Tunneling phenomena in solids

Lecture 2. Quantum-well states: exact solutions Quasiclassical WKB approximation

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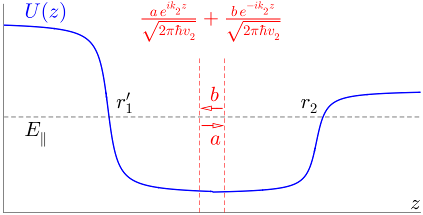
Part 1: Quantum-well states. Coupled potential wells

Quantum-well states in potential well: method 1

We proceed with calculation the energy of the localized states for 'particle-in-the-box' using the formalism of scattering matrix.

We assume that we can find area inside the potential well with (almost) constant potential. In this area there are two plane waves of amplitudes a and b.



Reflection of electron at the left and right edges of the potential well corresponds to the equations $a = r'_1 b$ и $b = r_2 a$, therefore

$$a = r'_1 b = r'_1 r_2\, a \qquad \text{or} \qquad (1 - r'_1 r_2)\, a = 0.$$

Non-trivial solution ($a \neq 0$) exists only if $1 - r'_1 r_2 = 0$.

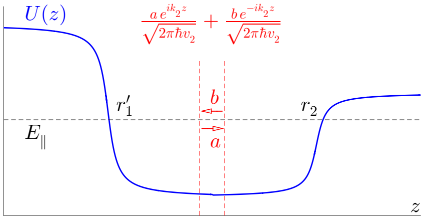
Since $r'_1 = |r'_1|\, e^{i \arg r'_1}$, $r_2 = |r_2|\, e^{i \arg r_2}$ and $|r'_1| = |r_2| = 1$, the above conditions $r'_1\, r_2 = 1$ can be written as a phase accumulation rule

$$\arg r'_1 + \arg r_2 = 2\pi n.$$

Quantum-well states in potential well: method 2

We calculate the energy of the localized states for 'particle-in-the-box' using the formalism of the scattering matrix.

For localized states the wave vectors inside the barrier area should be imaginary: $k_1 = i\varkappa_1$ и $k_3 = i\varkappa_3$.



The transformation of the solutions inside the left barrier:

$$a_1 e^{ik_1 z} \to a_1 e^{-\varkappa_1 z} \quad \text{and} \quad b_1 e^{-ik_1 z} \to b_1 e^{\varkappa_1 z}.$$

In order to avoid a divergency of the wave function deep inside the barrier (at $z \to -\infty$), we have to put $a_1 = 0$.

The transformation of the solutions inside the right barrier:

$$a_3 e^{ik_3 z} \to a_3 e^{-\varkappa_3 z} \quad \text{and} \quad b_3 e^{-ik_3 z} \to b_3 e^{\varkappa_3 z}.$$

In order to avoid a divergency of the wave function deep inside the barrier (at $z \to +\infty$), we have to put $b_3 = 0$.

Reminder: structure of the scattering matrix

$$\begin{pmatrix} b_1 \\ a_3 \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} a_1 \\ b_3 \end{pmatrix}$$

The scattering matrix in our case ($a_1 = 0$ and $b_3 = 0$)

$$\begin{pmatrix} b_1 \\ a_3 \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Non-zero solution exist provided that the coefficients of the scattering matrix have divergence at certain energies.

In the other words, the localized states have energies at which the amplitudes r and t have poles (singularities of complex-valued function).

Using the relationship

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

we find that the poles of the transmission amplitude corresponds to the condition

$$t = \infty \quad \text{and} \quad 1 - r_1' r_2 = 0.$$

Quantum-well states in potential well: method 3

We proceed with calculation the energy of the localized states for 'particle-in-the-box' using the formalism of transfer matrix.

Under the conditions $a_1 = 0$ и $b_3 = 0$ non-zero solution of the following matrix equation

$$\begin{pmatrix} 0 \\ b_1 \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} a_3 \\ 0 \end{pmatrix}$$

exists provided

$$T_{11} = 0.$$

Since $T_{11} = 1/t$, the conditions $T_{11} = 0$ and $t = \infty$ seem to be equivalent.

Quantum-well states in rectangular potential well

We consider asymmetric 1D potential well of finite height

$$U(z) = \begin{cases} U_1 \text{ at } z < z_1 \\ 0 \text{ at } z_1 < z < z_2 \\ U_3 \text{ at } z_2 < z < z_3 \end{cases}$$

The transmission amplitude for the double-scatter potential is equal (page 5)

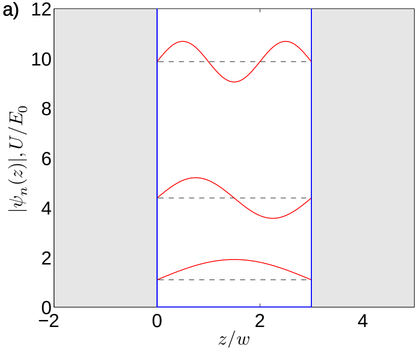
$$t = \frac{4\sqrt{k_1 k_2}\sqrt{k_2 k_3}\, e^{i(k_1-k_3)z_2}\, e^{-ik_2(z_2-z_1)}}{(k_1+k_2)(k_2+k_3)\, e^{-ik_2(z_2-z_1)} + (k_1-k_2)(k_2-k_3)\, e^{ik_2(z_2-z_1)}}.$$

Taking into account that $k_1 = i\varkappa_1$ and $k_3 = i\varkappa_3$ are imaginary values, k_2 is real-valued parameter, $w_2 = z_2 - z_1$ is the width of the potential well, we can find the poles of the transmission amplitude

$$(k_2 + i\varkappa_1)(k_2 + i\varkappa_3)\, e^{-ik_2 w_2} - (k_2 - i\varkappa_1)(k_2 - i\varkappa_3)\, e^{ik_2 w_2} = 0.$$

