Tunneling phenomena in solids

Lecture 3. Tunneling and quasiclassical approximation. Bardeen's approach. Quasistationary states

Prof. Alexey Yu. Aladyshkin

Moscow Institute of Physics and Technology, Dolgoprudny

Institute for Physics of Microstructures Russian Academy of Sciences, Nizhny Novgorod

Lobachevsky State University of Nizhny Novgorod, Nizhny Novgorod

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Part 1: Quasiclassical approximation. Barriers and wells

Correspondence rules 1 and 2

Correspondence rule 1 between exponentially decaying solution in the forbidden region and standing wave in the accessible region

$$\frac{1}{2}\frac{1}{\sqrt{|p(z)|}}\exp\left\{-\frac{1}{\hbar}\left|\int\limits_{z_0}^{z} p(z)\,dz\right|\right\} \quad \text{at} \quad E_{\|} < U(z) \quad \Longrightarrow$$

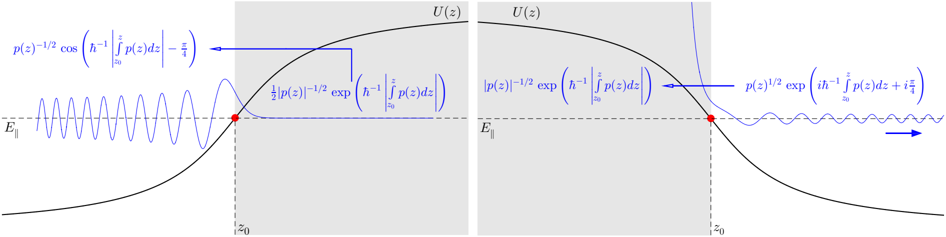
$$\frac{1}{\sqrt{p(z)}}\cos\left\{\frac{1}{\hbar}\left|\int\limits_{z_0}^{z} p(z)\,dz\right| - \frac{\pi}{4}\right\} \quad \text{at} \quad E_{\|} > U(z).$$

Correspondence rule 2 between travelling wave and decaying solution

$$\frac{1}{\sqrt{p(z)}}\exp\left\{\frac{i}{\hbar}\int\limits_{z_0}^{z} p(z)\,dz + i\frac{\pi}{4}\right\} \quad \text{при } E_{\|} > U(z) \quad \Longrightarrow$$

$$\frac{1}{\sqrt{|p(z)|}}\exp\left\{\frac{1}{\hbar}\left|\int\limits_{z_0}^{z} p(z)\,dz\right|\right\} \quad \text{при } E_{\|} < U(z).$$

Transmission through quasiclassical potential barrier



If incident wave runs from left to right, then there is outcoming travelling wave in the area behind the barrier ($z > z_2$)

$$\psi_{III}(z) = \frac{C}{\sqrt{p(z)}}\exp\left\{\frac{i}{\hbar}\int_{z_2}^{z} p(z)\,dz + i\frac{\pi}{4}\right\}.$$

Wave function inside the barrier ($z_1 < z < z_2$) can be found using the quasiclassical boundary condition 2

$$\psi_{II}(z) = \frac{C}{\sqrt{|p(z)|}}\exp\left\{\frac{1}{\hbar}\left|\int_{z_2}^{z} p(z)\,dz\right|\right\}.$$

Inside the barrier ($z < z_2$) we have

$$\left| \int_{z_2}^{z} p(z)\, dz \right| = \int_{z}^{z_2} |p(z)|\, dz = \int_{z_1}^{z_2} |p(z)|\, dz - \int_{z_1}^{z} |p(z)|\, dz.$$

We can rewrite the expression for the wave function inside the barrier in the form

$$\psi_{II}(z) = \frac{C}{\sqrt{|p(z)|}} \exp\left\{ \frac{1}{\hbar} \int_{z_1}^{z_2} |p(z)|\, dz \right\} \cdot \exp\left\{ -\frac{1}{\hbar} \int_{z_1}^{z} |p(z)|\, dz \right\}.$$

Using quasiclassical boundary condition 1, one can get the solution in the area in front of the barrier ($z < z_1$)

$$\psi_I(z) = \frac{2C}{\sqrt{p(z)}} \exp\left\{ \frac{1}{\hbar} \int_{z_1}^{z_2} |p(z)|\, dz \right\} \cdot \cos\left\{ \frac{1}{\hbar} \int_{z}^{z_1} p(z)\, dz - \frac{\pi}{4} \right\} =$$

$$= \frac{2C}{\sqrt{p(z)}} \exp\left\{ \frac{1}{\hbar} \int_{z_1}^{z_2} |p(z)|\, dx \right\} \cdot \cos\left\{ \frac{1}{\hbar} \int_{z_1}^{z} p(z)\, dz + \frac{\pi}{4} \right\}.$$

Taking into account $\cos\alpha = (e^{i\alpha} + e^{-i\alpha})/2$, we come to the solution in the form of two travelling waves (incident + reflected)

$$\psi_I(z) = \frac{C}{\sqrt{p(z)}} \exp\left\{\frac{1}{\hbar}\int_{z_1}^{z_2} |p(z)|\, dz\right\} \cdot \exp\left\{\frac{i}{\hbar}\int_{z_1}^{z} p(z)\, dz + i\frac{\pi}{4}\right\} +$$

$$+ \frac{C}{\sqrt{p(z)}} \exp\left\{\frac{1}{\hbar}\int_{z_1}^{z_2} |p(z)|\, dz\right\} \cdot \exp\left\{-\frac{i}{\hbar}\int_{z_1}^{z} p(z)\, dz - i\frac{\pi}{4}\right\}.$$

