

## STM Physical Backgrounds

### Tunneling Effect

The idea of particles tunneling appeared almost simultaneously with quantum mechanics. In **classical mechanics**, to describe a system of material points at a certain moment of time, it is enough to set every point coordinates and momentum components. In **quantum mechanics** it is in principle impossible to determine simultaneously coordinates and momentum components of even single point according to the Heisenberg uncertainty principle. To describe the system completely, an associated complex function is introduced in quantum mechanics (**the wavefunction**). The wavefunction  $\Psi$ , which is a function of time and all system particles position, is a solution of the wave Schrodinger equation. In order to use the system wavefunction, one should determine  $|\Psi|^2$  rather than  $\Psi$ . Then, the probability for finding particles in an elementary volume  $dx dy dz$  is given by  $|\Psi|^2 dx dy dz$ .

If particles impinge on a potential barrier of a limited width, the quantum mechanics predicts the effect of particles penetration through the potential barrier even if particle total energy is less than the barrier height which is unknown in classical physics.

Lets calculate the transparency of the rectangular barrier [1], [2]. Suppose that electrons of potential energy

$$U(z) = \begin{cases} 0, & \text{npu } z < 0; \\ U_0 \text{ npu } 0 \leq z \leq L; \\ 0, & \text{npu } z > L \end{cases} \quad (1)$$

impinge on the rectangular potential barrier and the total energy  $E$  is less than  $U_0$  (Fig. 1).

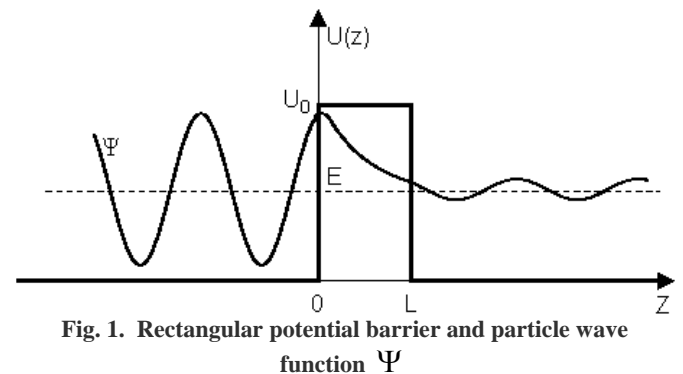


Fig. 1. Rectangular potential barrier and particle wave function  $\Psi$

The stationary Schrodinger equations can be written as follows

$$\begin{cases} \ddot{\Psi} + \kappa_1^2 \Psi = 0, & \text{npu } z < 0; \\ \ddot{\Psi} - \kappa_2^2 \Psi = 0, & \text{npu } z \in [0; L]; \\ \ddot{\Psi} + \kappa_1^2 \Psi = 0, & \text{npu } z > L \end{cases} \quad (2)$$

where  $\kappa_1 = \frac{\sqrt{2mE}}{\hbar}$ ,  $\kappa_2 = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$  – wave vectors,  $\hbar = 1,05 \cdot 10^{-34} \text{ Дж} \cdot \text{с} \cdot \text{с}$  – Planck's constant. The solution to the wave equation at  $z < 0$  can be expressed as a sum of incident and reflected waves  $\Psi = \exp(ik_1 z) + a \exp(-ik_1 z)$ , while solution at  $z > L$  – as a transmitted wave  $\Psi = b \exp(ik_1 z)$ . A general solution inside the potential barrier  $0 < z < L$  is written as  $\Psi = c \exp(k_2 z) + d \exp(-k_2 z)$ . Constants  $a$ ,  $b$ ,  $c$ ,  $d$  are determined from the wavefunction  $\Psi$  and  $\dot{\Psi}$  continuity condition at  $z = 0$  and  $z = L$ .

