II.2.4 Completeness of eigenfunctions of Hermitean operators.

Eigenfunctions form a complete set of functions. In other words it means that if we had some orthonormal system of eigenfunctions $\varphi_1, \varphi_2, \varphi_3,$ ... of some Hermitean operator $\hat{A}$, then an any function can be presented as linear combination of eigenfunctions. We have the same situation with vectors in three-dimensional space. Arbitrary three-dimensional vector can be represented by a combination of three basis orthonormal vectors. The basis vectors play the role of wave functions(eigenfunctions), and an arbitrary vector is an arbitrary function in quantum mechanics.

$$\psi = \sum_n c_n \varphi_n \,, \qquad \vec{A} = \vec{i} \cdot x + \vec{j} \cdot y + \vec{k} \cdot z$$

Geometrical interpretation: eigenfunctions φ_n is **treated as** a set of orthogonal unit vectors of some vector space and c_n are treated as coordinates of ψ.

where c_n are some numerical coefficients, obtained as

$$c_n = \int \varphi^* \cdot \psi \, dV$$

Geometrical interpretation: eigenfunctions φ_n is **treated as** a set of orthogonal unit vectors of some vector space and c_n are treated as coordinates of ψ.

Let us assume, that ψ is presented as

$$\psi = \sum_n c_n \varphi_n$$

.

To get c_m we find a scalar product with φ_m^* and use the orthonormality of

$$c_m = \int \varphi^* \cdot \psi \, dV \,.$$

II.2.5 Physical meaning. Let us give the physical meaning of sequence

$$\psi = \sum_n c_n \varphi_n \,,$$

where ψ is a state function (wave function) of some particle and φ_n are eigenfunctions of operator $\hat{A}$ corresponding to some physical quantity A (energy, momentum, etc).

If we perform measurements of *A*, the results are equal to the eigenvalues $a_1,\ldots,a_n,\cdots$. The probability of results depends on $c_1,\ldots,c_n,\cdots$. Namely – we get a_1 with probability $c_1{}^2$, a_2 with probability $c_2{}^2$, (and so on).

The sum of probabilities is equal to unity

$$\int \psi^* \psi \, dV = 1 = \sum_{m,n} c^*_m c \int \varphi^*_m \varphi_n dV \equiv \sum_{m,n} c_m * c_n \, \delta_{mn} = \sum_n |c_n|^2 \, .$$

If, for example, our measurements give only one value a_n of *A* then we have $\psi = \varphi_n$, in other cases the value of *A* is not uniquely determined. If we have the state ψ, which is expressed as

$$\psi = c_1\varphi_1 + c_2\varphi_2$$

and *A* is, for example energy, then the measurements of energy give us as a result two values: a_1 or a_2. a_1 has probability $c_1{}^2$, a_2 has probability $c_2{}^2$. It means that in microworld there exist states where the energy (or some other physical quantity) is not uniquely determined. Such states are more common that the states with a fixed energy.

<u>Comments, appendices:</u>

1. <u>Operator, linear operator.</u> Let us have some set of functions X. Operator is a prescription, which for every function $f \in X$ sets in corrspondence some other function $g \in X$ (from the same set of functions, in other words it is a function of functions). We denote it as $\hat{A}$ and write

$$g = \hat{A} f \quad .$$

In quantum mechanics we use only linear operators. By definition, linear operator satisfies the following two conditions

$$\hat{A}(f_1 + f_2) = \hat{A} f_1 + \hat{A} f_2 \quad ,$$

$$\hat{A}(af) = a \, \hat{A} f \quad ,$$

where $f_1, f_2, f \in X$ and $a \in C$ is some number (real or complex).