Comparing the amplitudes of the waves, we can find the amplitudes of reflection and transmission

$$r \simeq \exp\left(-i\frac{\pi}{2}\right) \quad \text{and} \quad t = \exp\left(-\frac{1}{\hbar}\int_{z_1}^{z_2} |p(z)|\, dz\right).$$

Coefficients of reflection and transmission are

$$\mathcal{R} = |r|^2 \simeq 1 \quad \text{and} \quad \mathcal{T} = |t|^2 = \exp\left(-\frac{2}{\hbar}\int_{z_1}^{z_2} |p(z)|\, dz\right).$$

Kemble formula*

Kemble formula for quasiclassical barrier and arbitrary energy of incident particle

$$\mathcal{T} = \left\{ 1 + \exp\left(\frac{2}{i\hbar} \int\limits_{z_1}^{z_2} p(z)\, dz \right) \right\}^{-1} .$$

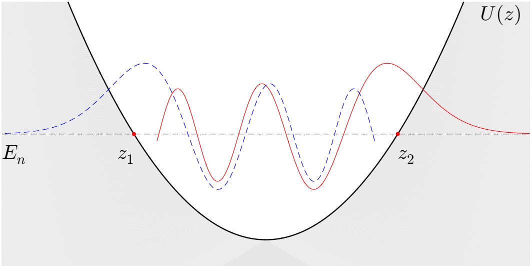
If the full energy is smaller than the barrier height, then both classical turning points can be found from the condition $U(z_{1,2}) = E$. Since in the barrier area $z_1 < z < z_2$ kinetic energy is formally negative, then $p(z) = i|p(z)|$ and

$$\mathcal{T} = \left\{ 1 + \exp\left(\frac{2}{\hbar} \int\limits_{z_1}^{z_2} |p(z)|\, dz \right) \right\}^{-1} , \quad \text{provided that} \quad E_{\|} < \max\ U(z).$$

If the barrier height significantly exceed the energy (limit of low-transmission barrier), then

$$\mathcal{T} = \exp\left(-\frac{2}{\hbar} \int\limits_{z_1}^{z_2} |p(z)|\, dz \right) , \quad \text{provided that} \quad E_{\|} \ll \max\ U(z).$$

Bohr-Sommerfeld quantization rule



Quantized states in one-dimensional potential well:

$U(z)$ is the profile of potential energy

E_n is n-th energy level

z_1 and z_2 are classical turning points for the n-th energy level

According to the quasiclassical boundary condition 1, the exponentially-decaying solution at $z > z_2$ gives us the following oscillating solution in the accessible region $z < z_2$

$$\psi(z) = \frac{C}{\sqrt{p(z)}} \cos\left\{ \frac{1}{\hbar} \int_{z}^{z_2} p(z)\, dz - \frac{\pi}{4} \right\}.$$

If we apply the same condition to the point z_1, we get an alternative expression for the wave function in the region $z > z_1$

$$\psi'(z) = \frac{C'}{\sqrt{p(z)}} \cos\left\{ \frac{1}{\hbar} \int_{z_1}^{z} p(z)\, dz - \frac{\pi}{4} \right\} = \frac{C'}{\sqrt{p(z)}} \cos\left\{ -\frac{1}{\hbar} \int_{z_1}^{z} p(z)\, dz + \frac{\pi}{4} \right\}.$$

In order to guarantee that both expressions

$$\psi(z) = \frac{C}{\sqrt{p(z)}} \cos\left\{ \frac{1}{\hbar} \int_{z}^{z_2} p(z)\, dz - \frac{\pi}{4} \right\}, \quad \psi'(z) = \frac{C'}{\sqrt{p(z)}} \cos\left\{ -\frac{1}{\hbar} \int_{z_1}^{z} p(z)\, dz + \frac{\pi}{4} \right\}$$

corresponds to the same wave function, the difference of the arguments of the cos-functions should be a multiple of π (provided that $C = (-1)^n C'$, where n is integer)

$$\left(\frac{1}{\hbar} \int_{z}^{z_2} p(z)\, dz - \frac{\pi}{4} \right) - \left(-\frac{1}{\hbar} \int_{z_1}^{z} p(z)\, dz + \frac{\pi}{4} \right) = \frac{1}{\hbar} \int_{z_1}^{z_2} p(z)\, dz - \frac{\pi}{2} = \pi n.$$

It leads to well-known Bohr-Sommerfeld quantization rule in the following form

$$\frac{1}{\pi\hbar} \int_{z_1}^{z_2} p(z)\, dz = n + \frac{1}{2}, \qquad n = 0, 1, 2, \ldots$$

or in the alternative form of closed integral

$$\frac{1}{2\pi\hbar} \oint p(z)\, dz = n + \frac{1}{2}, \qquad n = 0, 1, 2, \ldots$$

Illustrative example: particle in a parabolic potential well

Assume that the potential energy can be written in the form $U(z) = m^* \omega^2 z^2/2$, where ω is the frequency of oscillations.

Let E_n be the full energy of a particle at the n-th energy level.

From the condition $U(z) = E_n$ we find the coordinates of the turning points

$$z_{1,2} = \pm\sqrt{\frac{2E_n}{m^*\omega^2}}.$$

We apply Bohr-Sommerfeld quantization rule

$$\frac{1}{\pi\hbar}\int\limits_{-\sqrt{2E_n/(m^*\omega^2)}}^{\sqrt{2E_n/(m^*\omega^2)}} p(z)\,dz = \frac{2m^*\omega}{\pi\hbar}\int\limits_0^{\sqrt{2E_n/(m^*\omega^2)}} \sqrt{\frac{2E_n}{m^*\omega^2} - z^2}\,dz = \frac{2}{\pi}\frac{E_n}{\hbar\omega}\,arcsin\;1 = n + \frac{1}{2}.$$

Taking into account that $arcsin\;1 = \pi/2$, we get

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, \ldots$$

This result coincides with the exact solution of the quantum-mechanical problem.

