = \frac{2m^* D}{\hbar^2}\,\frac{1}{\sqrt{2\pi\hbar v_2}}\,t\,e^{ik_2 z_1}.$$

Amplitudes of reflection and transmission are the following:

$$r = \frac{\left(k_1 - k_2 - i\,2m^* D/\hbar^2\right)}{\left(k_1 + k_2 + i\,2m^* D/\hbar^2\right)}\;e^{2ik_1 z_1} \quad \text{and} \quad t = \frac{2\sqrt{k_1 k_2}}{\left(k_1 + k_2 + i\,2m^* D/\hbar^2\right)}\;e^{i(k_1 - k_2)z_1}.$$

◇ General solution for the 'right' scattering problem

$$\psi_R(z) = \begin{cases} t'\, e^{-ik_1 z} / \sqrt{2\pi\hbar v_1} & \text{at } z < z_1; \\ r'\, e^{ik_2 z} / \sqrt{2\pi\hbar v_2} + e^{-ik_2 z} / \sqrt{2\pi\hbar v_2} & \text{at } z > z_1. \end{cases}$$

Consequence of the boundary conditions for the z-problem:

$$\frac{1}{\sqrt{2\pi\hbar v_2}} \left\{ e^{-ik_2 z_1} + r'\, e^{ik_2 z_1} \right\} = \frac{1}{\sqrt{2\pi\hbar v_1}}\, t'\, e^{-ik_1 z_1}.$$

$$\frac{1}{\sqrt{2\pi\hbar v_2}} \left\{ -\, ik_2 e^{-ik_2 z_1} + ik_2 r'\, e^{ik_2 z_1} \right\} - \frac{(-ik_1)}{\sqrt{2\pi\hbar v_1}}\, t'\, e^{-ik_1 z_1} = \frac{2m^* D}{\hbar^2} \frac{1}{\sqrt{2\pi\hbar v_1}}\, t'\, e^{-ik_1 z_1}.$$

Amplitudes of reflection and transmission are the following:

$$r' = \frac{\left(k_2 - k_1 - i\, 2m^* D/\hbar^2\right)}{\left(k_1 + k_2 + i\, 2m^* D/\hbar^2\right)}\, e^{-2ik_2 z_1} \quad \text{and} \quad t' = \frac{2\sqrt{k_1 k_2}}{\left(k_1 + k_2 + i\, 2m^* D/\hbar^2\right)}\, e^{i(k_1 - k_2) z_1}.$$

◇ Scattering matrix for a single delta-step-potential has the following structure

$$\hat{S} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = \frac{1}{\left(k_1 + k_2 + i\, 2m^* D/\hbar^2\right)} \times$$

$$\begin{pmatrix} \left(k_1 - k_2 - i\, 2m^* D/\hbar^2\right)\, e^{2ik_1 z_1} & 2\sqrt{k_1 k_2}\, e^{i(k_1 - k_2) z_1} \\ 2\sqrt{k_1 k_2}\, e^{i(k_1 - k_2) z_1} & \left(k_2 - k_1 - i\, 2m^* D/\hbar^2\right)\, e^{-2ik_2 z_1} \end{pmatrix}$$

Unitarity of S-matrix

We would like to prove that the scattering matrix is an unitary matrix.

We introduce the vectors of the outcoming and incoming states:

$$|out\rangle = \begin{pmatrix} b_1 \\ a_2 \end{pmatrix} \quad \text{and} \quad |in\rangle = \begin{pmatrix} a_1 \\ b_2 \end{pmatrix}.$$

Since $|a_1|^2 + |b_2|^2 = \langle in|in\rangle$ and $|a_2|^2 + |b_1|^2 = \langle out|out\rangle$, the flux conservation constrain

$$|a_1|^2 + |b_2|^2 = |a_2|^2 + |b_1|^2$$

is equivalent to $\langle in|in\rangle = \langle out|out\rangle$.

Taking into account the definition $|out\rangle = \hat{S}\,|in\rangle$, we get

$$\langle out|out\rangle = \langle in|\hat{S}^{+}\hat{S}|in\rangle = \langle in|in\rangle.$$

As a result,

$$\hat{S}^{+}\hat{S} = 1 \quad \text{or} \quad \hat{S}\,\hat{S}^{+} = 1.$$

This is mathematical definition of an unitary matrix.

Number of independent coefficients for $\hat{S}$-matrix

Generally speaking, the $\hat{S}$ matrix seems to have four complex-valued parameters or eight real-valued parameters.

As a consequence of unitarity, we conclude

$$\hat{S}^{+}\hat{S} = \begin{pmatrix} r^* & t^* \\ t'^* & r'^* \end{pmatrix} \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = \begin{pmatrix} r^*r + t^*t & r^*t' + t^*r' \\ t'^*r + r'^*t & t'^*t' + r'^*r' \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

and

$$\hat{S}\hat{S}^{+} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} r^* & t^* \\ t'^* & r'^* \end{pmatrix} = \begin{pmatrix} rr^* + t't'^* & rt^* + t'r'^* \\ tr^* + r't'^* & tt^* + r'r'^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

therefore we get the following additional constrains

$$|r|^2 + |t|^2 = 1, \quad |r'|^2 + |t'|^2 = 1, \quad r^*t' + t^*r' = 0,$$
$$|r|^2 + |t'|^2 = 1, \quad |r'|^2 + |t|^2 = 1, \quad \text{and} \quad rt^* + t'r'^* = 0.$$

