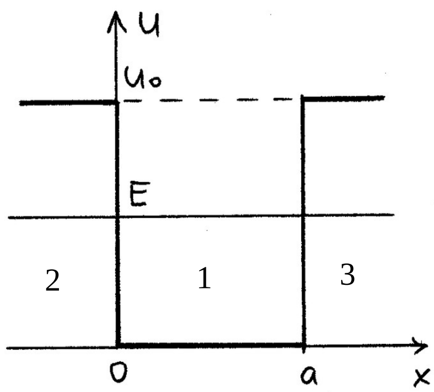
5.1 Infinite potential well. At first we deal with case $U_0 \to \infty$ (infinite well). In that case we have $\psi_2 = \psi_3 = 0$, i.e. particles may move only in region, where $U = 0$. It is the free particle case and the general solution of Schrödinger equation $\frac{\hbar^2}{2m}\psi'' = E\psi$ is:



$$\psi_1(x) = A\,e^{ikx} + B\,e^{-ikx} .$$

where

$$k = \frac{\sqrt{2ME}}{\hbar} .$$

Initial conditions are $\psi_1(0) = \psi_1(a) = 0$ and we get

$$A + B = 0 , \qquad Ae^{ika} + Be^{-ika} = 0 .$$

From the first one $B = - A$ and after substitution to the second one we have

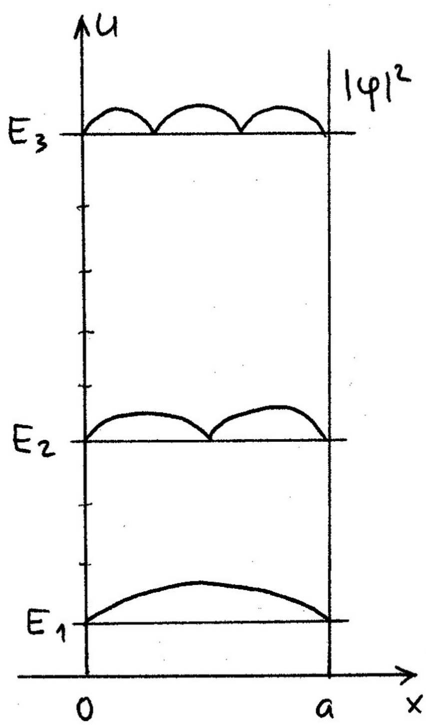
$$A(e^{ika} - e^{-ika}) \equiv 2iA\sin(ka) = 0 .$$

Since $A \neq 0$ (otherwise $\psi_1 = 0$ and there are no particles at all), we have

$$\sin(ka) = 0$$

from which

$$ka = n\pi , \quad n = 1, 2, 3, \ldots .$$



($n = 0$ is not allowed, since it gives $k = 0$ and $\varphi_I = 0$). Substituting k we obtain that the energy in infinite well is discrete

$$E_n = \frac{k^2\hbar^2}{2M} \equiv \frac{(\pi\hbar)^2}{2Ma^2}\cdot n^2 , \quad n = 1, 2, \ldots .$$

(In classical well energy is continuous $0 \leq E < \infty$.)

Orthonormed wave functions are

$$\psi_n(x) = i\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} .$$

Lowest energies and corresponding probability distribution:

$$E_1 = \frac{(\pi\hbar)^2}{2Ma^2} , \quad |\psi_1|^2 = \frac{2}{a}\sin^2\frac{\pi x}{a} ,$$

$$E_2 = 4E_1 , \quad |\psi_2|^2 = \frac{2}{a}\sin^2\frac{2\pi x}{a} ; \qquad E_3 = 9E_1 , \quad |\psi_3|^2 = \frac{2}{a}\sin^2\frac{3\pi x}{a} .$$

The wavefunctions are form the set of orthonormal functions. We can check it by calculation of corresponding integral:

$$\int_0^a \psi_n^* \psi_m \, dx = \frac{2}{a}\int_0^a \sin\frac{n\pi x}{a} \sin\frac{m\pi x}{a} \, dx$$ must be equal to δ_{nm} **Prove!**

<u>It is important to understand that the eigenfunctions for stationary states are standing waves. We have self-interfering wave functions reflected from the walls of the potential well. And only a stable result of this interference is realized as a stationary state.</u>

Additionally, we can calculate the average values of the coordinate and momentum of the particle.

Additional tasks:

Show that:

1.) $\langle x \rangle_n = \int_0^a \psi_n^* x \, \psi_n dx \quad = 0,$

2.) $\langle p_x \rangle_n = \int_0^a \psi_n^* \hat{p}_x \, \psi_n dx \quad = 0$

3.) Calculate the mean of the squared coordinate $\langle x^2 \rangle_n = \int_0^a \psi_n^* x^2 \, \psi_n \, dx \quad = ?$

4.) Calculate the mean of the squared momentum $\langle p_x^2 \rangle_n = \int_0^a \psi_n^* p_x^2 \, \psi_n dx \quad = ?$

Some tabular expressions:

$$\int x^2 \sin^2(x) \, dx = \frac{x^3}{6} - \left(\frac{x^2}{4} - \frac{1}{8}\right) \cdot \sin(2x) - \frac{x \cdot \cos(2x)}{4}$$

$$\int x \sin^2(x) \, dx = \frac{x^2}{4} - \frac{x \cdot \sin(2x)}{4} - \frac{\cos(2x)}{8}$$

$$\int \sin(x) \cos(x) \, dx = \frac{\sin^2(x)}{2}$$

$$\int \sin^2(x) \, dx = \frac{x}{2} - \frac{\sin(2x)}{4}$$

$$\int x \cos(x) \, dx = \cos(x) + x \cdot \sin(x)$$

$$2\sin(\alpha) \cdot \sin(\beta) = \cos(\alpha - \beta) - \cos(\alpha + \beta)$$