Illustrative example: particle in a square potential well

Assume that the potential energy can be written in the form $U(z) = 0$ for $0 < z < w$ and $U(z) = \infty$ outside this region; w is the width of the potential well.

The coordinates of the turning points do not depend on the particle energy

$$z_1 = 0 \quad \text{and} \quad z_2 = w.$$

We apply Bohr-Sommerfeld quantization rule

$$\frac{1}{\pi\hbar} \int\limits_0^w p(z)\, dz = \frac{\sqrt{2m^* E_n}}{\pi\hbar} \int\limits_0^w dz = n + \frac{1}{2} \quad \text{or} \quad E_n = \frac{\pi^2 \hbar^2}{2m^* w^2} \cdot \left(n + \frac{1}{2}\right)^2, \quad n = 0, 1, \ldots$$

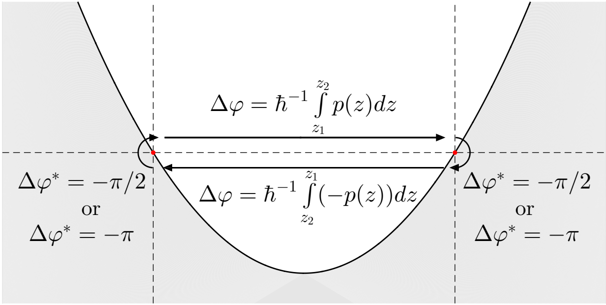
Reminder: the exact formula reads

$$E_n = \frac{\pi^2 \hbar^2}{2m^* w^2} \cdot n^2, \quad n = 1, 2, \ldots$$

Thus, the approximate WKB-result coincides with the exact solution only for $n \gg 1$.

Question: is it possible to improve the Bohr-Sommerfeld quantization rule?

Modified Bohr-Sommerfeld quantization rule*



The model of the accumulation of the total phase for the well with finite slope at the turning points

$$\frac{1}{\hbar}\int_{z_1}^{z_2} p(z)dz + \left(-\frac{\pi}{2}\right) + \frac{1}{\hbar}\int_{z_2}^{z_1} (-p(z))dz + \left(-\frac{\pi}{2}\right) = 2\pi n, \quad n = 0, 1, \dots \quad \Longrightarrow$$

$$\frac{1}{\pi\hbar}\int_{z_1}^{z_2} p(z)dz = n + \frac{1}{2}, \quad n = 0, 1, \dots$$

Modified Bohr-Sommerfeld quantization rule, taking into account the additional phase shift occurring at the turning points

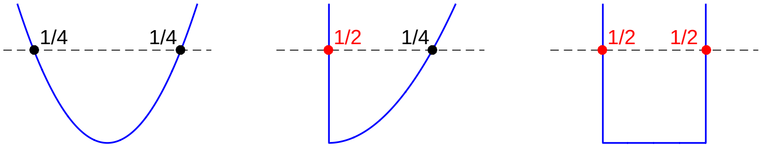
$$\frac{1}{\pi\hbar}\int\limits_{z_1}^{z_2} p(z)\,dz = n+\gamma \quad \text{or} \quad \frac{1}{2\pi\hbar}\oint p(z)\,dz = n+\gamma, \quad n = 1, 2, ...$$

where

$\gamma = 1/2$ for the potential well with finite slope at the turning points;

$\gamma = 3/4$ for the potential well with finite slope at one turning point and infinite slope at another turning point;

$\gamma = 1$ for the potential well with infinite slopes at the turning points.



Another form of Bohr-Sommerfeld quantization rule

$$\arg r_1' + \arg r_2 = 2\pi n \quad \Longrightarrow \quad \arg r_1' + \arg r_2 = \frac{2}{\hbar}\int\limits_{z_1}^{z_2} p(z)\,dz - 2\pi\gamma = 2\pi n, \quad n = 0, 1, \ldots$$

Part 2: Tunneling in low-transmission systems: Bardeen's approach

Fermi's golden rule and tunneling current

The rate of quantum transitions (i. e. the number of quantum transition per unit of time) from the initial state i to the final state of discrete spectrum f is essentially constant and it is known to be given by the formula

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}\,|\,T_{i\to f}|^2\,\delta\big(E_i - E_f\big),$$

where $T_{i\to f}$ is the matrix element of a stationary perturbing Hamiltonian $\hat{H}'$ applied to the system

$$T_{n,m} = \int \Psi_n^*(\boldsymbol{r},t)\,\hat{H}'\,\Psi_m(\boldsymbol{r},t)\,d\boldsymbol{r} = e^{-i(E_n-E_m)t/\hbar}\cdot\int \psi_m^*(\boldsymbol{r})\,\hat{H}'\,\psi_n(\boldsymbol{r})\,d\boldsymbol{r},$$

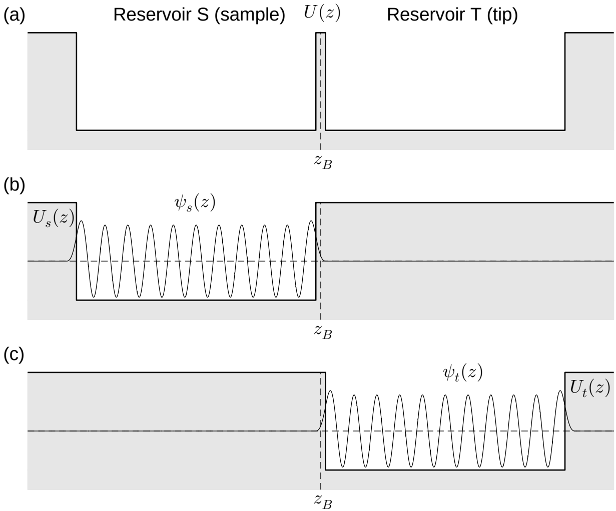
and the delta-function $\delta\big(E_i - E_f\big)$ accounts the conservation of energy at quantum transitions.