The barrier transmission coefficient can be naturally considered as a ratio of the transmitted electrons probability flux density to that one of the incident electrons. In the case under consideration this ratio

is just equal to the squared wavefunction module at  $z > L$  because the incident wave amplitude is assumed to be 1 and wave vectors of both incident and transmitted waves coincide.

$$D = bb^* = \left( ch^2(k_2L) + \frac{1}{4} \left( \frac{k_2}{k_1} - \frac{k_1}{k_2} \right)^2 sh^2(k_2L) \right)^{-1} \quad (3)$$

If  $k_2L \gg 1$ , then both  $ch(k_2L)$  and  $sh(k_2L)$  can be approximated to  $\exp(k_2L)/2$  and (3) will be written as

$$D(E) = D_0 \exp \left\{ -\frac{2L}{\hbar} \sqrt{2m(U_0 - E)} \right\} \quad (4)$$

where 
$$D_0 = 4 \left[ 1 + \frac{1}{4} \left( \frac{k_2}{k_1} - \frac{k_1}{k_2} \right)^2 \right]^{-1}.$$

Thus, analytical calculation of the rectangular barrier transmission coefficient is rather a simple task. However, in many quantum mechanical problems it is necessary to find the transmission coefficient of the more complicated shape barrier. In this case, there is no common analytical solution for the  $D$  coefficient. Nevertheless, if the problem parameters satisfy the quasiclassical condition, the transmission coefficient can be calculated in a general form. (see chapter [Tunneling Effect in Quasiclassical Approximation](#)).

#### Summary

- In quantum mechanics tunneling effect is particles penetration through the potential barrier even if particle total energy is less than the barrier height.
- To calculate the transparency of the potential barrier, one should solve Shrodinger equation at continuity condition of wavefunction and its first derivative.
- The transparency coefficient of the rectangular barrier decreases exponentially with the barrier width, when wave vectors of both incident and transmitted waves coincide.

#### References

1. Sivuhin D.V. A General course of physics. Nauka, volume 5, chapter 1, 1988 (In Russian)
2. Goldin L.L., Novikova H.I. The introduction in quantum physics. Nauka, 1988 (In Russian).

#### Tunneling Effect in Quasiclassical Approximation

The quasiclassical qualitative condition imply that de Broglie wavelength of the particle  $\lambda$  is less than characteristic length  $L$  determining the conditions of the problem. This condition means that the particle wavelength should not change considerably within the length of the wavelength order

$$\left| \frac{d\tilde{\lambda}}{dz} \right| \ll 1 \quad (1)$$

where  $\tilde{\lambda} = \lambda/2\pi$ ,  $\lambda(z) = 2\pi\hbar/p(z)$  – de Broglie wavelength of the particle expressed by way of the particle classical momentum  $p(z)$  [1].

Condition (1) can be expressed in another form taking into account that

$$\frac{dp}{dz} = \frac{d}{dz} \sqrt{2m(W - U)} = -\frac{m}{p} \frac{dU}{dz} = \frac{mF}{p} \quad (2)$$

where  $F = -dU/dz$  means classical force acting upon the particle in the external field.

Introducing this force, we get

$$\frac{m\hbar|F|}{p^3} \ll 1 \quad (3)$$

From (3) it is clear that the quasiclassical approximation is not valid at too small momentum of the particle. In particular, it is deliberately invalid near positions in which the particle, according to classical mechanics, should stop, then start moving in the opposite direction. These points are the so called "turning points". Their coordinates  $z_1$  and  $z_2$  are determined from the condition  $E=U(z)$ .

It should be emphasized that condition (3) itself can be insufficient for the permissibility of the quasiclassical approach. One more condition should be met: the barrier height should not change much over the length  $L$ .

Let us consider the particles move in the field shown in Fig. 1 which is characterized by the presence of the potential barrier with potential energy  $U(z)$  exceeding particle total energy  $E$  and meeting all the quasiclassics conditions. In this case points  $z_1$  and  $z_2$  are the turning points.