<u>The sum and product of operators</u>. Sum

$$\left(\hat{A}+\hat{B}\right)\cdot f=\hat{A}\,f+\hat{B}\,f \quad ,$$

product

$$\hat{A}\,\hat{B}\,f=\hat{A}\left(\hat{B}\,f\right) \quad .$$

2. <u>δ-function.</u> 1-dimensional case. δ-function (Dirac δ-function) is defined as follows

$$\delta(x)=0 \quad if \quad x\neq 0, \qquad \delta(x)\neq 0 \quad if \quad x=0$$

and

$$\int_a^b \delta(x)\,dx=1 \quad if \quad x=0\in[a,b] \quad .$$

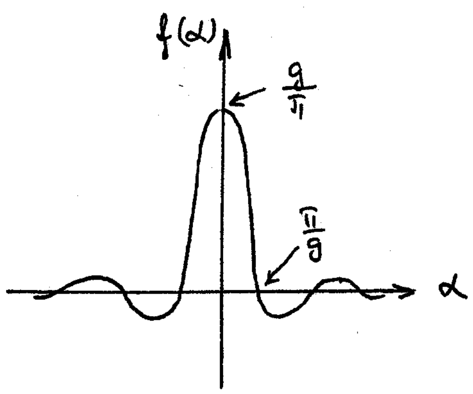
From the definition it follows, tha for arbitrary function $f(x)$

$$\int_a^b f(x)\,\delta(x)\,dx=f(0) \quad ,$$

and

$$\int_a^b f(x)\,\delta(x-c)\,dx=f(c) \quad if \quad c\in[a,b] \quad .$$

<u>δ-function as integral</u>.



Since

$$\int_{-\infty}^{+\infty}\frac{\sin(g\,\alpha)}{\pi\,\alpha}\,d\alpha=1 \quad ,$$

δ-fuction is expressed as limit

$$\delta(x)=\frac{\sin(g\,\alpha)}{\pi\,\alpha} \quad .$$

Since

$$\frac{\sin(g\,\alpha)}{\pi\,\alpha}=\frac{1}{2\,\pi}\int_{-g}^{+g}e^{i\,\alpha\,\beta}d\,\beta \quad ,$$

we have

$$\delta(\alpha)=\frac{1}{2\,\pi}\int_{-\infty}^{+\infty}e^{i\,\alpha\,\beta}\,d\,\beta \quad .$$

δ-function as a limit. In the following we also use the definition of δ-funktsiooni as the following limit

$$\delta(x)=\frac{\sin^2(A\ x)}{\pi\ A\ x^2}$$

III. Uncertainty principle

In a microworld it is common that not all physical quantities can be are simultaneously exactly measurable. And for that quantities we have some uncertainty relations.

If operators of two physical quantities *A* and *B* - $\hat{A}$ and $\hat{B}$ commute (the order of acting of the operators on the wave function can be changed)

$$[\hat{A},\hat{B}]=0\ ,$$

($\hat{A}\hat{B}=\hat{B}\hat{A}$, i.e. for each ψ we have $\hat{A}\hat{B}\psi=\hat{B}\hat{A}\psi$), the physical quantities *A* ja *B* are at the same time (simultaneously) exactly measureable. But if operators do not commute

$$[\hat{A},\hat{B}]=i\hat{C}$$

($\hat{C}$ is some nonzero Hermitean operator) *A* and *B* are not simultaneously measureable, and we have certain restrictions on measurements, called uncertainty principles. If physical quantities cannot be exactly measured simultaneously, we need to calculate the lower accuracy limit of these measurements.

3.1 Simultaneous measurements, exact values of observables.

If two operator are commute

$$[\hat{A},\hat{B}]=0\ ,$$

we prove, that *A* ja *B* are simultaneusly measureable.

If we assume, that measurements of *A* ja *B* give simultaneously certain exact values *a* and *b*, then opeators commute. Mathematically it means, that there exist such state function (wave function) ψ , for which

$$\hat{A}\psi=a\psi\ \ and\ \ \hat{B}\psi=b\psi\ .$$

Therefore, operators have common eigenfunctions. Now it is easy to demonstrate that $\hat{A}\hat{B}=\hat{B}\hat{A}$ **(prove it!)**.