Recommended methodological notes for educational reading: Emmanuel N. Koukara, *Fermi's Golden Rule*, http://staff.ustc.edu.cn/∼yuanzs/teaching/Fermi-Golden-Rule-No-II.pdf

Question: How to introduce the tunneling Hamiltonian $\hat{H}'$ in such a way to calculate tunneling current using the Fermi's golden rule $I = e\sum\Gamma_{i,f}$?

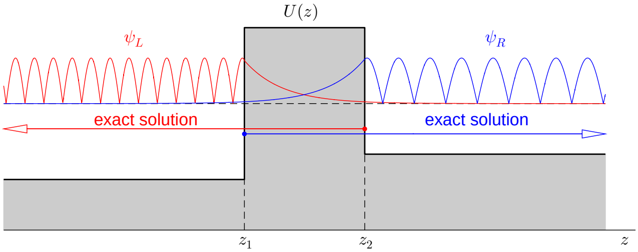
Tunneling through low-transmission 1D potential barrier: Bardeen's approach

John Bardeen, Nobel prize in physics in 1956 (with Shockley and Brattain for the invention of the transistor) and in 1972 (with Cooper and Schrieffer for microscopic theory of superconductivity)



Bardeen, Phys. Rev. Lett., vol. 6, 57 (1961).

Main idea: the partial wave functions $\psi_{L,n}(z)$ and $\psi_{R,m}(z)$ in a non-interacting system are non-overlapping and thus form the full and orthonormal basises, describing the localization of electrons in the left and right electronic reservoirs, respectively.



Following the Bardeen's idea, we consider the *approximate* wave functions for the electrons in the left and right reservoirs (limit of weekly-interacting subsystems)

$$\psi_{L,n} = \begin{cases} \hat{H}\psi_{L,n} = E_{L,n}\psi_{L,n} & \text{при } z \le z_2; \\ const \cdot e^{-\varkappa_2 z} & \text{при } z > z_2, \end{cases} \qquad \psi_{R,n} = \begin{cases} const \cdot e^{+\varkappa_2 z} & \text{при } z \le z_1; \\ \hat{H}\psi_{R,n} = E_{R,n}\psi_{R,n} & \text{при } z > z_1, \end{cases}$$

where $\hat{H}$ is the exact Hamiltonian of the problem.

We start with the assumption that the electron at initial moment (at $t = 0$) is in the left reservoir in the state, described by one of the localized functions $\psi_{L,n}(z)$. We estimate a probability for this electron to transfer to one of possible electronic states described by the localized wave function $\psi_{R,m}(z)$ in the right reservoir.

We seek for the solution of time-dependent Schrödinger equation in the form of the linear combination of non-perturbed wave functions

$$\Psi(z,t) = c_n(t)\,\psi_{L,n}(z)\,e^{-iE_n t/\hbar} + \sum_{m'} d_{m'}(t)\,\psi_{R,m'}(z)\,e^{-iE_{m'} t/\hbar},$$

where E_n и E_m are eigenenergies of the initial and final states.

After substitution of the trial function $\Psi(z,t)$ into the non-stationary Schrödinger equation $i\hbar\,\partial\Psi/\partial t = \hat{H}\Psi$, we get

$$i\hbar\,\dot{c}_n(t)\,\psi_{L,n}(z)\,e^{-iE_n t/\hbar} + \sum_{m'} i\hbar\,\dot{d}_{m'}(t)\,\psi_{R,m'}(z)\,e^{-iE_{m'} t/\hbar} =$$

$$= c_n(t)\,e^{-iE_n t/\hbar}\,(\hat{H} - E_n)\,\psi_{L,n}(z) + \sum_{m'} d_{m'}(t)\,e^{-iE_m t/\hbar}\,(\hat{H} - E_{m'})\,\psi_{R,m'}(z) \quad (*),$$

where $\dot{c}_n(t) \equiv dc_n/dt$.

After multiplying the equation (*) at $\psi^*_{R,m}(z)$ and integration over z, we get

$$\sum_{m'} i\hbar\,\dot{d}_{m'}(t)\,\langle\psi^*_{R,m}(z)|\psi_{R,m'}(z)\rangle\,e^{-iE_{m'}t/\hbar} \simeq c_n(t)\,e^{-iE_nt/\hbar}\,\langle\psi^*_{R,m}(z)|(\hat{H}-E_n)\,\psi_{L,n}(z)\rangle.$$

The expression

$$T_{L\to R} = \langle\psi^*_{R,m}(z)\,|(\hat{H}-E_n)\,\psi_{L,n}(z)\rangle$$

can be viewed as a matrix element of quantum transition for the effective Hamiltonian $\hat{H}' = \hat{H} - E_n$ from the initial state $\psi_{L,n}(z)$ (electron in the left box) to the state $\psi_{R,m}(z)$ (electron in the right box).

Provided that $\psi_{R,m}(z)$ are orthonormal functions, we arrive

$$\sum_{m'} i\hbar\,\dot{d}_{m'}(t)\,\delta_{m,m'}\,e^{-iE_{m'}t/\hbar} = i\hbar\,\dot{d}_m(t)\,e^{-iE_{m'}t/\hbar} \simeq c_n(t)\,e^{-iE_nt/\hbar}\,T_{L\to R}.$$

This means that the evolution of the coefficients d_m is similar to the expression typical for quantum-mechanical problems

$$i\hbar\,\dot{d}_m \simeq e^{-i(E_n-E_m)t/\hbar}\cdot T_{L\to R}.$$

Thus, the matrix element in the Bardeen's problem is equal to

$$T_{L\to R} = \langle \psi^*_{R,m}(z) | (\hat{H} - E_n) \psi_{L,n}(z) \rangle = \int\limits_{-\infty}^{\infty} \psi^*_{R,m}(z)\, (\hat{H} - E_n)\, \psi_{L,n}(z)\, dz =$$

$$= \int\limits_{z_B}^{\infty} \psi^*_{R,m}(z)\, (\hat{H} - E_n) \psi_{L,n}(z)\, dz,$$

where z_B is an arbitrary point inside the tunneling barrier ($z_1 \le z_B \le z_2$).