We rewrite the last expression keeping in mind that $|r| = |r'|$ and $|t| = |t'|$

$$rt^* + t'r'^* = 0 \quad \Longrightarrow \quad |r|e^{i \arg r} \cdot |t|e^{-i \arg t} + |r'|e^{-i \arg r'} \cdot |t'|e^{i \arg t'} = 0 \quad \Longrightarrow$$
$$e^{i \arg r} e^{-i \arg t} e^{i \arg r'} e^{-i \arg t'} = -1 = e^{i\pi} \quad \Longrightarrow \quad \arg r - \arg t + \arg r' - \arg t' = \pi.$$

Thus, there are four independent constrains

$$|r|^2 + |t|^2 = 1, \quad |r| = |r'|, \quad |t| = |t'| \quad \text{and} \quad arg\, r - arg\, t + arg\, r' - arg\, t' = \pi.$$

As a consequence, there are $8 - 4 = 4$ independent real-valued parameters.

Let $\mathcal{T} \equiv |t|^2$ be the coefficient of transmission. Since

$$t = |t|\, e^{i\, arg\, t} = \sqrt{\mathcal{T}}\, e^{i\, arg\, t}, \quad r = |r|\, e^{i\, arg\, r} = \sqrt{1 - \mathcal{T}}\, e^{i\, arg\, r},$$

$$t' = |t'|\, e^{i\, arg\, t'} = \sqrt{\mathcal{T}'}\, e^{i\, arg\, t'} \quad \text{and} \quad r' = |r'|\, e^{i\, arg\, r'} = \sqrt{1 - \mathcal{T}'}\, e^{i\, arg\, r'},$$

therefore a possible general parametrization of the scattering matrix for single-channel scattering problem is as follows

$$\hat{S} = \begin{pmatrix} \sqrt{1-\mathcal{T}}\ e^{i\, \arg r} & \sqrt{\mathcal{T}}\ e^{i\, \arg t'} \\ \sqrt{\mathcal{T}}\ e^{i\, \arg t} & \sqrt{1-\mathcal{T}}\ e^{i\, \arg r'} \end{pmatrix}$$

provided that $\quad \arg t + \arg t' - \arg r - \arg r' = \pi.$

If the considered quantum system has additional symmetry properties, then the number of independent parameters can be less than four!

$\hat{S}$-matrix for system with time-reversal symmetry*

For simplicity we assume that magnetic field is absent ($\boldsymbol{B} = 0$ and $\boldsymbol{A} = 0$).

The operation of complex conjugate for a stationary wave function is equivalent to time inversion ($t \to -t$). Indeed,

$$\psi^*(z) = \left(a\, e^{ikz}\right)^* = a^*\, e^{-ikz}.$$

In the other words, the plane wave running in a certain direction transforms to the wave running in the opposite direction. By definition, we conclude formally

$$\begin{pmatrix} b_1 \\ a_2 \end{pmatrix} = \hat{S} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix} \quad \Longrightarrow \quad \begin{pmatrix} b_1^* \\ a_2^* \end{pmatrix} = \hat{S}^* \begin{pmatrix} a_1^* \\ b_2^* \end{pmatrix}.$$

Provided that $\hat{H} = \hat{H}^*$ and $\hat{H}\,\psi^*(z) = E_{||}\,\psi^*(z)$, we conclude that both $\psi(z)$ and $\psi^*(z)$ meet the same equation, therefore

$$\begin{pmatrix} a_1^* \\ b_2^* \end{pmatrix} = \hat{S} \begin{pmatrix} b_1^* \\ a_2^* \end{pmatrix} \quad \Longrightarrow \quad \begin{pmatrix} a_1^* \\ b_2^* \end{pmatrix} = \hat{S} \begin{pmatrix} b_1^* \\ a_2^* \end{pmatrix} = \hat{S}\hat{S}^* \begin{pmatrix} a_1^* \\ b_2^* \end{pmatrix} \quad \Longrightarrow \quad \hat{S}\,\hat{S}^* = 1.$$

Comparing this with the definition of unitarity $\hat{S}\,\hat{S}^+ = 1$, we get $\hat{S}^* = \hat{S}^+$ or $\hat{S} = \hat{S}^\tau$, where τ is the operation of matrix transposing. In particular, for one-dimensional scattering problem we get $t' = t$.

$\hat{S}$-matrix for system with spatial-inversion symmetry*

If the potential energy is symmetric function $U(z) = U(-z)$, then wave functions $\psi(z)$ and $\psi(-z)$ meet the same Schrödinger equation

$$\hat{H}\psi(z) = E_{\|}\psi(z) \quad \text{and} \quad \hat{H}\psi(-z) = E_{\|}\psi(-z).$$

As a result, we get the same matrix equation for the direct and inverted problems

$$\begin{pmatrix} b_1 \\ a_2 \end{pmatrix} = \hat{S} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix} \qquad \text{и} \qquad \begin{pmatrix} a_2 \\ b_1 \end{pmatrix} = \hat{S} \begin{pmatrix} b_2 \\ a_1 \end{pmatrix}.$$

We introduce an auxiliary matrix

$$\hat{\Sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

which has the same structure as the Pauli matrix $\hat{\sigma}_x$ in theory of magnetism.