And vice versa, if

$$[\hat{A},\hat{B}]=0 \quad ,$$

$$\hat{A}\psi_a = a\psi_a$$

and demonstrate that these are also eigenfunctions of operator $\hat{B}$. Let us apply operator $\hat{B}$

$$\hat{B}(\hat{A}\psi_a)=a(\hat{B}\psi_a) .$$

Since operators commute, we have $\hat{B}(\hat{A}\psi_a)=\hat{A}(\hat{B}\psi_a)$, and therefore

$$\hat{A}(\hat{B}\psi_a)=a(\hat{B}\psi_a) .$$

Now we see that $\hat{B}\psi_a$ is the eigenfunction of operator $\hat{A}$ with the eigenvalue *a*, and therefore

$$\hat{B}\psi_a \sim \psi_a \quad .$$

We can find a constant *b*, that

$$\hat{B}\psi_a = b\psi_a \ .$$

Therefore each eigenfunction of $\hat{A}$ is at the same time also eigenfunction of $\hat{B}$ .Therefore the quantities have simultaneous observables *a* and *b*.

3.2 Mean values of physical quantities. The mean value of physical quatity in the state, described by wave function ψ, is calculated from

$$\langle A\rangle = \int \psi * \hat{A}\psi \, dV .$$

<u>**Proof.**</u> Using eigenfunctions of $\hat{A}$ we have an expansion

$$\psi = \sum_n c_n \varphi_n .$$

Since c_n ^{2} is probability, that we obtain the result a_n (n = 1,2, ...), the mean value is calculated as

$$\langle A\rangle = \sum_n a_n |c_n|^2 .$$

From the above given $\int \psi * \hat{A}\psi \, dV$. If we replace one ψ and use $c_n * = \langle \varphi_n|\psi\rangle * = \langle \psi|\varphi_n\rangle$ we have

$$\langle A\rangle = \langle\psi\,|\,\hat{A}\psi\rangle \equiv \left\langle\psi\,\middle|\,\hat{A}(\sum_n c_n\varphi_n)\right\rangle = \left\langle\psi\,\middle|\,\sum_n c_n a_n \varphi_n\right\rangle =$$

$$= \sum_n a_n c_n \langle\psi\,|\,\varphi_n\rangle = \sum_n a_n |c_n|^2 \quad .$$

3.3 Uncertainty relations. Let us assume that

$$\left[\hat{A}, \hat{B}\right] = i\hat{C}$$

and derive uncertainty formulas for measurements of quantities A ja B . It is obvious, that the deviations from mean value are not usable, since its mean value is zero, therefore we consider the mean value of its square, which we define as follows (root mean square deviation)

$$\left\langle(\Delta A)^2\right\rangle = \int\psi^*(\hat{A} - \langle A\rangle)^2\psi\, dV \quad ,$$

$$\left\langle(\Delta B)^2\right\rangle = \int\psi^*(\hat{B} - \langle B\rangle)^2\psi\, dV \quad .$$

For these quantities one can prove the following general result

$$\left\langle(\Delta A)^2\right\rangle\left\langle(\Delta B)^2\right\rangle \geq (\frac{1}{2}\langle C\rangle)^2 \quad ,$$

which means the root mean square deviations cannot be simultaneusly equal to zero and therefore we have no exact simultaneous values of observables A and B.

<u>Proof.</u> We present the simpler version, assuming that the mean values of A ja B are equal to zero

$$< A > = < B > = 0 \quad .$$

Now the root mean square deviations are

$$< (\Delta A)^2 > = < A^2 > = \int\psi^*\hat{A}^2\psi\, dV \qquad \text{ja} \qquad < (\Delta B)^2 > = < B^2 > = \int\psi^*\hat{B}^2\psi\, dV \quad .$$

Let us take the nonnegative integral, where α is some real parameter

$$J(\alpha) = \int |(\alpha\,\hat{A} - i\,\hat{B})\,\psi|^2 dV \ \geq\ 0 \quad .$$

Since $\hat{A}$ ja $\hat{B}$ are Hermitean, one may write

$$J(\alpha)=\int((\alpha\hat{A}-i\hat{B})\psi)^*(\alpha\hat{A}-i\hat{B})\psi\ dV=$$

$$=\int\psi(\alpha^2\hat{A}^2-i\alpha(\hat{A}\hat{B}-\hat{B}\hat{A})+\hat{B}^2)\psi\ dV$$