Since $k_2 \pm i\varkappa_1 = \sqrt{k_2^2 + \varkappa_1^2}\, e^{\pm i\,\mathrm{arctg}(\varkappa_1/k_2)}$ and $k_2 \pm i\varkappa_3 = \sqrt{k_2^2 + \varkappa_3^2}\, e^{\pm i\,\mathrm{arctg}(\varkappa_3/k_2)}$, we arrive at

$$k_2 w_2 = \pi m + \mathrm{arctg}\,\frac{\varkappa_1}{k_2} + \mathrm{arctg}\,\frac{\varkappa_3}{k_2}, \quad \text{where} \quad m = 0,\, 1,\, 2, \ldots$$



Limiting case: rectangular quantum well with infinite barriers ($U_1 \to \infty$ and $U_3 \to \infty$)

Since $\varkappa_1 \to \infty$ and $\varkappa_3 \to \infty$, then $\mathrm{arctg}\, \varkappa_1/k_2 \to \pi/2$ and $\mathrm{arctg}\, \varkappa_3/k_2 \to \pi/2$, therefore

$$k_2 w_2 = \pi m + \mathrm{arctg}\, \frac{\varkappa_1}{k_2} + \mathrm{arctg}\, \frac{\varkappa_3}{k_2} \simeq \pi m + \frac{\pi}{2} + \frac{\pi}{2} = \pi\,(m+1), \qquad m = 0,\, 1,\, 2, \ldots$$

or

$$k_2 w_2 = \pi\, n \quad \Longrightarrow \quad E_n = \frac{\hbar^2 k_n^2}{2m^*} = \frac{\pi^2 \hbar^2 n^2}{2m^* w^2}, \quad \text{where} \quad n = 1,\, 2 \ldots$$

Quantum-well states in parabolic potential well

We can write the potential energy in the form $U(z) = m\omega^2 z^2/2$, where ω is the frequency of oscillations. The stationary Schroedinger can be written as follows

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dz^2} + \frac{m\omega^2 z^2}{2}\psi(z) = E\psi(z).$$

We will find the solution by the method of trial functions.

1. Let us assume that $\psi(z) = A\,e^{-bz^2/2}$, where A and b are fitting parameters. It is easy to see that

$$\frac{d\psi}{dz} = A\,e^{-bz^2/2}\cdot(-bz) \quad \text{and} \quad \frac{d^2\psi}{dz^2} = A\,e^{-bz^2}\cdot(-bz)^2 + A\,e^{-bz^2}\cdot(-b).$$

After substitution we get

$$-\frac{\hbar^2}{2m}A\,e^{-bz^2/2}\,(-bz)^2 + \frac{\hbar^2}{2m}A\,e^{-bz^2/2}\,b + \frac{m\omega^2 z^2}{2}A\,e^{-bz^2/2} = EA\,e^{-bz^2/2}$$

or

$$-\frac{\hbar^2 b^2}{2m}\cdot z^2 + \frac{\hbar^2}{2m}\,b + \frac{m\omega^2}{2}\cdot z^2 = E.$$

In order to exclude z-dependence in the latter equation we have to put $b = m\omega/\hbar$, therefore

$$\psi(z) = A\, e^{-m\omega z^2/(2\hbar)} \quad \Longrightarrow \quad E = \frac{\hbar^2}{2m}\, b = \hbar\omega\, \frac{1}{2}.$$

2. Let us assume that $\psi(z) = A\, z\, e^{-bz^2}$, where A and b are fitting parameters. Repeating all calculations, we get

$$\psi(z) = A\, z\, e^{-m\omega z^2/(2\hbar)} \quad \Longrightarrow \quad E = \hbar\omega\, \frac{3}{2}.$$

3. Finally, we come to the conclusion that

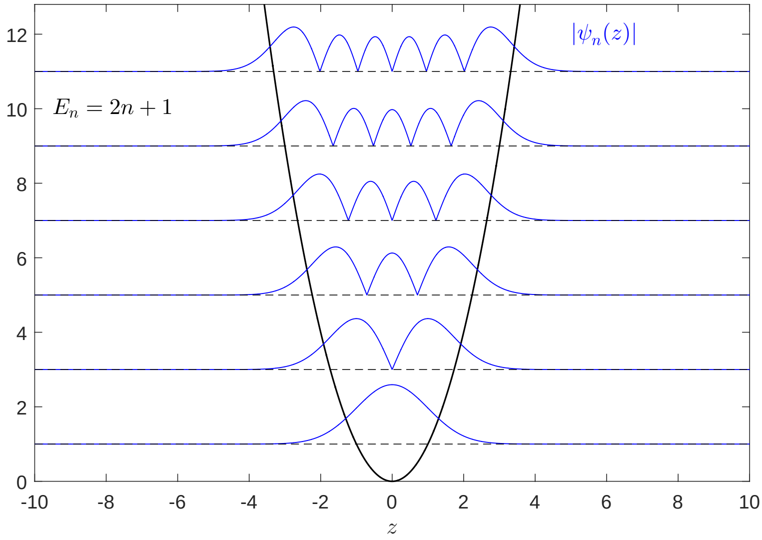
$$\psi(z) = A\, H_n\left(\sqrt{\frac{m\omega}{\hbar}} z\right)\, e^{-m\omega z^2/(2\hbar)} \quad \Longrightarrow \quad E = \hbar\omega\, \left(n + \frac{1}{2}\right), \quad n = 0, 1, \ldots$$

where $H_n(z)$ are the Hermite's polynoms of the n-order:
$H_0(z) = 1,\ H_1(z) = 2z,\ H_2(z) = 4z^2 - 2,\ H_3(z) = 8z^3 - 12z$ etc

Main conclusion: the energy spectrum for a particle in the parabolic potential well is equidistant!

Alternatively, you may solve the Schroedinger equation using special mathematical functions and prove this solution.

Quantum-well states in parabolic potential well: numerical simulations



Landau problem for the electron in uniform magnetic field*

see lectures of Prof. Irina Bobkova on magnetism

The stationary Schroedinger equation for the electron in uniform magnetic field described by the vector potential $\boldsymbol{A}$ has the form

$$\left\{ \frac{1}{2m} \left(\hat{\boldsymbol{p}} - \frac{e}{c} \boldsymbol{A}(\boldsymbol{r}) \right)^2 - \hat{\boldsymbol{\mu}} \boldsymbol{B}(\boldsymbol{r}) + e\varphi(\boldsymbol{r}) \right\} \psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}),$$

where $\hat{\boldsymbol{\mu}}$ is magnetic moment and $\psi(\boldsymbol{r})$ is local electrical potential. For simplicity take $\varphi(\boldsymbol{r}) = 0$.

