Quasi-classical approximation	One and three-dimensional problems, the correspondence principle, the calculation of matrix elements for highly oscillating functions.

Lecture 8-10

Tunneling Effect in Quasi-classical Approximation

The quasi-classical qualitative condition imply that de Broglie wavelength of the particle λ 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

$$\left|\frac{d\bar{\lambda}}{dz}\right| \ll 1 \tag{1}$$

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

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

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

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

Introducing this force, we get

$$\frac{m\hbar|F|}{p^3} \ll 1 \tag{3}$$

From (3) it is clear that the quasi-classical 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 quasi-classical 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 quasi-classics conditions. In this case points z_1 and z_2 are the turning points.

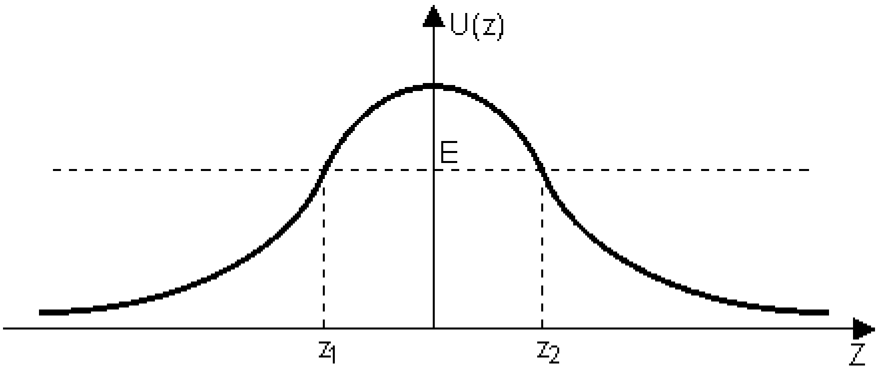

Fig. 1. Potential barrier of arbitrary shape.

The approximation technique of the Schrodinger equation solution when quasi-classical conditions are met was first used by Wentzel, Kramers and Brillouin. This technique is known as WKB approximation or quasi-classical quantization method. 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

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

Comparing expressions (5) in next chapter for transmission coefficients of rectangular barrier (precise solution of Shrodinger equation) and (4) for quasi-classical 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 quasi-classical 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 quasi-

classical 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)
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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 wave function**). The wave function Ψ, 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 wave function, one should determine $|\Psi|^2$ rather than Ψ. Then, the probability for finding particles in an elementary volume *dxdydz* is given by $|\Psi|^2 dxdydz$.

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

$$U(z) = \begin{cases} 0, & \text{при} \quad z < 0; \\ U_0, & \text{при} \quad 0 \le z \le L; \\ 0, & \text{при} \quad z > L, \end{cases} \tag{5}$$

impinge on the rectangular potential barrier and the total energy E is less than U_0 **(Fig. 2)**.

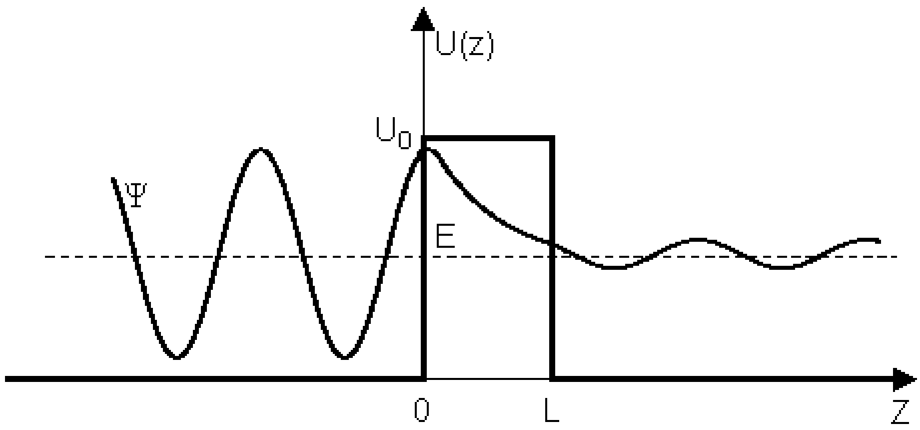

Fig. 2. Rectangular potential barrier and particle wave function Ψ .

The stationary Schrodinger equations can be written as follows

$$\begin{cases} \ddot{\Psi} + k_1^2 \Psi = 0, & \text{при } z < 0; \\ \ddot{\Psi} - k_2^2 \Psi = 0, & \text{при } z \in [0; L]; \\ \ddot{\Psi} + k_1^2 \Psi = 0, & \text{при } z > L, \end{cases} \tag{6}$$

where $k_1 = \frac{\sqrt{2mE}}{\hbar}$, $k_2 = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$ – wave vectors, $\hbar = 1{,}05 \cdot 10^{-34}$ Дж $\cdot$ 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 wave function Ψ 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 wave function module at $z > L$ because the incident wave amplitude is assumed to be 1 and wave vectors of both incident and transmitted waves coincide.

$$D = bb^* = \left(\mathrm{ch}^2(k_2 L) + \frac{1}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2} \right)^2 \mathrm{sh}^2(k_2 L) \right)^{-1} \tag{7}$$

If $k_2 L >> 1$, then both $\mathrm{ch}(k_2 L)$ and $\mathrm{sh}(k_2 L)$ can be approximated to $\exp(k_2 L)/2$ and (3) will be written as

$$D(E) = D_0 \exp\left\{ -\frac{2L}{\hbar}\sqrt{2m(U_0 - E)} \right\} \tag{8}$$

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 quasi-classical condition, the transmission coefficient can be calculated in a general form.

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 wave function 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.

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3. Quasiclassical methods, eds. Jeffrey Rauch, Barry Simon; Springer, 1997, ISBN0387983104, 9780387983103; p. 224