This expression can be written in a symmetric form

$$T_{L\to R} = \int\limits_{z_B}^{\infty} \left\{ \psi^*_{R,m}(z)\, (\hat{H} - E_n)\, \psi_{L,n}(z) - \psi_{L,n}(z)\, (\hat{H} - E_m)\, \psi^*_{R,m}(z) \right\} dz.$$

Taking into account the conservation of the energy at tunneling process ($E_n = E_m$) and after integration by parts, we get a simple expression for the matrix element

$$T_{L\to R} = -\frac{\hbar^2}{2m^*} \left\{ \psi_{L,n} \frac{d}{dz} \psi^*_{R,m} - \psi^*_{R,m} \frac{d}{dz} \psi_{L,n} \right\}_{z=z_B}$$

Bardeen's approach: summary

The matrix elements for the direct and reverse tunneling processes in 1D case are equal to

$$T_{L\to R} = -\frac{\hbar^2}{2m^*}\left\{\psi_{L,n}\frac{d}{dz}\psi^*_{R,m} - \psi^*_{R,m}\frac{d}{dz}\psi_{L,n}\right\}_{z=z_B}$$

$$T_{R\to L} = -\frac{\hbar^2}{2m^*}\left\{\psi_{R,m}\frac{d}{dz}\psi^*_{L,n} - \psi^*_{L,n}\frac{d}{dz}\psi_{R,m}\right\}_{z=z_B},$$

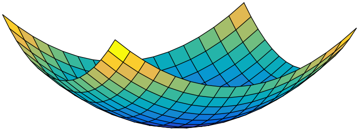
where z_B is the arbitrary point inside the tunneling barrier.

These expressions look like probability flux in quantum mechanics (up to numerical coefficient)

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

Generalization for three-dimensional case:

$$T_{L\to R} = -\frac{\hbar^2}{2m^*}\iint\limits_S \left\{\psi_{L,n}\nabla\psi^*_{R,m} - \psi^*_{R,m}\nabla\psi_{L,n}\right\}_{\boldsymbol{n}}\cdot d\boldsymbol{S},$$



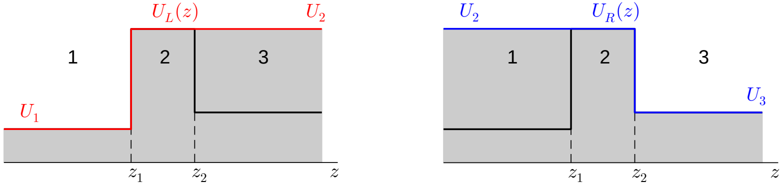
where S is an arbitrary surface inside the barrier, $\boldsymbol{n}$ is the normal vector.

Homework for inspired students: estimate of the transmission coefficient of one-dimensional square barrier

A model potential has the following form

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

The auxiliary potentials for the 'left' and 'right' problems, which can be considered separately



It is possible to demonstrate that the transmission coefficient (do not mix it with the matrix element) are equal to

$$\mathcal{T} = \frac{16 k_1 \varkappa_2^2 k_3}{(k_1^2 + \varkappa_2^2)(\varkappa_2^2 + k_3^2)} \, e^{-2\varkappa_2 (z_2 - z_1)}.$$

It perfectly coincides with the exact answer for the transmission coefficient in the limit of low-transmission barrier ($\varkappa_2 (z_2 - z_1) \gg 1$).

Part 3: Quasistationary states

Stationary and quasi-stationary states in quantum mechanics

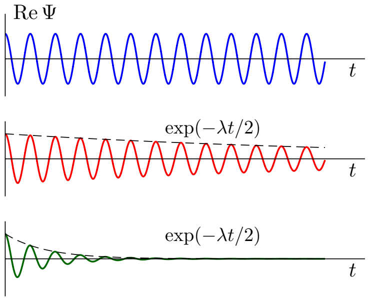
We start with time-dependent Schroedinger equation $i\hbar\,\partial\Psi/\partial t = \hat{H}\,\Psi$.

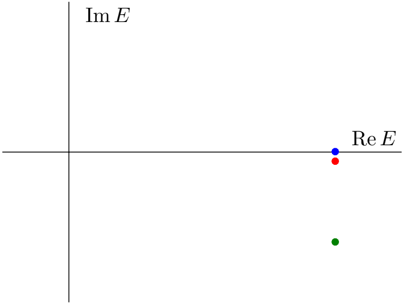
If $\Psi(\boldsymbol{r},t) = \psi(\boldsymbol{r}) \cdot e^{-iEt/\hbar}$, then we come to $\hat{H}\,\psi(\boldsymbol{r}) = E\,\psi(\boldsymbol{r})$.

For decaying state $\Psi(\boldsymbol{r},t) = \psi(\boldsymbol{r}) \cdot e^{-\lambda t/2} \cdot e^{-iEt/\hbar}$ we get $\hat{H}\,\psi(\boldsymbol{r}) = (E - i\cdot\lambda\hbar/2)\,\psi(\boldsymbol{r})$.