Uniform magnetic field $\boldsymbol{B} = B\boldsymbol{e}_z$ corrsponds to linearly increasing vector potential. Assume

$$A_x(\boldsymbol{r}) = -B \cdot y, \quad A_y(\boldsymbol{r}) = 0 \quad and \quad A_z(\boldsymbol{r}) = 0,$$

then the Schroedinger equation can be rewritten in the following form

$$\frac{1}{2m} \left(\hat{p}_x + \frac{e}{c} By \right)^2 \psi(\boldsymbol{r}) + \frac{\hat{p}_y^2}{2m} \psi(\boldsymbol{r}) + \frac{\hat{p}_z^2}{2m} \psi(\boldsymbol{r}) - \hat{\mu} B \psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}).$$

Due to the symmetry of the problem, we can find the solution in the form

$$\psi(x, y, z) = e^{i(p_x x + p_z z)/\hbar} \cdot \xi(y),$$

corresponding to the conservation of x- and z-components of momentum.

For the auxiliary function $\chi(y)$ there is a simpler equation, which coincides with the eigenvalue problem for a particle in the parabolic potential well

$$-\frac{\hbar^2}{2m}\frac{d^2\chi}{dy^2} + \frac{m\omega^2}{2}(y - y_0)^2 = E'\chi(y),$$

where

$$y_0 = -\frac{cp_x}{eB}, \quad \omega = \frac{eB}{mc} \quad \text{and} \quad E' = E + \frac{\mu}{s}\sigma B - \frac{p_z^2}{2m}.$$

Based on the considered solution for the particle in the parabolic potential well, we automatically conclude that

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

therefore the full energy is equal to

$$E = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{\mu}{s}\sigma B + \frac{p_z^2}{2m}, \quad n = 0, 1, \ldots$$

The fact that E is independent of y_0 (or p_x) means that there is degeneracy of all localized states (so-called Landau levels) of infinite order.

Research project 2: particle-in-the-box problem

We can write the Schrödinger equation in the dimensionless form:

$$-\frac{d^2}{dz^2}\psi(z) + U(z)\psi(z) = E\psi(z), \qquad (*)$$

If we introduce an equidistant grid $(z_1, z_2, \ldots, z_N)$, then the problem (*) can be rewritten in the form of finite-difference equation

$$-\frac{\psi_{n-1} - 2\psi_n + \psi_{n+1}}{\Delta_z^2} + U_n\psi_n = E\psi_n, , \qquad (**)$$

where $\psi_n = \psi(z_n)$, $U_n = U(z_n)$, and $\Delta_z = z_{n+1} - z_n$ is the interval between neighbour points.

The eigenvalue problem (**) can be formulated in the matrix form

$$\hat{L}\begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_N\end{pmatrix} = E\begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_N\end{pmatrix},$$

where $\hat{L}$ is square matrix (size $N \times N$), and $(\psi_1, \ldots \psi_N)$ is the vector to be determined.

The matrix of the finite difference problem $\hat{L} = \hat{L}_1 + \hat{L}_2$ is a combination of three-diagonal matrix

$$\hat{L}_1 = \begin{pmatrix} A/\Delta_z^2 & -1/\Delta_z^2 & 0 & \dots & \dots \\ -1/\Delta_z^2 & 2/\Delta_z^2 & -1/\Delta_z^2 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & 0 & -1/\Delta_z^2 & 2/\Delta_z^2 & -1/\Delta_z^2 \\ \dots & \dots & 0 & -1/\Delta_z^2 & B/\Delta_z^2 \end{pmatrix},$$

and single-diagonal matrix

$$\hat{L}_2 = \begin{pmatrix} U_1 & 0 & \dots & \dots & \dots \\ 0 & U_2 & 0 & \dots & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & \dots & 0 & U_{N-1} & 0 \\ \dots & \dots & \dots & 0 & U_N \end{pmatrix}.$$

Constants A and B depend on considered boundary conditions:

$A = 1$ and $B = 1$ for zero-gradient boundary condition ($\psi' = 0$ at end points),

$A = 2$ and $B = 2$ for zero boundary condition ($\psi = 0$ at end points).

Strategy: we have to diagonalize the matrix $\hat{L}$, thus we get the set of the eigenvalues E_m and the eigenfunctions ψ_m.

Matlab built-in function: $[eigenfunctions, eigenvalues] = \texttt{eig}(L)$,
where *eigenfunctions* and *eigenvalues* are $N \times N$ matrices.

Python built-in function (import packages numpy and numpy.linalg):

$$eigenvalues, eigenfunctions = \texttt{numpy.linalg.eig}(L),$$

where *eigenfunctions* is $N \times N$ matrix, while *eigenvalues* is N-element vector.

Potential problems for analysis:

1. Calculate the energy spectrum for double-parabolic well $U(z) = (|z| - z_0)^2$. Using the calculated dependence $E_0(z_0)$, consider the appearance of bulk and surface superconductivity.

2. Calculate the energy spectrum for a particle localized in rectangular potential well. Analyze the dependence of the error on the grid size and the number of the quantum level.

3. Find the energy spectrum for a particle localized in triangular and semi-triangular potential wells numerically and analytically using Bohr-Sommerfeld quantization rule.

4. Calculate energy spectrum and wave functions for a particle localized in a cylindrical quantum well.

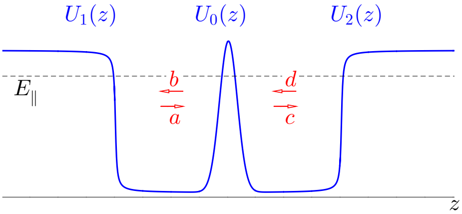
5. Calculate the energy spectrum for a particle localized near the edge of the semi-infinite periodic potential.