(We have used the commutation relation for $\hat{A}$ and $\hat{B}$,)

Using mean values it is

$$J(\alpha)=\alpha^2<(\Delta A)^2>+\alpha<C>+<(\Delta B)^2> \ .$$

Since $J(\alpha)\geq 0$, the cofiicients must satify

$$4<(\Delta A)^2><(\Delta B)^2> \ \geq \ <C>^2 \ ,$$

which is our uncertainty relation.

Example. Let us have operators (coordinate and momentum)

$$\hat{A}=\hat{x}\equiv x \qquad ja \qquad \hat{B}=\hat{p}_x\equiv -i\hbar\frac{\partial}{\partial x}.$$

We have

$$\left|x,\hat{p}_x\right|=i\hbar\ , \ \textbf{Prove!}$$

therefore $\hat{C}=\hbar$. Uncertainty relation is

$$\left\langle(\Delta x)^2\right\rangle\left\langle(\Delta p_x)^2\right\rangle\geq\frac{\hbar^2}{4} \ .$$

Usually it is written in simpler form. If we define

$$\Delta x=\sqrt{\left\langle(\Delta x)^2\right\rangle} \qquad and \qquad \Delta p_x=\sqrt{\left\langle(\Delta p_x)^2\right\rangle}\ ,$$

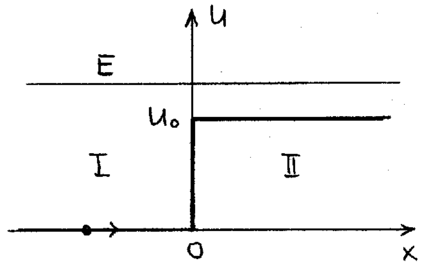
then we have

$$\Delta x\ \Delta p_x\geq\frac{\hbar}{2}.$$

(Similar expressions we have also for y- ja z-coordinates and correponding momenta.)

4. Potential barriers, tunneling

4.1 Potential barrier (E > U). Consider the following potential energy



$$U = \begin{cases} U_0\,, & x \geq 0, \\ 0\,, & x < 0. \end{cases}$$

Let us consider the flux of particles moving from the left to right and analyze their behaviour if the energy of particles E is higher than U_o.

For classical particles we know that all particles moving from left (region I) continue their moving in the region II, but for microparticles the behaviour of particles is different, some particles always reflect back and do not reach the II region.

We find the solutions of the Schrödinger equation in regions I and II and then apply the continuity of solutions for x = 0.

<u>Region I.</u> Since $U = 0$, the Schrödinger equation may be written as

$$\psi_1'' + k_1^2\,\psi_1 = 0 \quad ,$$

where $k_1^2 = 2mE/\hbar^2$. General solution is

$$\psi_1(x) = e^{ik_1 x} + Be^{-ik_1 x} \quad .$$

e^{ikx} describes particles moving from left to right. We assume that the initial flux of particles moving toward the barrier is known and take the coefficient before it equal to one (A = 1) and the flux of particles moving towards the barrier is equal to k/m. The second term Be^{-ikx} describes the particles that are reflected back. The flux of reflected particles is equal to $k_1|B|^2$ /m.

<u>Region II</u>. Now $U = U_o$, and the Schrödinger equation is

$$\psi_2''(x) + k_2 \psi_2(x) = 0 \quad ,$$

where $k_2 = 2m(E - U_0)/\hbar^2$. Special solutions are

$$e^{ik_2 x} \;\; and \;\; e^{-ik_2 x} \quad .$$

Since in the region II there are particles moving from left to right, the general solution is

$$\psi_2(x) = Ce^{ik_2 x} \quad .$$

In order to find the general solution to our problem, we must use the continuity conditions, which means that $\psi_1(0) = \psi_2(0)\ ,\ \psi'_1(0) = \psi'_2(0)$.