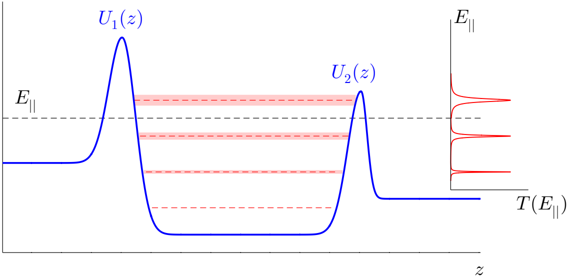
Such slowly-decaying states ($E = Re\,E + i\,Im\,E$ and $|Im\,E| \ll Re\,E$) are typically called quasistationary states. Imaginary part of the eigenenergy determines the decay constant λ:

$$|\Psi(\boldsymbol{r},t)|^2 = |\psi(\boldsymbol{r})|^2 \cdot e^{-\lambda t}, \quad \text{where} \quad \lambda \equiv -\frac{2}{\hbar}\,Im\,E.$$





Decaying states in double-barrier structure



Stationary states, which satisfy the Schroedinger equation $\hat{H}\,\psi = E\,\psi$ for the double-barrier systems, corresponds to the poles of the transmission coefficient $\mathcal{T}$.

The shape of the transmission line near the quantum-well resonance

$$\mathcal{T} \simeq \frac{\Gamma_n^2}{\Gamma_n^2 + \left(E - E_n^{(0)}\right)^2}, \quad \text{where} \quad \Gamma_n = \left| \frac{d}{dE}\left(\arg r_1' + \arg r_2\right)\Big|_{E=E_n^{(0)}} \right|^{-1} \frac{\left(1 - \mathcal{R}\right)}{\sqrt{\mathcal{R}}},$$

The pole for the dependence $\mathcal{T}(E)$ corresponds to complex-valued energy: $E = E_n^{(0)} - i\Gamma_n$, where $E_n^{(0)}$ is the energy and Γ_n is the transmission linewidth for the n-th quantum-well state.

We can Bohr-Sommerfeld quantization rule for one-dimensional potential well as follows

$$\arg r_1' + \arg r_2 = \frac{2}{\hbar}\int\limits_{z_1}^{z_2} p(z)\,dz - \pi, \quad n = 0, 1, \ldots$$

It is easy to demonstrate that

$$\frac{d}{dE}\big(\arg r_1' + \arg r_2\big)\Big|_{E=E_n^{(0)}} \simeq \frac{d}{dE}\left(\frac{2}{\hbar}\int\limits_{z_1}^{z_2} p(z)dz\right)_{E=E_n^{(0)}} \simeq$$

$$\simeq \frac{2}{\hbar}\sqrt{2m^*}\int\limits_{z_1}^{z_2}\frac{d}{dE}\sqrt{E-U(z)}\,dz \simeq \frac{1}{\hbar}\sqrt{2m^*}\int\limits_{z_1}^{z_2}\frac{dz}{\sqrt{E-U(z)}} \simeq \frac{1}{\hbar}\oint\frac{dz}{v_n(z)} \simeq \frac{T}{\hbar},$$

where $T = 2L/v_n$ is the period of oscillations of a particle in the area L between two potential barriers, $f_n = 1/T$ is so-called attempt frequency, v_n is mean quasiclassical velocity at n-th energy level. As a result, for $T_n \ll 1$ we get

$$\Gamma_n = \left|\frac{d}{dE}\big(\arg r_1' + \arg r_2\big)\Big|_{E=E_n^{(0)}}\right|^{-1}\frac{(1-\mathcal{R}_n)}{\sqrt{\mathcal{R}_n}} \simeq \left|\frac{1}{\hbar}\cdot\frac{1}{f_n}\right|^{-1}\frac{\mathcal{T}_n}{\sqrt{1-\mathcal{T}_n}} \simeq \hbar\cdot f_n\cdot\mathcal{T}_n.$$

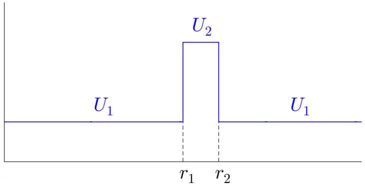
Decay constant is equal to the product of attempt frequency f_n and the transmission coefficient $\mathcal{T}_n$

$$\lambda = -\frac{2}{\hbar}\,Im\,E \simeq \frac{2}{\hbar}\Gamma_n \simeq \frac{2}{\hbar}\cdot\hbar\cdot f_n\cdot\mathcal{T}_n \quad\Longrightarrow\quad \lambda \simeq \frac{f_n}{2}\cdot\mathcal{T}_n \simeq \frac{v_n}{L}\cdot\mathcal{T}_n.$$

Decay constant for $s-$state in spherical potential well*

We consider spherical potential well

$$U(r) = \begin{cases} U_1 \text{ at } r < r_1 \\ U_2 \text{ at } r_1 < r < r_2 \\ U_1 \text{ at } r > r_2 \end{cases}$$



For spherically-symmetrical wave function $\psi(x, y, z) = \psi(r)$ we get the following differential equation with variable coefficients

$$\frac{d^2}{dr}\psi(r) + \frac{2}{r}\frac{d}{dr}\psi(r) + \frac{2m^*}{\hbar^2}\Big(E - U(r)\Big)\psi(r) = 0.$$

After change of variable $\psi(r) = \chi(r)/r$ we come to an ordinary differential equation, which resembles one-dimensional problem $(r \to x)$

$$\frac{d^2}{dr^2}\chi(r) + \frac{2m^*}{\hbar^2}\Big(E - U(r)\Big)\chi(r) = 0.$$

In order to solve this equation we need to apply an additional condition $\chi = 0$ at $r = 0$ to avoid divergency of the wave function $\psi(r)$ at origin.