6. Calculate the energy spectrum for a particle localized near metallic surface taking into account the Coulomb-like image potential.

Quantum-well states in coupled potential wells*

We would like to calculate the energy spectrum for a particle localized in the coupled potential wells.

We use a formalism of scattering matrix



Scattering at the left and right edges of the complex potential well:

$$a = r_1' \, b \quad \text{and} \quad d = r_2 \, c.$$

These two equations can be rewritten in the form of a matrix equation for the effective states

$$\begin{pmatrix} a \\ d \end{pmatrix} = \begin{pmatrix} r_1' & 0 \\ 0 & r_2 \end{pmatrix} \begin{pmatrix} b \\ c \end{pmatrix} = \hat{S}_{eff} \begin{pmatrix} b \\ c \end{pmatrix}, \qquad \text{where} \qquad \hat{S}_{eff} = \begin{pmatrix} r_1' & 0 \\ 0 & r_2 \end{pmatrix}$$

Scattering at the central (separating) barrier $\hat{S}_0$

$$\begin{pmatrix} b \\ c \end{pmatrix} = \begin{pmatrix} r_0 & t_0' \\ t_0 & r_0' \end{pmatrix} \begin{pmatrix} a \\ d \end{pmatrix} = \hat{S}_0 \begin{pmatrix} a \\ d \end{pmatrix}$$

By merging two matrix equations, we get

$$\begin{pmatrix} a \\ d \end{pmatrix} = \hat{S}_{eff} \begin{pmatrix} b \\ c \end{pmatrix} = \hat{S}_{eff} \hat{S}_0 \begin{pmatrix} a \\ d \end{pmatrix} \quad \text{or} \quad \left(\hat{S}_{eff} \hat{S}_0 - 1 \right) \begin{pmatrix} a \\ d \end{pmatrix} = 0.$$

The criterion of the existence of nontrivial solution: $det \, (\hat{S}_{eff} \hat{S}_0 - \hat{1}) = 0$.

To get further, we assume that the potential is symmetric $[U(z) = U(-z)]$, therefore $r_0 = r_0'$, $t_0 = t_0'$ and

$$\hat{S}_0 = \begin{pmatrix} \sqrt{1-\mathcal{T}_0} \; e^{i \arg r_0} & \sqrt{\mathcal{T}_0} \; e^{i\pi/2 + i \arg r_0} \\ \sqrt{\mathcal{T}_0} \; e^{i\pi/2 + i \arg r_0} & \sqrt{1-\mathcal{T}_0} \; e^{i \arg r_0} \end{pmatrix} = e^{i \arg r_0} \begin{pmatrix} \sqrt{1-\mathcal{T}_0} & i\sqrt{\mathcal{T}_0} \\ i\sqrt{\mathcal{T}_0} & \sqrt{1-\mathcal{T}_0} \end{pmatrix},$$

where $\mathcal{T}_0$ is the transmission coefficient through the cental barrier. Due to the inversion symmetry $r_1' = 1 \cdot e^{i \, arg \, r}$ and $r_2 = 1 \cdot e^{i \, arg \, r}$, therefore

$$\hat{S}_{eff} = e^{i \arg r} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Since

$$\hat{S}_{eff}\,\hat{S}_0 - \hat{1} = \begin{pmatrix} e^{i\arg r + i\arg r_0}\sqrt{1-\mathcal{T}_0} - 1 & e^{i\arg r + i\arg r_0}\, i\sqrt{\mathcal{T}_0} \\ e^{i\arg r + i\arg r_0}\, i\sqrt{\mathcal{T}_0} & e^{i\arg r + i\arg r_0}\sqrt{1-\mathcal{T}_0} - 1 \end{pmatrix},$$

the criterion $\det\left(\hat{S}_{eff}\cdot\hat{S}_0 - \hat{1}\right) = 0$ is equivalent to the condition

$$\left(e^{i\arg r + i\arg r_0}\sqrt{1-\mathcal{T}_0} - 1\right)^2 - \left(e^{i\arg r + i\arg r_0}\, i\sqrt{\mathcal{T}_0}\right)^2 = 0 \quad \text{или}$$

$$e^{-i\arg r - i\arg r_0} = \sqrt{1-\mathcal{T}_0} \pm i\sqrt{\mathcal{T}_0}.$$

Taking into account that $\sqrt{1-\mathcal{T}_0} \pm i\sqrt{\mathcal{T}_0} = e^{\pm i\,\mathrm{arctg}\left(\sqrt{\mathcal{T}_0}/\sqrt{1-\mathcal{T}_0}\right)}$, we get

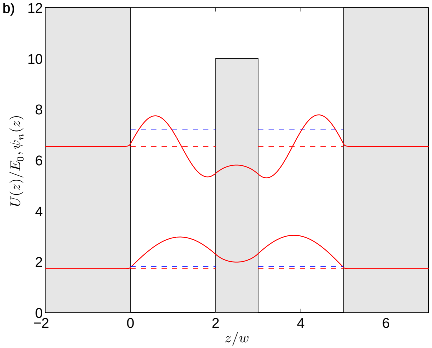
$$\arg r + \arg r_0 = 2\pi n \pm \mathrm{arctg}\,\frac{\sqrt{\mathcal{T}_0}}{\sqrt{1-\mathcal{T}_0}} \simeq 2\pi n \pm \sqrt{\mathcal{T}_0} \quad \text{при} \quad \mathcal{T}_0 \ll 1.$$

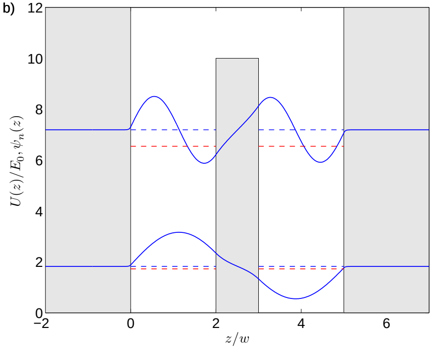
Expending this sum into a Taylor series

$$\arg r + \arg r_0 \simeq \left(\arg r^{(0)} + \arg r_0^{(0)}\right) + \frac{d}{dE}\left(\arg r^{(0)} + \arg r_0^{(0)}\right)_{E=E_n^{(0)}} \cdot \left(E - E_n^{(0)}\right),$$

we get the following estimate for energy of quantum-well states

$$E \simeq E_n^{(0)} \pm \delta E_n, \quad \text{где} \quad \delta E_n = \sqrt{\mathcal{T}_0}\Big|_{E=E_n^{(0)}} \left\{\frac{d}{dE}\left(\arg r^{(0)} + \arg r_0^{(0)}\right)_{E=E_n^{(0)}}\right\}^{-1}.$$





The deeper the non-perturbed energy levels, the smaller the energy splitting is, and vice versa.