Using these conditions we after some algebra get that

$$B = \frac{k_1 - k_2}{k_1 + k_2}\ ,\ \ C = \frac{2k_1}{k_1 + k_2} \quad .$$

Therefore the general solution is

$$\psi(x) = \begin{cases} e^{ik_1 x} + \dfrac{k_1 - k_2}{k_1 + k_2} e^{-ik_1 x}\ ,\ \ x < 0\ , \\ \dfrac{2k_1}{k_1 + k_2} e^{ik_2 x}\ ,\ x \geq 0\ . \end{cases}$$

The main result we obtained is that $B \neq 0$ and therefore some particles indeed reflect at x = 0 back.

Let us calculate the flux of particles. The flux of particles, moving towards the barrier (incident particles) is

$$j_i = \frac{i\hbar}{2m}\left(\psi \frac{d\psi^*}{dx} - \psi^* \frac{d\psi}{dx}\right) = \frac{\hbar k_1}{m} \quad .$$

The flux of reflected particles and particles moving to region II are correspondingly

$$j_r=\frac{\hbar\, k_1}{m}\,|B|^2\ ,\ \ j_t=\frac{\hbar\, k_2}{m}\,|C|^2\ .$$

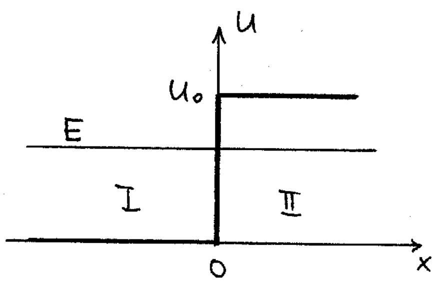
If we define the reflection coefficients and transition coefficients (R and T) (as a ratio of densities of current of probabilities)

$$R=\frac{j_r}{j_i}=|B|^2\ ,\ \ T=\frac{j_t}{j_i}=\frac{k_2}{k_1}\,|C|^2\ ,$$

it is possible to verify that

$$R+T=1\ .$$

4.2 Potential barrier (E < U_0). Barrier is the same, but now we assume that $E < U_o$. The classical particles must reflect at x = 0 back, since classical particles can move only in regions where $E \geq U$. Microparticles have some probability to move in regions where $E < U$ (in regions where kinetic energy is negative!).



Region I. The general solution is the same as in the previous case

$$\psi_1(x)=e^{ik_1x}+Be^{-ik_1x}\ .$$

Region II. Schrodinger equation is

$$\psi_1''-\kappa_1^2\psi_1=0\ ,$$

where $\kappa_1^2=2m(U_0-E)/\hbar^2$. Special solutions are $e^{\kappa x}$ and $e^{-\kappa x}$. Since the solution must exist in the region $0 \leq x < \infty$, the first one is not applicable, since in $x \to \infty$ case $e^{\kappa x} \to \infty$, the second solution is applicable, since it is finite. Therefore the general solution is

$$\psi_2(x)=Ce^{-\kappa_2 x}\ .$$

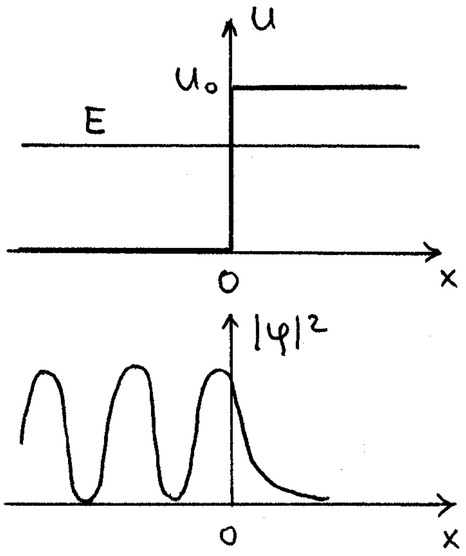
Applying the conditions $\psi_1(0)=\psi_2(0)\ ,\ \ \psi'_1(0)=\psi'_2(0)$, we get B and C

$$B=\frac{k-i\kappa}{k+i\kappa}\ ,\quad C=\frac{2k}{k+i\kappa}$$

and the general solution is

$$\psi(x)=\begin{cases} e^{ikx}+\dfrac{k-i\kappa}{k+i\kappa}e^{-ikx}\ , & x<0,\\[2ex] \dfrac{2k}{k+i\kappa}e^{-\kappa x}\ , & x\geq 0\,. \end{cases}$$