For piece-wise potential $U(r)$ we get the following solution

$$\begin{array}{ll} \text{Region 1 } (r < r_1): & \chi_1(r) = a_1\, e^{ik_1 r} - a_1\, e^{-ik_1 r} \\ \text{Region 2 } (r_1 < r < r_2): & \chi_2(r) = a_2\, e^{ik_2 r} + b_2\, e^{-ik_2 r} \\ \text{Region 3 } (r > r_2): & \chi_3(r) = a_3\, e^{ik_3 r} + 0\, e^{-ik_3 r}. \end{array}$$

Criterion for localized states in terms of transfer-matrices $\hat{T} = \hat{T}^{(1)}\,\hat{T}^{(2)}$

$$\left(\begin{array}{c} a_1 \\ -a \end{array}\right) = \hat{T} \left(\begin{array}{c} a_3 \\ 0 \end{array}\right) \quad \Longrightarrow \quad T_{11} = -T_{21}.$$

It is easy to obtain the spectrum of the localized states

$$\left\{(k_1+k_2)(k_2+k_3)\, e^{i(-k_1+k_2)r_1}\, e^{i(-k_2+k_3)r_2} + (k_1-k_2)(k_2-k_3)\, e^{i(-k_1-k_2)r_1}\, e^{i(k_2-k_3)r_2}\right\} =$$
$$-\left\{(k_1-k_2)(k_2+k_3)\, e^{i(k_1+k_2)r_1}\, e^{i(-k_2+k_3)r_2} + (k_1+k_2)(k_2-k_3)\, e^{i(k_1-k_2)r_1}\, e^{i(k_2-k_3)r_2}\right\}.$$

Simplified expression for symmetric spherical barrier ($k = k_{1,3} = \sqrt{2m^*(E-U_{1,3})}/\hbar$ and $k_2 = i\varkappa_2$):

$$\left\{(k+i\varkappa_2)(i\varkappa_2+k)\, e^{i(-k+i\varkappa_2)r_1}\, e^{i(-i\varkappa_2+k)r_2} + (k-i\varkappa_2)(i\varkappa_2-k)\, e^{i(-k-i\varkappa_2)r_1}\, e^{i(i\varkappa_2-k)r_2}\right\} =$$
$$-\left\{(k-i\varkappa_2)(i\varkappa_2+k)\, e^{i(k+i\varkappa_2)r_1}\, e^{i(-i\varkappa_2+k)r_2} + (k+i\varkappa_2)(i\varkappa_2-k)\, e^{i(k-i\varkappa_2)r_1}\, e^{i(i\varkappa_2-k)r_2}\right\}.$$

As a result, we get the following equation

$$\left(\frac{\varkappa}{k}\tan kr_1 + 1\right) = -e^{-2\varkappa w}\left(\frac{k-i\varkappa}{k+i\varkappa}\right)\cdot\left(\frac{\varkappa}{k}\tan kr_1 - 1\right), \qquad (*)$$

where $w = r_2 - r_1$ is the barrier width, $\varphi = \arctan(\varkappa/k)$ is the phase shift.

1. For completely impenetratable barrier ($e^{-2\varkappa w} \lll 1$) we get the spectrum of quantum-well states in the spherical potential well:

$$\left(\frac{\varkappa_n}{k_n}\tan k_n r_1 + 1\right) = 0.$$

2. For low-transmission barrier ($e^{-2\varkappa w} \ll 1$) we can calculate the spectrum of quantum-well states using theory of perturbation, formally considering the offset $\Delta k = k - k_n$ from the stationary-state value.

Left-hand side of Eq. (*): we expand over Δk and take into account that $(d\varkappa/dk)_n = -k_n/\varkappa_n$, $\operatorname{tg} k_n r_1 = -k_n/\varkappa_n$ и $\cos^{-2} k_n r_1 = (k_n^2 + \varkappa_n^2)/\varkappa_n^2$, тогда

$$\text{LHS:} \quad \left(\frac{\varkappa}{k}\tan kr_1 + 1\right) \simeq \frac{\left(k_n^2+\varkappa_n^2\right)}{k_n\varkappa_n^2}\left(1+\varkappa_n r_1\right)\Delta k.$$

Right-hand side of Eq. (*): we put here the unperturbed values k_n and $\varkappa_n$

$$\text{RHS:} \quad -e^{-2\varkappa_n w}\left(\frac{k_n-i\varkappa_n}{k_n+i\varkappa_n}\right)\cdot\left(\frac{\varkappa_n}{k_n}\tan k_n r_1 - 1\right) \simeq 2\,e^{-2\varkappa_n w}\frac{\left(k_n-i\varkappa_n\right)^2}{k_n^2+\varkappa_n^2}.$$

Combining two previous expressions, we get the equation for the offset Δk

$$\Delta k_n = \frac{2k_n \varkappa_n^2}{(1+\varkappa_n r_1)} \frac{(k_n - i\varkappa_n)^2}{(k_n^2+\varkappa_n^2)^2} e^{-2\varkappa_n w}.$$

It is obvious that the offset is complex-valued parameter. We can write the imaginary part of the offset as follows

$$Im\,\Delta k_n = \frac{2k_n \varkappa_n^2}{(1+\varkappa_n r_1)} \cdot \frac{-2\,k_n\,\varkappa_n}{(k_n^2+\varkappa_n^2)^2} \cdot e^{-2\varkappa_n w} < 0.$$

One can substitute $k = k_n + i\,Im\,\Delta k$ in the expression for energy

$$E = \frac{\hbar^2}{2m} k^2 \simeq \frac{\hbar^2}{2m^*} (k_n + i\,Im\,\Delta k)^2\,, \quad \Longrightarrow \quad Im\,E = \frac{\hbar^2}{m^*} k_n \cdot Im\,\Delta k < 0.$$