From the following set of transformations

$$\begin{pmatrix} b_1 \\ a_2 \end{pmatrix} = \hat{\Sigma}_x \begin{pmatrix} a_2 \\ b_1 \end{pmatrix} = \hat{\Sigma}_x \, \hat{S} \begin{pmatrix} b_2 \\ a_1 \end{pmatrix} = \hat{\Sigma}_x \, \hat{S} \, \hat{\Sigma}_x \begin{pmatrix} a_1 \\ b_2 \end{pmatrix},$$

we get $\hat{\Sigma}_x \, \hat{S} \, \hat{\Sigma}_x = \hat{S}$. In particular, for one-dimensional scattering problem $r = r'$.

Summary: structure of $\hat{S}$-matrix and $\hat{T}$-matrix for delta-step-potential

Scattering matrix is

$$\hat{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{22} & S_{22} \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = \frac{1}{\left(k_1 + k_2 + i\,2m^* D/\hbar^2\right)} \times$$

$$\begin{pmatrix} \left(k_1 - k_2 - i\,2m^* D/\hbar^2\right)\, e^{2ik_1 z_1} & 2\sqrt{k_1 k_2}\, e^{i(k_1 - k_2)z_1} \\ 2\sqrt{k_1 k_2}\, e^{i(k_1 - k_2)z_1} & \left(k_2 - k_1 - i\,2m^* D/\hbar^2\right)\, e^{-2ik_2 z_1} \end{pmatrix}.$$

Here z_1 is the location of the delta-step barrier.

Transfer-matrix is

$$\hat{T} = \begin{pmatrix} T_{11} & T_{12} \\ T_{22} & T_{22} \end{pmatrix} = \begin{pmatrix} 1/t & -r'/t \\ r/t & t' - r\,r'/t \end{pmatrix} =$$

$$\frac{1}{2\sqrt{k_1 k_2}} \cdot \begin{pmatrix} \left(k_1 + k_2 + i\,2m^* D/\hbar^2\right)\, e^{i\,(-k_1 + k_2)z_1} & \left(k_1 - k_2 + i\,2m^* D/\hbar^2\right)\, e^{i\,(-k_1 - k_2)z_1} \\ \left(k_1 - k_2 - i\,2m^* D/\hbar^2\right)\, e^{i\,(+k_1 + k_2)z_1} & \left(k_1 + k_2 - i\,2m^* D/\hbar^2\right)\, e^{i\,(+k_1 - k_2)z_1} \end{pmatrix}.$$

Question for home-work: check the general symmetry properties for this particular case.

Transmission coefficient and reflection coefficient

Definitions:

Reflection coefficient for a particle moving from left ro right: $\mathcal{R} = |r|^2$ (if k_1 is real).

Transmission coefficient for a particle moving from left ro right: $\mathcal{T} = |t|^2$ (if k_2 is real).

Reflection coefficient for a particle moving from right ro left: $\mathcal{R}' = |r'|^2$ (if k_2 is real).

Transmission coefficient for a particle moving from right to left: $\mathcal{T}' = |t'|^2$ (if k_1 is real).

Example 1: Scattering matrix for delta-step potential has the following structure

$$\hat{S} = \frac{1}{\left(k_1 + k_2 + i\, 2m^* D/\hbar^2\right)} \times \begin{pmatrix} \left(k_1 - k_2 - i\, 2m^* D/\hbar^2\right)\, e^{2ik_1 z_1} & 2\sqrt{k_1 k_2}\, e^{i(k_1 - k_2) z_1} \\ 2\sqrt{k_1 k_2}\, e^{i(k_1 - k_2) z_1} & \left(k_2 - k_1 - i\, 2m^* D/\hbar^2\right)\, e^{-2ik_2 z_1} \end{pmatrix}.$$

For single delta-barrier we should take $k_1 = k_2 = k$ and $D \neq 0$, therefore

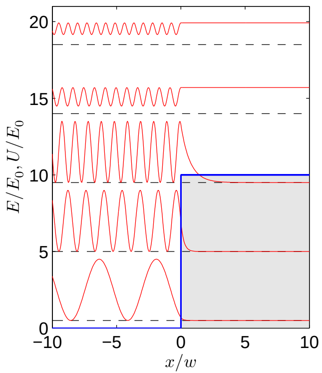
$$\mathcal{R} = \left| \frac{-i\, 2m^* D/\hbar^2}{\left(2k + i\, 2m^* D/\hbar^2\right)}\; e^{2ik_1 z_1} \right|^2 = \frac{(m^* D/\hbar^2)^2}{k^2 + (m^* D/\hbar^2)^2} = \frac{m^* D^2/(2\hbar^2)}{E_\parallel + m^* D^2/(2\hbar^2)}.$$

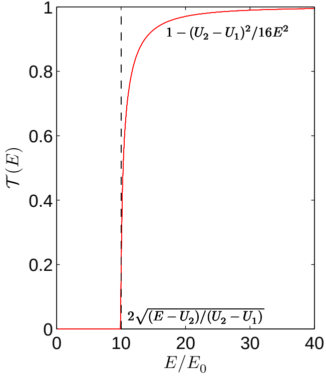
$$\mathcal{T} = \left| \frac{2\sqrt{k^2}}{\left(2k + i\, 2m^* D/\hbar^2\right)}\; e^{i(k_1 - k_2) z_1} \right|^2 = \frac{k^2}{k^2 + (m^* D/\hbar^2)^2} = \frac{E_\parallel}{E_\parallel + m^* D^2/(2\hbar^2)}.$$