Important to note that there are symmetrical and antisymmetrical solutions, describing the localization of a particle in coupled potential wells simultaneously.

Simple estimate of tunneling rate

We consider two potential wells of the same shape. Let $\psi_n^{(0)}(z)$ be the non-perturbed wave function corresponding to the $n-$th energy level of a particle in the right potential well without taking into account tunneling between the potential wells.

In the limit of low-transparency separating barrier ($\mathcal{T}_0 \ll 1$), the wave functions of a particle at the $n-$th level in the coupled potential wells can be viewed as symmetric and antisymmetric combinations of non-perturbed wave functions $\psi_n^{(0)}(z)$ for the right well and $\psi_n^{(0)}(-z)$ for the left well.

Let $\psi_{sym}(z)$ be the symmetric solution corresponding to the ground state of a particle in double-well potential with energy $E = E_0 - \delta E_0$

$$\psi_{sym}(z) = \psi_0^{(0)}(z) + \psi_0^{(0)}(-z) \quad \text{and} \quad \Psi_{sym}(z,t) = \left[\psi_0^{(0)}(z) + \psi_0^{(0)}(-z)\right] \cdot e^{-i(E_0 - \delta E_0)t/\hbar},$$

where E_0 is the ground energy for isolated potential well.

Let $\psi_{asym}(z)$ be the asymmetric solution corresponding to the first excited state of a particle in double-well potential with energy $E = E_0 + \delta E_0$

$$\psi_{asym}(z) = \psi_0^{(0)}(z) - \psi_0^{(0)}(-z) \quad \text{and} \quad \Psi_{asym}(z,t) = \left[\psi_0^{(0)}(z) - \psi_0^{(0)}(-z)\right] \cdot e^{-i(E_0 + \delta E_0)t/\hbar}.$$

We emphasize that the wave functions $\Psi_{sym}(z,t)$ and $\Psi_{asym}(z,t)$ are stationary solutions and they describe the localization of a particle in two potential wells simultaneously.

In order to estimate the tunneling rate without considering the time-dependent Schrödinger equation, we compose a linear combination of stationary wave functions $\Psi_{sym}(z,t)$ and $\Psi_{asym}(z,t)$ in such a way to describe the localization of a particle at the right potential well at $t=0$

$$\Psi(z,t) = \frac{1}{2}\left\{\Psi_{sym}(z,t) + \Psi_{asym}(z,t)\right\} =$$
$$= e^{-iE_0 t/\hbar}\,\frac{1}{2}\left\{\psi_0^{(0)}(z)\,\left(e^{i\delta E_0 t/\hbar} + e^{-i\delta E_0 t/\hbar}\right) + \psi_0^{(0)}(-z)\,\left(e^{i\delta E_0 t/\hbar} - e^{-i\delta E_0 t/\hbar}\right)\right\}.$$

Using trigonometric formulas we rewrite this relation as follows

$$\Psi(z,t) = e^{-iE_0 t/\hbar}\left\{\psi_0^{(0)}(z)\,\cos\left(\frac{\delta E_0\, t}{\hbar}\right) + i\,\psi_0^{(0)}(-z)\,\sin\left(\frac{\delta E_0\, t}{\hbar}\right)\right\}.$$

If the particle at $t=0$ was located in the right well, then it will be at the left well after time interval $\pi\hbar/(2\delta E_0)$. Such changes are periodic in time.

Typical frequency of a particle relocation between wells can be estimated as

$$\omega = \frac{\delta E_0}{\hbar} \propto \sqrt{\mathcal{T}_0}.$$

The tunneling speed depends exponentially on the transparency of the barrier: the lower the level of the localized state in the potential well, the lower the frequency of oscillations.

Part 2: Quasiclassical approximation. Boundary conditions

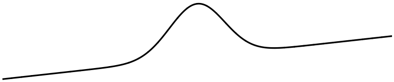
Reasons to study quasiclassical approximation

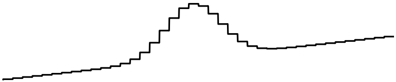
- Scattering problem in an inhomogeneous potential of arbitrary shape does not have an universal analytical solution unlike from piecewise potential.
- Exact analytical solutions for a piecewise potential seem to be useless for describing real systems. For example, according to the Ohm's law the electric potential should be linearly increasing function for systems with constant current

$$\boldsymbol{j} = -\sigma \nabla \varphi \quad \Longrightarrow \quad \varphi(z) = -\frac{j_z}{\sigma} \cdot z.$$

  This circumstance prevents the decomposition of the complicated potential into the sum of localized scatters.

- The transition from smooth potentials to a piecewise functions allows us to solve scattering problems numerically using transfer-matrix approach (research project 1). However, such the discretization could lead to unphysical oscillations of the reflection and transmission coefficients as a function of energy.