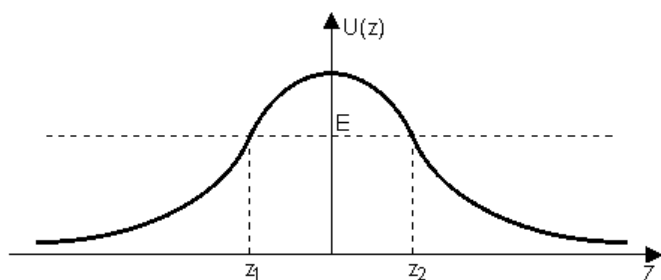


Fig. 1. Potential barrier of arbitrary shape

The approximation technique of the Schrodinger equation solution when quasiclassical conditions are met was first used by Wentzel, Kramers and Brillouin. This technique is known as WKB approximation or quasiclassical quantization method. In this textbook we do not present the Schrodinger equations solution for the given case. However, it can be found in [1], [2] and the barrier transparency in this case is

$$D(E) \propto \exp \left\{ -\frac{2}{\hbar} \int_{z_1}^{z_2} \sqrt{2m(U(z) - E)} dz \right\} \quad (4)$$

Comparing expressions (3) in chapter [Tunneling Effect](#) for transmission coefficients of rectangular barrier (precise solution of Shrodinger equation) and (4) for quasiclassical approximation, we can notice that there is no qualitative difference between them. In both cases the transparency decreases exponentially with the barrier width.

#### Summary

- If the problem parameters satisfy quasiclassical conditions, then transmission coefficient can be calculated in a general form using (4).
- In case of the square barrier there is no qualitative difference between transmission coefficients calculated using quantum mechanics and quasiclassical approximation. In both cases the transparency decreases exponentially with the barrier width.

#### References

1. Landau L.D., Lifshitz E. M. Quantum mechanics. Nauka, 1989 (In Russian)
2. Mott N., Sneddon I. Wave mechanics and its application. Nauka, 1966 (In Russian)

### Metal Energy-Band Structure

To derive the formula of tunneling current in the metal-insulator-metal (MIM) system (John G. Simmons formula, see [chapter "John G. Simmons Formula"](#)), we must make some assumptions and remind of metal electronic theory fundamentals.

- Firstly, let us consider that the solid (metal) is a three-dimensional potential well with a plain bottom (the so called Sommerfeld model) and electrons do not interact with each other. The energy of the electron resting at the bottom of such potential well is less than vacuum level – the energy of electron resting infinitely far from the solid surface. The well depth  $U$  is determined by the averaged field of all positive ions of the lattice and of all electrons.
- Secondly, because all electrons are considered to be noninteracting, the solution to the Schrodinger equation for the system of electrons is turned to the solution to the Schrodinger equation for single electron moving in the averaged field which allows to use formulas (3) in chapter [Tunneling Effect](#) or (4) in chapter [Tunneling Effect in Quasiclassical Approximation](#).
- Thirdly, in the potential box with the plain bottom, the dependence of energy allowed values on wave vector allowed values looks like points on the parabolic dependence of the energy on the wave vector components  $E = p^2 / 2m = (\hbar k)^2 / 2m$  for the free electron in void. If electrons mass  $m$  is isotropic in space, then the following expression is valid  $E = p_x^2 / 2m + p_y^2 / 2m + p_z^2 / 2m = p^2 / 2m$ , where  $P_x, P_y, P_z$  – axial electron momentum components.

From the statistical physics [1] it is known that in a system in thermodynamic equilibrium all quantum states with the same energy level  $E$  are occupied with electrons equally. The mean number of electrons in one quantum state with energy  $E$  at

temperature  $T$  is given by the Fermi-Dirac distribution:

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} \quad (1)$$

where  $k_B = (11600)^{-1} \text{ eV/K}$  – Boltzmann's constant,  $\mu$  – parameter having the dimension of energy and called chemical potential.

The chemical potential  $\mu$  is defined by the normalization condition

$$\int_0^{\infty} n(E) f(E) dE = n_e \quad (2)$$

where  $n_e$  – number of conduction band electrons per volume unit (concentration),

$$n(E) dE = 2(2\pi)^3 \iiint_{[E, E+dE]} d^3k = \frac{1}{2\pi^2} \left(\frac{\sqrt{2m}}{\hbar}\right)^3 \sqrt{E} dE -$$

number of electron states per volume unit in the energy range from  $E$  to  $E + dE$ .  $n(E)$  function is called the energetic density of states.