Example 2: Scattering at single step-barrier ($k_1 \neq k_2$ and $D = 0$)

$$\mathcal{R} = \left| \left(\frac{k_1 - k_2}{k_1 + k_2} \right) \, e^{2ik_1 z_1} \right|^2 = \begin{cases} 1 \text{ at } Im\, k_2 \neq 0, \\ (k_1 - k_2)^2/(k_1 + k_2)^2 \text{ at } Im\, k_2 = 0. \end{cases}$$

$$\mathcal{T} = \left| \frac{2\sqrt{k_1 k_2}}{k_1 + k_2} \, e^{i(k_1 - k_2) z_1} \right|^2 = \begin{cases} 0 \text{ at } Im\, k_2 \neq 0, \\ 4 k_1 k_2/(k_1 + k_2)^2 \text{ at } Im\, k_2 = 0. \end{cases}$$





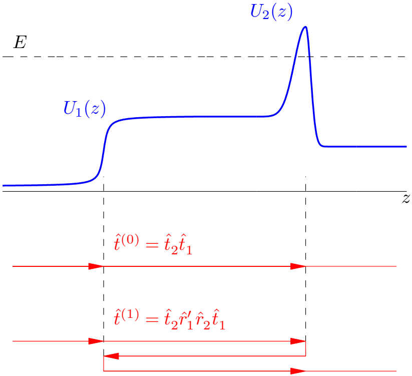
Oscillations of $|\psi(z)|$ are due to the interference of incident and reflected waves.

Part 3: scattering at two localized defects

Scattering at two localized defects: method 1

We would like to calculate the transmission amplitude for the potential equivalent to the sum of two localized potentials with known scattering matrices based on perturbation theory.

We formally assume that all reflection coefficients are rather small, while all transmission coefficients are close to unity.



Summary:

zero-order term: $t^{(0)} = t_2\, t_1$

first-order term: $t^{(1)} = t_2\, r_1'\, r_2\, t_1$

$n-$th order term: $t^{(n)} = t_2\, (r_1'\, r_2)^n\, t_1$

Summation of all contributions:

$$t = \sum_{n=0}^{\infty} t^{(n)} = t_2\, t_1 \sum_{n=0}^{\infty} \left(r_1' r_2\right)^n = \frac{t_2\, t_1}{(1 - r_1' r_2)},$$

provided that $\quad 1 - r_1' r_2 \neq 0.$

The obtained result is valid for the scatters of arbitrary reflection/transmission.

Scattering at two localized defects: method 2

We would like to calculate the transmission amplitude for the potential equivalent to sum of two localized potentials with known scattering matrices based on a formal solution of matrix equations.

Two matrix equations

$$\begin{pmatrix} b_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} r_1 & t_1' \\ t_1 & r_1' \end{pmatrix} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix}, \qquad \begin{pmatrix} b_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} r_2 & t_2' \\ t_2 & r_2' \end{pmatrix} \begin{pmatrix} a_2 \\ b_3 \end{pmatrix}$$

are equivalent to four scalar equations

$$b_1 = r_1 a_1 + t_1' b_2, \quad a_2 = t_1 a_1 + r_1' b_2, \quad b_2 = r_2 a_2 + t_2' b_3 \quad \text{and} \quad a_3 = t_2 a_2 + r_2' b_3.$$

Expressing the amplitudes of outcoming waves (b_1 and a_2) via the amplitudes of incoming waves (a_1 and b_2), we find

$$b_1 = \left\{ r_1 + t_1' \, r_2 \left(1 - r_1' r_2\right)^{-1} t_1 \right\} \cdot a_1 + \left\{ t_1' \, r_2 \left(1 - r_1' r_2\right)^{-1} r_1' t_2' + t_1' \, t_2' \right\} \cdot b_3,$$

$$a_3 = t_2 \left(1 - r_1' r_2\right)^{-1} t_1 \cdot a_1 + \left\{ t_2 \left(1 - r_1' r_2\right)^{-1} r_1' t_2' + r_2' \right\} \cdot b_3$$

As a result, the transmission and reflection amplitudes for two scatters are equal to

$$t = \frac{t_1 t_2}{1 - r_1' r_2} \quad \text{and} \quad r = r_1 + \frac{t_1' \, r_2 \, t_1}{1 - r_1' r_2}.$$

Scattering at two localized defects: method 3

We would like to calculate the transmission amplitude for the potential equivalent to sum of two localized potentials with known scattering matrices using transfer-matrix approach.

According to the definition of the transfer matrix

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \hat{T}_1 \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \hat{T}_2 \begin{pmatrix} a_3 \\ b_3 \end{pmatrix}.$$

Combining this expressions, we conclude that the resulting transfer matrix $\hat{T}$ is the product of matrices $\hat{T}^{(1)}$ and $\hat{T}^{(2)}$

$$\hat{T} = \hat{T}^{(1)}\hat{T}^{(2)} = \begin{pmatrix} t_1^{-1} & -t_1^{-1}r_1' \\ r_1 t_1^{-1} & t_1' - r_1 t_1^{-1} r_1' \end{pmatrix} \begin{pmatrix} t_2^{-1} & -t_2^{-1}r_2' \\ r_2 t_2^{-1} & t_2' - r_2 t_2^{-1} r_2' \end{pmatrix} =$$

$$= \begin{pmatrix} t_1^{-1}t_2^{-1} - t_1^{-1}r_1' r_2 t_2^{-1} & -t_1^{-1}t_2^{-1}r_2' - t_1^{-1}r_1'\left(t_2' - r_2 t_2^{-1} r_2'\right) \\ \left(t_1' - r_1 t_1^{-1} r_1'\right) r_2 t_2^{-1} & -r_1 t_1^{-1} t_2^{-1} r_2' + \left(t_1' - r_1 t_1^{-1} r_1'\right)\left(t_2' - r_2 t_2^{-1} r_2'\right) \end{pmatrix}$$