Wentzel-Kramer-Brillouin (WKB) approximation

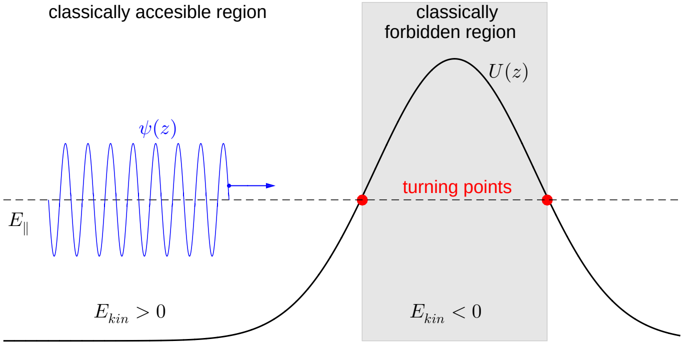
We consider one-dimensional stationary Schrödinger equation

$$-\frac{\hbar^2}{2m^*}\,\frac{d^2\psi}{dz^2} + U(z)\,\psi = E_{\parallel}\psi,$$

which is a second-order linear differential equation with variable coefficients.

Such equation has no universal analytical solution.

Terminology:



After the change of variables $\psi(z) = \exp(iS(z)/\hbar)$ in the Schrödinger equation

$$-\frac{\hbar^2}{2m^*}\,\frac{d^2\psi}{dz^2} + U(z)\,\psi = E_{\parallel}\psi,$$

we get a new differential equation for unknown function $S(z)$ (also known as an eikonal)

$$\frac{1}{2m^*}\left(\frac{dS}{dz}\right)^2 - \frac{i\hbar}{2m^*}\left(\frac{d^2S}{dz^2}\right) = E_{\parallel} - U(z).$$

Assuming that the quantum system under consideration is close to classical one, we will look for a solution in the form of a series in powers of $\hbar$, formally considering $\hbar$ as a small parameter:

$$S(z) = S_0(z) + \frac{\hbar}{i}\,S_1(z) + \left(\frac{\hbar}{i}\right)^2\,S_2(z) + \ldots$$

In the zeroth order of the perturbation theory we obtain

$$\frac{1}{2m^*}\left(\frac{dS_0}{dz}\right)^2 = E_{\parallel} - U(z) \quad \Longrightarrow \quad \frac{dS_0}{dz} = \pm\,p(z), \quad \text{where} \quad p(z) = \sqrt{2m^*(E_{\parallel} - U(z))}.$$

The zeroth order equation $dS_0/dz = \pm\,p(z)$ can be easily integrated

$$S_0(z) = \pm\int p(z)\,dz.$$

In the first order of the perturbation theory we obtain

$$\frac{dS_0}{dz}\frac{dS_1}{dz}+\frac{1}{2}\frac{d^2S_0}{dz^2}=0 \quad \Longrightarrow \quad \frac{dS_1}{dz}=-\frac{1}{2}\,\frac{S_0''}{S_0'}=-\frac{1}{2}\,\frac{p'(z)}{p(z)}.$$

By integrating the latter equation, we get

$$S_1(z)=-\frac{1}{2}\int\frac{p'(z)}{p(z)}\,dz=-\frac{1}{2}\,\ln p(z)=-\ln\sqrt{p(z)}.$$

Thus, we come to the following expressions for the eikonal

$$S(z)=S_0(z)+\frac{\hbar}{i}\,S_1(z)=\pm\int p(z)\,dz+i\hbar\,\ln\sqrt{p(z)}$$

and for the set of linearly independent solutions of the Schrödinger equation

$$\psi(z)=\exp\left(\frac{i}{\hbar}S(z)\right)=\exp\left(\frac{i}{\hbar}S_0(z)\right)\cdot\exp\left(\frac{i}{\hbar}\,\frac{\hbar}{i}\,S_1(z)\right)=$$

$$=\frac{1}{\sqrt{p(z)}}\,\exp\left(\pm\frac{i}{\hbar}\int p(z)dz\right).$$

It is important to consider two cases.

1. If $E_{\|} > U(z)$ in a certain region, then the classical momentum $p(z) = \sqrt{2m^*(E_{\|} - U(z))}$ is real-valued function of the z-coordinate. This region can be called as classically allowed area. In this area the first-order WKB-approximation is a linear combination of the two nonuniform travelling electronic waves:

$$\psi(z) = \frac{C_1}{\sqrt{p(z)}} \exp\left(\frac{i}{\hbar}\int p(z)dz\right) + \frac{C_2}{\sqrt{p(z)}} \exp\left(-\frac{i}{\hbar}\int p(z)dz\right),$$

where C_1 and C_2 are constants.

2. If $E_{\|} < U(z)$ in a certain region, then the classical momentum becomes complex-valued function of the z-coordinate: $p(z) = i|p(z)|$. This region can be called as classically forbidden area. In this area the first-order WKB-approximation is a linear combination of the two exponentially decaying functions:

$$\psi(z) = \frac{C_1'}{\sqrt{|p(z)|}} \exp\left(\frac{1}{\hbar}\int |p(z)|dz\right) + \frac{C_2'}{\sqrt{|p(z)|}} \exp\left(-\frac{1}{\hbar}\int |p(z)|dz\right),$$

where C_1' and C_2' are constants.

The main problem is how to determine the coefficients C_1, C_2, C_1', and C_2'.

Criterion of applicability of the quasiclassical expressions

Zeroth order of perturbation theory:

$$\psi(z) = const \cdot \exp\left(\pm\frac{i}{\hbar}\int p(z)dz\right).$$

Zeroth and first orders of perturbation theory:

$$\psi(z) = \frac{const}{\sqrt{p(z)}} \cdot \exp\left(\pm\frac{i}{\hbar}\int p(z)dz\right).$$

Zeroth, first and second orders of perturbation theory:

$$\psi(z) = \frac{const}{\sqrt{p(z)}} \cdot \left\{1 - \frac{i\hbar m^*}{4}\frac{F(z)}{p^3(z)} - \frac{i\hbar m^{*2}}{8}\int\frac{F^2(z)}{p^5(z)}dz\right\} \cdot \exp\left(\pm\frac{i}{\hbar}\int p(z)\,dz\right),$$

where $F(z) = -dU/dz$ is classical force acting on a quantum particle.