The result is physically very interesting. The fact, that particles reflect back is obvious, but the fact that $C \neq 0$ is shocking, because it is possible to obtain particles inside the barrier (which is forbidden to classical particles). Probability density of finding particles inside the barrier is



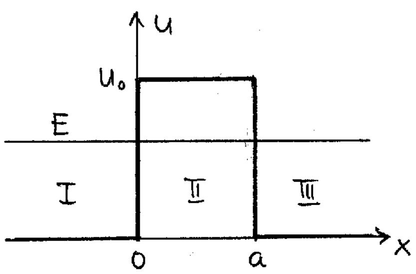
$$|\psi_{II}(x)|^2 = \frac{4k^2}{k^2+\kappa^2} e^{-2\kappa x} \cdot$$

The probability density is increasing exponentially. Probability distribution $|\psi|^2$ graph. On the left side there is the interference picture of particles (waves) moving towards the barrier and reflected particles.

It appears, that finally all particles reflect back, since the reflection coefficient is equal to 1. Indeed, the simple calculation gives (**prove!**)

$$R = \frac{j_p}{j_l} = |B|^2 = B^* B = 1 \cdot$$

4.3 Tunnel effect (tunneling). Consider the next potential barrier



$$U = \begin{cases} U_0 \,, \; 0 \le x \le a \,, \\ 0 \,, \; x < 0 \,, \; x > a \,. \end{cases}$$

Let us consider the flux of particles moving in the region I from left to right (toward the barrier) with energy E that is less than U_0 ($E < U_0$). Since the with of barrier is finite there is nonzero transition probability and some particles may move to the region III. That effect is called the tunnel effect or tunneling. Of course, in classical physics there is no tunneling, since all classical particles must reflect back at x = 0.

In order to prove tunneling we find general solutions for each region and then apply the **continuity** conditions for x = 0 and x = a. Region I

$$\psi_I(x) = e^{ikx} + Be^{-ikx} \;.$$

Region II

$$\psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x} \;.$$

(Since $0 \le x \le a$ both special solutions must be used). Region III

$$\psi_{III}(x) = F\, e^{ikx} \ .$$

Continuity conditions

$$1 + B = C + D\,, \quad C\,e^{\kappa a} + D\,e^{-\kappa a} = F\,e^{ika}\ ,$$

$$ik(1 - B) = \kappa(C - D)\,, \quad \kappa(C\,e^{\kappa a} - D\,e^{-\kappa a}) = ikF\,e^{ika}\ ,$$

gives solutions

$$B = \frac{(k^2 + \kappa^2)\,sh(\kappa a)}{(k^2 - \kappa^2)\,sh(\kappa a) - 2ik\kappa\, ch(\kappa a)}\ ,$$

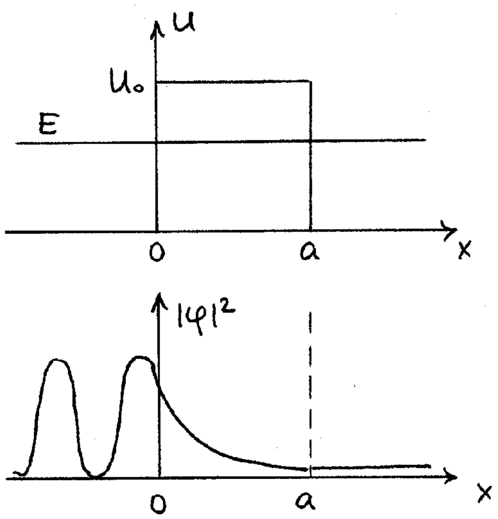
$$F = \frac{2ik\kappa\, e^{-ika}}{(k^2 - \kappa^2)\,sh(\kappa a) + 2ik\kappa\, ch(\kappa a)}\ .$$

Since $F \neq 0$ there exists tunneling, particles have nonzero probability to „go through“ barrier.