The coefficient $T_{11} = t_1^{-1}t_2^{-1}\left(1 - r_1' r_2\right)$ should be equal to t^{-1}, therefore

$$t = \frac{t_1 t_2}{1 - r_1' r_2}.$$

Scattering at rectangular potential barrier: method 1

We consider the following model potential

$$U(z) = \begin{cases} U_1 \text{ at } z < z_1, \\ U_2 \text{ at } z_1 < z < z_2, \\ U_3 \text{ at } z > z_2 \end{cases}$$

as a combination of two localized step-barriers, $w_2 = z_2 - z_1$ is the width of the barrier.

General structure of the scattering matrix without delta-barriers is

$$\hat{S} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = \frac{1}{(k_1 + k_2)} \cdot \begin{pmatrix} (k_1 - k_2)\, e^{2ik_1 z_1} & 2\sqrt{k_1 k_2}\, e^{i(k_1 - k_2) z_1} \\ 2\sqrt{k_1 k_2}\, e^{i(k_1 - k_2) z_1} & (k_2 - k_1)\, e^{-2ik_2 z_1} \end{pmatrix}.$$

The amplitude of transmission through double-step barrier is equal to

$$t = \frac{t_1 t_2}{(1 - r_1' r_2)} = \frac{4\sqrt{k_1 k_2}\sqrt{k_2 k_3}\, e^{i(k_1 - k_3) z_2}\, e^{-ik_2 (z_2 - z_1)}}{(k_1 + k_2)(k_2 + k_3)\, e^{-ik_2 (z_2 - z_1)} + (k_1 - k_2)(k_2 - k_3)\, e^{ik_2 (z_2 - z_1)}}.$$

The coefficient of transmission is equal

$$\mathcal{T} = |t|^2 = \frac{16\, k_1\, |k_2|^2\, k_3}{\left| (k_1 + k_2)(k_2 + k_3)\, e^{-ik_2 w_2} + (k_1 - k_2)(k_2 - k_3)\, e^{ik_2 w_2} \right|^2}.$$

Here $w_2 = z_2 - z_1$ is the width of the barrier and k_3 is assumed to be real-valued.

Scattering at rectangular potential barrier: method 2

We would like to calculate the transmission amplitude for the rectangular potential barrier using the theory of transfer matrices.

General structure of the transfer matrices for step barriers (without delta-barrier)

$$\hat{T}^{(1)} = \frac{1}{2\sqrt{k_1 k_2}} \cdot \begin{pmatrix} (k_1 + k_2)\; e^{i\,(-k_1+k_2)z_1} & (k_1 - k_2)\; e^{i\,(-k_1-k_2)z_1} \\ (k_1 - k_2)\; e^{i\,(+k_1+k_2)z_1} & (k_1 + k_2)\; e^{i\,(+k_1-k_2)z_1} \end{pmatrix},$$

$$\hat{T}^{(2)} = \frac{1}{2\sqrt{k_2 k_3}} \cdot \begin{pmatrix} (k_2 + k_3)\; e^{i\,(-k_2+k_3)z_2} & (k_2 - k_3)\; e^{i\,(-k_2-k_3)z_2} \\ (k_2 - k_3)\; e^{i\,(+k_2+k_3)z_2} & (k_2 + k_3)\; e^{i\,(+k_2-k_3)z_2} \end{pmatrix}.$$

The resulting transfer matrix $\hat{T} = \hat{T}^{(1)}\,\hat{T}^{(2)}$ can be written as follows

$$T_{11} = T_{11}^{(1)}\,T_{11}^{(2)} + T_{12}^{(1)}\,T_{21}^{(2)} =$$

$$= \frac{e^{-ik_1 z_1 + ik_3 z_2}}{4\sqrt{k_1 k_2}\,\sqrt{k_2 k_3}} \left\{ (k_1 + k_2)(k_2 + k_3)\, e^{-ik_2 w_2} + (k_1 - k_2)(k_2 - k_3)\, e^{ik_2 w_2} \right\} = \frac{1}{t}.$$

The coefficient of transmission is equal

$$\mathcal{T} = |t|^2 = \frac{16\, k_1\, |k_2|^2\, k_3}{\left| (k_1 + k_2)(k_2 + k_3)\, e^{-ik_2 w_2} + (k_1 - k_2)(k_2 - k_3)\, e^{ik_2 w_2} \right|^2}.$$

Scattering at rectangular potential barrier: limiting cases

Using the expression

$$\mathcal{T} = |t|^2 = \frac{16\, k_1\, |k_2|^2\, k_3}{\left|(k_1 + k_2)(k_2 + k_3)\, e^{-ik_2 w_2} + (k_1 - k_2)(k_2 - k_3)\, e^{ik_2 w_2}\right|^2}$$

we consider the important limiting cases of low and high energies of the scattered particle.

1. If $E_{\|} > U_2$ and all k values are real-valued (over-the-barrier transmission), then

$$\mathcal{T} = \frac{16\, k_1 k_2^2 k_3}{4k_2^2(k_1 + k_3)^2 + 4(k_2^2 - k_1^2)(k_2^2 - k_3^2)\, \sin^2 k_2 w_2}.$$

In this case the transmission coefficient oscillates as $E_{\|}$ and k_2 increases with the period $\delta k_2 \cdot w_2 = \pi n$. Such oscillations are due to constructive and destructive interference of the electronic waved reflected by the left and right sides of the barrier.