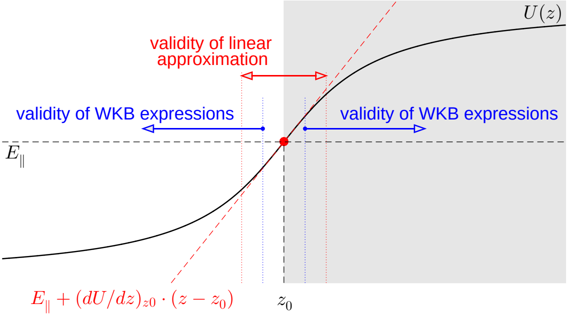
Criterion of applicability: accounting of the higher-order terms is excessive provided that

$$\left|m^*\hbar\,\frac{F(z)}{p^3(z)}\right| \ll 1 \qquad \text{or} \qquad \left|\frac{1}{2\pi}\frac{d\lambda}{dz}\right| \ll 1.$$

This means that the quasiclassical expression are not valid near the turning points, where $E_{||} = U(z)$ and the classical momentum of the particle $p(z)$ is close to zero.

Matching quasiclassical expressions near turning point (1)

We compare the WKB approximate solutions in classically accessible and forbidden regions with the exact solution:



Near the turning point $z = z_0$ the potential energy $U(z)$ can be linearized

$$U(z) \simeq E_\| + \left(\frac{dU}{dz}\right)_{z_0} (z - z_0).$$

The Schrödinger equation near this point can be written in the form of Airy equation

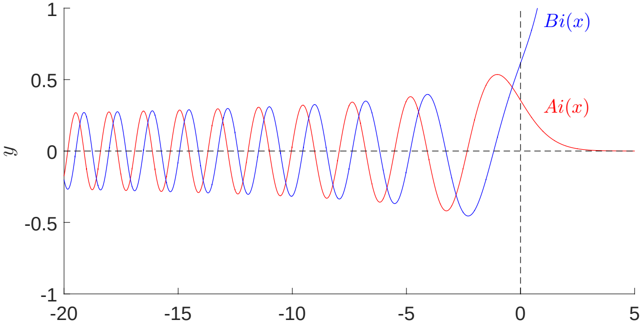
$$\frac{d^2\psi}{dz^2} + \frac{2m^*}{\hbar^2}\left(E_\| - U(z)\right)\psi = 0 \quad \Longrightarrow \quad \frac{d^2\psi}{d\xi^2} - \xi \cdot \psi = 0, \quad \xi = (z - z_0)\sqrt[3]{\frac{2m^*}{\hbar^2}\left|\frac{dU}{dz}\right|_{z_0}}.$$

Model Airy equation $\psi'' - \xi \cdot \psi = 0$ has two independent solutions $Ai(\xi)$ and $Bi(\xi)$ with the following asymptotes

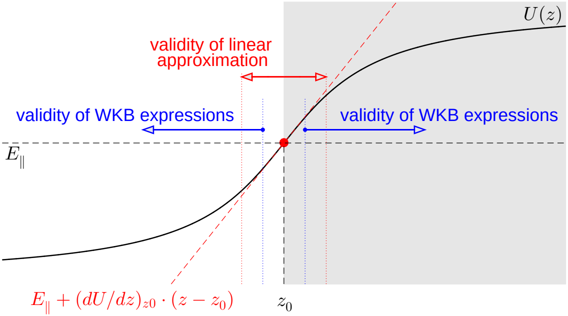
$$Ai(\xi) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{u^3}{3} + u\xi\right) du = \frac{1}{\sqrt{\pi}|\xi|^{1/4}} \times \begin{cases} \exp\left(-2\xi^{3/2}/3\right) / 2 & \text{at } \xi \to +\infty, \\ \sin\left(-2\xi^{3/2}/3 + \pi/4\right) & \text{at } \xi \to -\infty; \end{cases}$$

$$Bi(\xi) = \frac{1}{\pi} \int_0^\infty \left\{ \exp\left(-\frac{u^3}{3} + u\xi\right) + \sin\left(\frac{u^3}{3} + u\xi\right) \right\} du =$$

$$= \frac{1}{\sqrt{\pi}|\xi|^{1/4}} \times \begin{cases} \exp\left(2\xi^{3/2}/3\right) & \text{at } \xi \to +\infty, \\ \cos\left(-2\xi^{3/2}/3 + \pi/4\right) & \text{at } \xi \to -\infty. \end{cases}$$



To be specific, we consider the case when the forbidden region is to the right of the turning point, and the allowed region is to the left:



In this case the solution of the Schroedinger within the region with the linear approximation should be $Ai(\xi)$ function.

The correspondence rule for asymptotes of the $Ai(\xi)$ function

$$\frac{1}{2} \cdot \frac{1}{\sqrt{\pi}|\xi|^{1/4}} \exp\left(-\frac{2}{3}\,\xi^{3/2}\right) \quad \text{at} \quad \xi \to +\infty \quad \Longrightarrow$$

$$1 \cdot \frac{1}{\sqrt{\pi}|\xi|^{1/4}} \sin\left(-\frac{2}{3}\,\xi^{3/2} + \frac{\pi}{4}\right) \quad \text{at} \quad \xi \to -\infty.$$

WKB solution to the right of the turning point in the classically forbidden region in the domain of applicability of the linear approximation is

$$\psi_{II}(z) = \frac{C_2'}{\sqrt{|p(z)|}} \exp\left(-\frac{1}{\hbar}\int_{z_0}^{z} |p(z)|dz\right) = \left(2m^*\hbar\left(\frac{dU}{dz}\right)_{z_0}\right)^{-1/6} \frac{C_2'}{\xi^{1/4}} \exp\left(-\frac{2}{3}\,\xi^{3/2}\right).$$

WKB solution to the left of the turning point in the classically accessible region in the domain of applicability of the linear approximation is

$$\psi_I(z) = \frac{C_1}{\sqrt{p(z)}} \exp\left(\frac{i}{\hbar}\int_{z_0}^{z} p(z)\,dz\right) + \frac{C_2}{\sqrt{p(z)}} \exp\left(-\frac{i}{\hbar}\int_{z_0}^{z} p(x)\,dx\right) =$$

$$= \left(2m^*\hbar\left(\frac{dU}{dz}\right)_{z_0}\right)^{-1/6} \left\{\frac{C_1}{|\xi|^{1/4}} \exp\left(-\frac{2}{3}\,i\,|\xi|^{3/2}\right) + \frac{C_2}{|\xi|^{1/4}} \exp\left(\frac{2}{3}\,i\,|\xi|^{3/2}\right)\right\}.$$