Decay constant is equal to

$$\lambda = -\frac{2}{\hbar} Im\,E \simeq \frac{8\hbar k_n}{m^*} \frac{k_n^2 \varkappa_n^3}{(k_n^2+\varkappa_n^2)^2} \frac{e^{-2\varkappa_n w}}{(1+\varkappa_n r_1)}.$$

For low-transmission barrier $\varkappa_n r_1 \gg 1$, therefore

$$\lambda \simeq \frac{\hbar k_n}{m^*} \cdot \frac{1}{2r_1} \cdot \frac{16 k_n \varkappa_n^2 k_n}{(k_n^2+\varkappa_n^2)^2}\; e^{-2\varkappa_n w} \simeq \frac{v_n}{2r_1} \cdot \mathcal{T}_n.$$

As before, the decay constant equal to the product of the attempt frequency $(v_n/2r_1)$ and the transmission coefficient $\mathcal{T}_n$ for n−th quantum-well state.

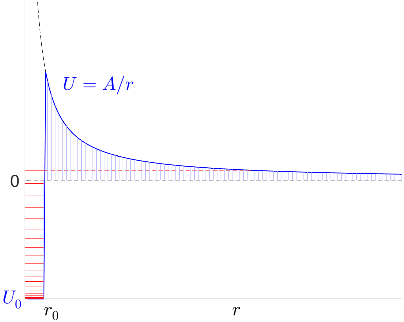
Alpha-decay as a tunneling process

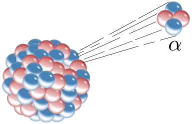
Alpha decay is a type of radioactive decay in which an atomic nucleus emits an alpha particle ${}^4_2He$ and thereby transforms into a different atomic nucleus, with a mass number that is reduced by four and an atomic number that is reduced by two.

In order to estimate the decay constant, we calculate the transmission coefficient through the following Coulomb potential barrier

$$U(r) = \begin{cases} -U_0 \text{ при } r < r_0 \\ A/r \text{ при } r > r_0, \end{cases} \quad \text{where} \quad A = (Z-2)e \cdot 2e,$$

r_0 is typical radius of strong nuclear forces, Z is atomic number of parent nucleus.





We consider the Coulomb barrier as quasiclassical barrier and estimate the transmission of such barrier for α-particle of energy E using WKB-theory

$$\mathcal{T} = \exp\left(-\frac{2}{\hbar}\int\limits_a^b |p(r)|\,dr\right) = \exp\left(-\frac{2\sqrt{2m^*}}{\hbar}\int\limits_{r_0}^{A/E}\sqrt{\frac{A}{r} - E}\,dr\right),$$

where $a = r_0$ and $b = A/E$ are classical turning points, $|p(r)| = \sqrt{2m^*}\sqrt{U(r) - E}$ is classical momentum.

This integral can be easily calculated by means of change of variables $x = b\cos^2 u$ and the following standard integral

$$\int\sqrt{\frac{b}{x} - 1}\cdot dx = -b\,arccos\sqrt{\frac{r}{b}} + b\sqrt{\frac{r}{b} - \frac{r^2}{b^2}}.$$

As a result, we get the transmission coefficient of the Coulomb barrier

$$\mathcal{T} \simeq \exp\left(-\frac{2A}{\hbar}\sqrt{\frac{2m^*}{E}}\left\{\arccos\sqrt{\frac{Er_0}{A}} - \sqrt{\frac{Er_0}{A}\left(1 - \frac{Er_0}{A}\right)}\right\}\right).$$

For low-energy emitting α-particles one can come to a simplified formula

$$\mathcal{T} \simeq \exp\left(-\frac{2A}{\hbar}\sqrt{\frac{2m^*}{E}}\cdot\frac{\pi}{2}\right), \quad \text{provided that} \quad \frac{Er_0}{A} \ll 1.$$

Now we can estimate the decay constant

$$\lambda = \frac{v_n}{2r_0} \cdot \mathcal{T} = const \cdot \exp\left(-\frac{\pi A}{\hbar}\sqrt{\frac{2m^*}{E}}\right)$$

and half-life time $T_{1/2} = \ln 2/\lambda$ for heavy nucleus (Gamow, 1928)

$$\ln T_{1/2} \simeq -\ln const + \frac{\pi(Z-2)2e^2}{\hbar}\sqrt{\frac{2m^*}{E}}.$$

Gamow's formula explains well the experimental dependence of the half-life time on atomic number and energy (Geiger and Nuttal, 1911)

$$\ln T_{1/2} \simeq -const_1 + const_2 \cdot \frac{Z}{\sqrt{E}}.$$

Examples of alpha-decay:

${}^{232}_{90}\mathrm{Th} \to {}^{228}_{88}\mathrm{Ra} + \alpha\ (1.4 \cdot 10^{10}\ \mathrm{yr})$,
${}^{238}_{92}\mathrm{U} \to {}^{234}_{90}\mathrm{Th} + \alpha\ (4.5 \cdot 10^{9}\ \mathrm{yr})$,
${}^{236}_{92}\mathrm{U} \to {}^{232}_{90}\mathrm{Th} + \alpha\ (2.3 \cdot 10^{7}\ \mathrm{yr})$,
${}^{226}_{88}\mathrm{Ra} \to {}^{222}_{86}\mathrm{Re} + \alpha\ (1600\ \mathrm{yr})$
${}^{241}_{95}\mathrm{Am} \to {}^{237}_{93}\mathrm{Np} + \alpha\ (433\ \mathrm{yr})$,
${}^{210}_{84}\mathrm{Po} \to {}^{208}_{82}\mathrm{Pb} + \alpha\ (138\ \mathrm{day})$,
${}^{222}_{86}\mathrm{Rn} \to {}^{218}_{84}\mathrm{Po} + \alpha\ (3.8\ \mathrm{day})$.