We calculate the maximum of the transmission coefficient at one of resonant energy values

$$\max \mathcal{T} = \left(\frac{16\, k_1 k_2^2 k_3}{4k_2^2(k_1 + k_3)^2 + 4(k_2^2 - k_1^2)(k_2^2 - k_3^2)\, \sin^2 k_2 w_2} \right)_{k_2 w_2 = \pi n} = \frac{4\, k_1 k_3}{(k_1 + k_3)^2}.$$

Apparently it reaches unity for the symmetrical barrier ($k_1 = k_3$).

For all other values $T < 1$ and therefore there is over-the-barrier reflection.

Scattering at rectangular potential barrier: limiting cases

2. If $E_{\|} < U_2$ and $k_2 = i\varkappa_2$ is a complex-valued parameter (sub-barrier tunneling), then

$$k_2^2 \to -\varkappa_2^2 \quad \text{and} \quad \sin^2 k_2 w_2 \to -\sinh^2 \varkappa_2 w_2 .$$

As a result,

$$\mathcal{T} = \frac{16\, k_1 \varkappa_2^2 k_3}{4\varkappa_2^2 (k_1 + k_3)^2 + 4(\varkappa_2^2 + k_1^2)(\varkappa_2^2 + k_3^2) \sinh^2 \varkappa_2 w_2}.$$

3. Low-transmission barrier ($e^{w_2 \varkappa_2} \gg e^{-w_2 \varkappa_2}$): $\sinh \varkappa_2 w_2 \to e^{-\varkappa_2 w_2}/2$ and

$$\mathcal{T} \simeq \frac{16\, k_1\, \varkappa_2^2\, k_3}{(k_1^2 + \varkappa_2^2)(\varkappa_2^2 + k_3^2)}\, e^{-2\varkappa_2 w_2}.$$

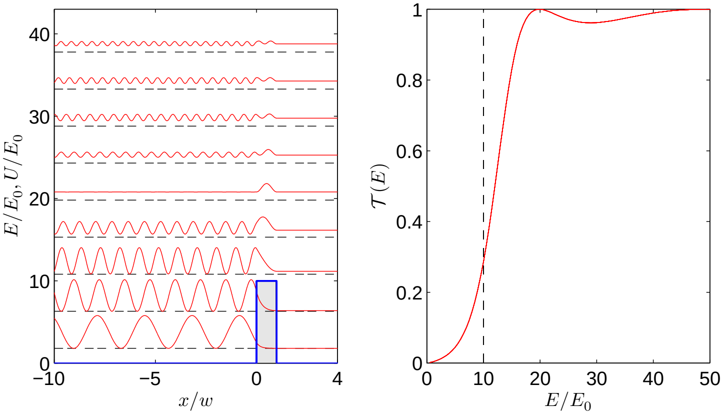
We get exponential suppression of the probability flux by the barrier of a finite width.

4. Tunneling via thin and high symmetrical barrier ($k_1 = k_3 = k$, $\varkappa_2 \gg k$ and $\varkappa_2 w_2 \to 0$):

$$\mathcal{T} = \left(\frac{16\, k_1 \varkappa_2^2 k_3}{4\varkappa_2^2 (k_1 + k_3)^2 + 4(\varkappa_2^2 + k_1^2)(\varkappa_2^2 + k_3^2) \sinh^2 \varkappa_2 w_2} \right)_{\varkappa_2 w_2 \to 0} = \frac{k^2}{k^2 + \varkappa_2^4 w_2^2 / 4}.$$

Compare this expression with that for the delta-barrier (lecture 1, page 28)

$$\mathcal{T} = \frac{E_{\|}}{E_{\|} + m^* D^2 / 2\hbar^2} = \frac{k^2}{k^2 + m^{*2} D^2 / \hbar^4} \quad \Longrightarrow \quad D = U_2 w_2 .$$



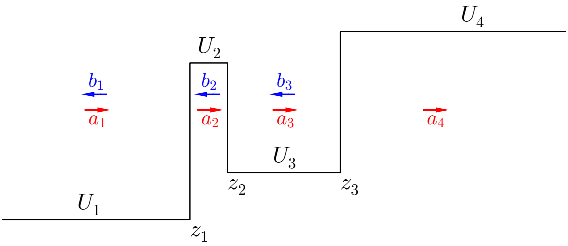
Oscillations of $|\psi(z)|$ in the region to the left from the barrier are due to the interference of incident and reflected waves.

Oscillations of $\mathcal{T}(E_{\parallel})$ at $E_{\parallel} > U_2$ are due to the interference of waves reflected by the left and right edges of the potential barrier.