In order the expression $\psi_I(z)$ has the form of standing wave $\sin\left(-2\xi^{3/2}/3 + \pi/4\right)$ and thus coincides with asymptotic expression for the Airy function at $\xi \to -\infty$, we need to assume $C_1 = -C_0\, e^{-i\pi/4}/(2i)$ and $C_2 = C_0\, e^{i\pi/4}/(2i)$. As a result, we get

$$\psi_I(z) = \left(2m^*\hbar\left(\frac{dU}{dz}\right)_{z_0}\right)^{-1/6} \frac{C_0}{|\xi|^{1/4}} \sin\left(-\frac{2}{3}\xi^{3/2} + \frac{\pi}{4}\right).$$

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

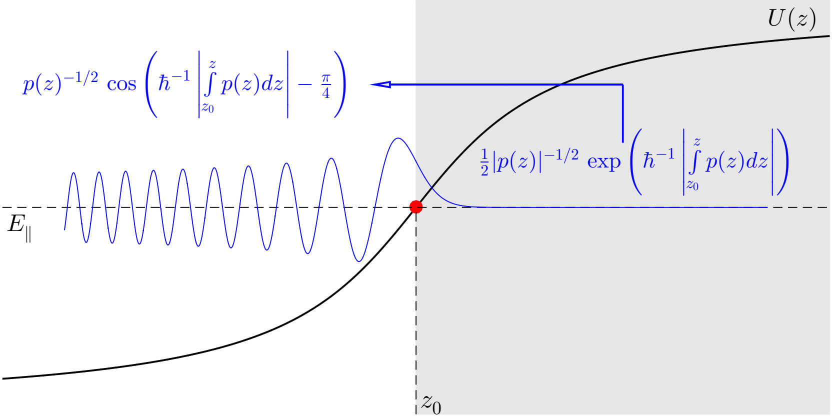
$$\frac{1}{2}\,\frac{1}{\sqrt{|p(z)|}}\,\exp\left\{-\frac{1}{\hbar}\int\limits_{z_0}^{z}|p(z)|\,dz\right\} \quad \text{at} \quad E_\parallel < U(z) \quad \Longrightarrow$$

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

The correspondence rule can be written in the form regardless on the particular location of the forbidden region (to the left of to the right from the turning point)

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

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

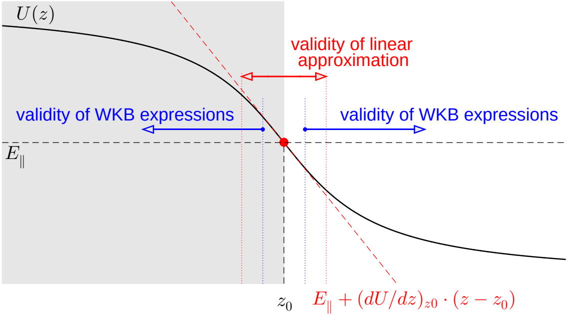


Reminder: the sign of the absolute value is defined as follows

$$|a| = \begin{cases} a & \text{if } a > 0, \\ -a & \text{if } a < 0, \end{cases}$$

Matching quasiclassical expressions near turning point (2)

Now we consider the case when the forbidden region is to the left of the turning point, and the allowed region is to the right:



We assume that there is a solution in the form of nonuniform travelling wave in the classically accessible region ($z > z_0$ and $\xi > 0$). Such the solution corresponds to a linear combination of the Airy functions $Ai(-\xi)$ and $Bi(-\xi)$

$$i\,Ai(-\xi) + Bi(-\xi) = \frac{1}{\sqrt{\pi}|\xi|^{1/4}} \times \begin{cases} \exp\left(-2\xi^{3/2}/3\right) & \text{at } \xi \to -\infty, \\ \exp\left(2i\,\xi^{3/2}/3 + i\pi/4\right) & \text{at } \xi \to +\infty. \end{cases}$$

In the other words,

$$\frac{1}{\sqrt{\pi}|\xi|^{1/4}}\,\exp\left(i\frac{2}{3}\,\xi^{3/2}+i\frac{\pi}{4}\right)\quad \text{at}\quad \xi\to+\infty \quad\Longrightarrow$$

$$\frac{1}{\sqrt{\pi}|\xi|^{1/4}}\,\exp\left(-\frac{2}{3}\,\xi^{3/2}\right)\quad \text{at}\quad \xi\to-\infty.$$

Quasiclassical solution in classically accessible region in the domain of applicability of the linear approximation is

$$\psi_{II}(z)=\frac{C_1}{\sqrt{p(z)}}\,\exp\left\{\frac{i}{\hbar}\int\limits_{z_0}^{z}p(z)\,dz+i\frac{\pi}{4}\right\}=$$

$$=\left(2m^*\hbar\left(\frac{dU}{dz}\right)_{z_0}\right)^{-1/6}\,\frac{C_1}{\xi^{1/4}}\,\exp\left(\frac{2}{3}\,i\,\xi^{3/2}+i\frac{\pi}{4}\right),$$

where the phase shift $\pi/4$ is introduced for convenience.

Quasiclassical solution in classically forbidden region is

$$\psi_I(z)=\frac{C_2'}{\sqrt{|p(z)|}}\,\exp\left(-\frac{1}{\hbar}\int\limits_{z_0}^{z}|p(x)|\,dx\right)\simeq\left(2m^*\hbar\left(\frac{dU}{dz}\right)_{z_0}\right)^{-1/6}\,\frac{C_2'}{|\xi|^{1/4}}\,\exp\left(-\frac{2}{3}\,\xi^{3/2}\right)$$

Correspondence rule between travelling wave and decaying solution

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

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