In a metal at the temperature close to absolute zero, electrons occupy all quantum states with energies up to the level  $\mu_0 = \mu(0)$  called the Fermi level. All quantum states above the Fermi level are not occupied with electrons. In a metal, the chemical potential slightly depends on temperature, therefore it can be approximated by  $\mu_0$  at  $T = 0$ :

$$\mu(T) \approx \mu_0 = \frac{\hbar^2}{2m} (3\pi^2 n_e)^{2/3} \quad (3)$$

where  $m$  – electron mass. If  $n_e$  is expressed in C.G.S. units, then  $\mu_0 = 0,36 \cdot 10^{-14} n_e^{2/3} \text{ eV}$ .

If a system is in thermal equilibrium and consists of some sub-systems, the Fermi levels of subsystems should be the same (Fig. 1). If voltage  $V$  is applied between two subsystems (solids), the Fermi level of the solid connected to the positive pole decreases, while for the other solid it increases. The difference in Fermi levels between solids is  $eV$  (Fig. 2).

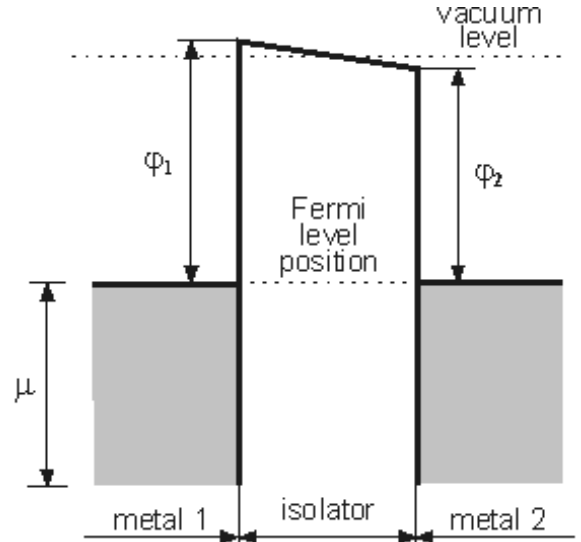


Fig. 1. Diagram of MIM system in equilibrium.  $j_1$  and  $j_2$  – work function of the left and right metals, respectively

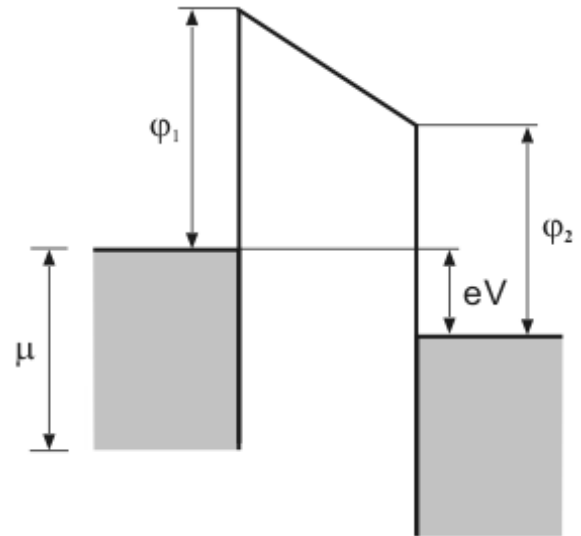


Fig. 2. Model of MIM system then positive potential is applied to the right metal

#### Summary

To derive the formula of tunneling current in the MIM system ([chapter "John G. Simmons Formula"](#)) we assume that:

- Sommerfeld model is correct for all solid bodies.
- Each electron from the solid move in averaged field of all positive ions of the lattice and of all electrons.
- Isotropic square-law of dispersion as for free electron in void is correct (1).
- In a metal at  $T \rightarrow 0K$ , electrons occupy all quantum states with energies up to the Fermi level  $\mu_0$  (3). All quantum states above the Fermi level are not occupied with electrons.

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## References

1. Landau L.D., Lifshitz E. M. Statistical physics. Nauka, 1976 (in Russian)
2. Kittel Ch. Introduction in solid-state physics. Nauka, 1978 (in Russian)

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