Research project 1: one-dimensional scattering problem

Structure of the transfer-matrix for the single step-barrier located at the point z_n

$$\hat{T}^{(n)} = \frac{1}{2\sqrt{k_n\, k_{n+1}}} \cdot \begin{pmatrix} \left(k_n + k_{n+1}\right)\, e^{i\,(-k_n+k_{n+1})\,z_n} & \left(k_n - k_{n+1}\right)\, e^{i\,(-k_n-k_{n+1})\,z_n} \\ \left(k_n - k_{n+1}\right)\, e^{i\,(+k_n+k_{n+1})\,z_n} & \left(k_n + k_{n+1}\right)\, e^{i\,(+k_n-k_{n+1})\,z_n} \end{pmatrix}.$$



The resulting transfer-matrix, describing the scattering at series of the step barriers at the points z_1, $z_2, \ldots z_N$ is equal to the product of the matrices $\hat{T}_n$ in the same order

$$\hat{T} = \hat{T}^{(1)}\,\hat{T}^{(2)}\ldots\hat{T}^{(N)}.$$

Transmission coefficient and reflection coefficient are equal to

$$T = \frac{1}{|\,\hat{T}_{11}|^2} \quad \text{and} \quad R = \frac{|\,\hat{T}_{21}|^2}{|\,\hat{T}_{11}|^2}.$$

Strategy to find the profile of the wave function

$$\psi(z) = \begin{cases} a_1\, e^{ik_1 z}/\sqrt{k_1} + b_1\, e^{-ik_1 z}/\sqrt{k_1} & \text{at } z < z_1, \\ a_2\, e^{ik_2 z}/\sqrt{k_2} + b_2\, e^{-ik_2 z}/\sqrt{k_2} & \text{at } z_1 < z < z_2, \\ \ldots & \end{cases}$$

It is clear that the amplitudes of the normalized waves in each region can be found step by step

$$a_1 = 1 \quad \Longrightarrow \quad b_1 = a_1\, \frac{\hat{T}_{21}}{\hat{T}_{11}} \quad \Longrightarrow$$

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \hat{T}^{(1)} \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} \quad \Longrightarrow \quad \begin{aligned} a_2 &= \left(a_1\, \hat{T}^{(1)}_{2,2} - b_1\, \hat{T}^{(1)}_{1,2}\right) / \left(\hat{T}^{(1)}_{1,1}\, \hat{T}^{(1)}_{2,2} - \hat{T}^{(1)}_{1,2}\, \hat{T}^{(1)}_{2,1}\right) \\ b_2 &= \left(-a_1\, \hat{T}^{(1)}_{2,1} + b_1\, \hat{T}^{(1)}_{1,1}\right) / \left(\hat{T}^{(1)}_{1,1}\, \hat{T}^{(1)}_{2,2} - \hat{T}^{(1)}_{1,2}\, \hat{T}^{(1)}_{2,1}\right) \end{aligned}$$

and so on for all regions.

Potential problems for analysis:

1. Consider scattering of a particle at single rectangular barrier. Compare your numerical solution with the analytical solutions and consider important limiting cases.

2. Consider scattering of a particle at double rectangular barrier. Consider the suppression of the resonant tunneling by the difference in amplitudes/widths of the barriers.

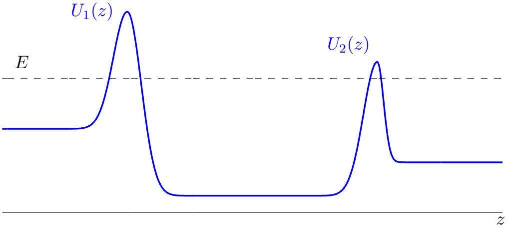
3. Using the formalism of the transfer-matrix, solve the problem of band spectrum of a particle in the periodic potential, consisting of single rectangular barriers (so-called Kronig-Penney problem).

Resonant tunneling in double-barrier potential

We calculate the transmission coefficient for a double-barrier potential.

The transmission amplitude is equal to

$$t = \frac{t_1 t_2}{(1 - r_1' r_2)}$$



According to the definition, the coefficient of transmission is equal ($e^{i\alpha} = \cos\alpha + i\sin\alpha$)

$$\mathcal{T} = |t|^2 = \frac{\mathcal{T}_1\,\mathcal{T}_2}{\left|1 - \sqrt{\mathcal{R}_1\,\mathcal{R}_2}\,e^{i(\arg r_1' + \arg r_2)}\right|^2} = \frac{\mathcal{T}_1\,\mathcal{T}_2}{1 + \mathcal{R}_1\mathcal{R}_2 - 2\sqrt{\mathcal{R}_1\mathcal{R}_2}\cos\left(\arg r_1' + \arg r_2\right)},$$

where $\mathcal{R}_{1,2}$ and $\mathcal{T}_{1,2}$ are coefficients of reflection and transmission through the first and second barriers, correspondingly.

Maximal and minimal values

$$\mathcal{T}_{max} \simeq \frac{\mathcal{T}_1\,\mathcal{T}_2}{\left(1 - \sqrt{\mathcal{R}_1\mathcal{R}_2}\,\right)^2} \simeq \frac{\mathcal{T}_1\,\mathcal{T}_2}{\left(1 - \sqrt{(1-\mathcal{T}_1)\,(1-\mathcal{T}_2)}\,\right)^2} \quad \text{at} \quad \arg r_1' + \arg r_2 \simeq 2\pi n$$

$$\mathcal{T}_{min} \simeq \frac{\mathcal{T}_1\,\mathcal{T}_2}{\left(1 + \sqrt{\mathcal{R}_1\mathcal{R}_2}\,\right)^2} \simeq \frac{\mathcal{T}_1\,\mathcal{T}_2}{\left(1 + \sqrt{(1-\mathcal{T}_1)\,(1-\mathcal{T}_2)}\,\right)^2} \quad \text{at} \quad \arg r_1' + \arg r_2 \simeq \pi + 2\pi n.$$

Limiting case of two low-transmission barriers ($\mathcal{T}_1 \ll 1$ and $\mathcal{T}_2 \ll 1$)

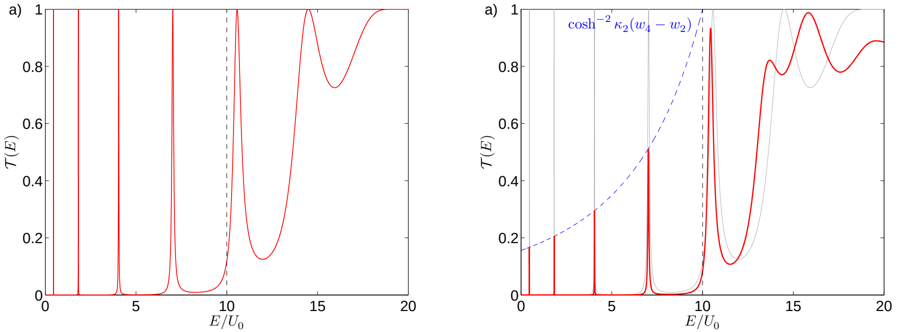
$$\mathcal{T}_{max} \simeq \frac{4\,\mathcal{T}_1\,\mathcal{T}_2}{\left(\mathcal{T}_1 + \mathcal{T}_2\right)^2} \qquad \text{and} \qquad \mathcal{T}_{min} \simeq \frac{\mathcal{T}_1\,\mathcal{T}_2}{4}.$$

Limiting case of two identical low-transmission barriers ($\mathcal{T}_1 = \mathcal{T}_2 \ll 1$)

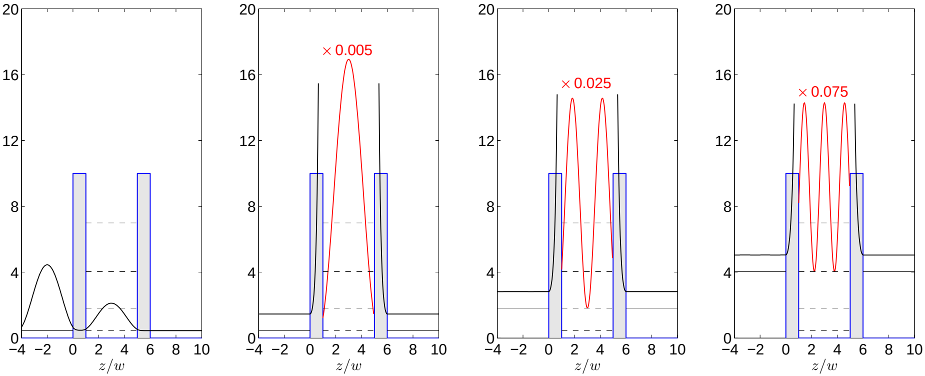
$$\mathcal{T}_{max} \simeq 1 \qquad \text{and} \qquad \mathcal{T}_{min} \simeq \frac{\mathcal{T}^2}{4} \ll 1.$$

The transmission coefficient through two barriers of the same shape (even in the low-transmission case) can be close to unity!

Similar effects: parallel plate (Fabri-Perot) resonator, standing waves in waveguides



Interference of electronic waves in double-barrier structure



Shape of the resonant transmission line

Let E_n be one of possible solutions of the equation $\arg r_1' + \arg r_2 \simeq 2\pi n$. Let $\delta E_n = E - E_n$ be the difference between the energy and the resonant energy. Since $\cos x \simeq 1 - x^2/2$

$$\cos\left(\arg r_1' + \arg r_2\right) = \cos\left(\left(\arg r_1' + \arg r_2\right)_{E=E_n} + \frac{d}{dE}\left(\arg r_1' + \arg r_2\right)_{E=E_n} \cdot (E - E_n)\right)$$

$$\approx 1 - \frac{1}{2}\,\beta_n^2\,(\delta E_n)^2, \qquad \text{where} \quad \beta_n = \frac{d}{dE}\left(\arg r_1' + \arg r_2\right)\Big|_{E=E_n},$$

and therefore in the limit $E \simeq E_n$

$$\mathcal{T} \simeq \frac{\mathcal{T}_1\,\mathcal{T}_2}{\left(1 - \sqrt{\mathcal{R}_1\mathcal{R}_2}\right)^2 + \sqrt{\mathcal{R}_1\mathcal{R}_2}\,\beta_n^2\,(\delta E_n)^2}.$$

Thus, it is a Lorentz-like dependence!

We can introduce the half-width of the transmission line at half-maximum

$$\Gamma_n = \frac{1}{|\beta_n|}\,\frac{\left(1 - \sqrt{\mathcal{R}_1\mathcal{R}_2}\right)}{\sqrt[4]{\mathcal{R}_1\mathcal{R}_2}} = \left|\frac{d}{dE}\left(\arg r_1' + \arg r_2\right)\Big|_{E=E_n}\right|^{-1} \frac{\left(1 - \sqrt{\mathcal{R}_1\mathcal{R}_2}\right)}{\sqrt[4]{\mathcal{R}_1\mathcal{R}_2}},$$

and then we rewrite the dependence $\mathcal{T}(E)$ in the form of Lorentian

$$\mathcal{T}(E) \simeq \frac{\mathcal{T}_1\,\mathcal{T}_2}{\left(1 - \sqrt{\mathcal{R}_1\mathcal{R}_2}\right)^2} \cdot \frac{\Gamma_n^2}{\left(\Gamma_n^2 + (E - E_n)^2\right)} \simeq T_{max} \cdot \frac{\Gamma_n^2}{\left(\Gamma_n^2 + (\delta E_n)^2\right)}.$$