Transition coefficient

$$L = \frac{j_e}{j_I} = |F|^2 = F^* F = \frac{4k^2\kappa^2}{(k^2 - \kappa^2)^2 sh^2(\kappa a) + 4k^2\kappa^2 ch^2(\kappa a)}\ .$$

It depends on $\kappa = \dfrac{\sqrt{2M(U_0 - E)}}{\hbar}$ and a.



The general solution is quite complicated and we therefore consider the simpler specific case where $\kappa a >> 1$. Then $\mathrm{sh}^2\kappa a \approx \mathrm{ch}^2\kappa a \approx e^{2\kappa a}/4$ and we get

$$L = |F|^2 = \frac{16k^2\kappa^2}{(k^2 + \kappa^2)^2} e^{-2\kappa a}\ .$$

Transition probability decreases exponentially

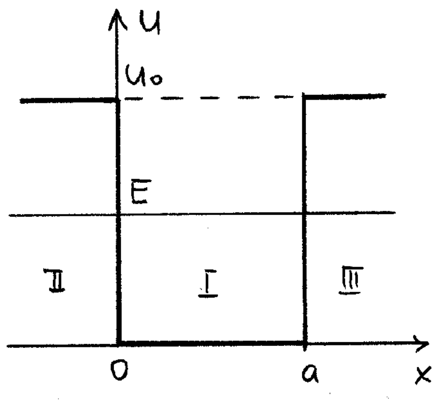
$$L \approx e^{-2\kappa a}\ ,$$

Calculating $R = |B|^2$, it is possible to verify that

$$R + L = 1\ .$$

5. Potential well

5.1 Infinite potential well. At first we deal with case $U_0 \to \infty$ (infinite well). In that case we have $\psi_{II} = \psi_{III} = 0$, i.e. particles may move only in region, where U = 0. It is the free particle case and the general solution is



$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \cdot$$

where

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

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

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

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

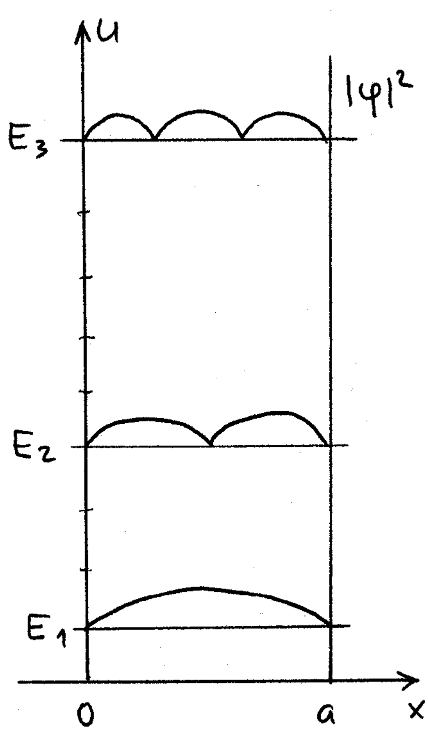
$$A(e^{ika} - e^{-ika}) \equiv 2iA\sin(ka) = 0 \ .$$

Since $A \neq 0$ (otherwise $\varphi_I = 0$ 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

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

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

Orthonormed wave functions are

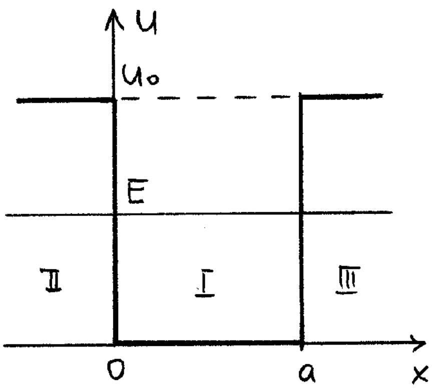
$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} \ .$$

Lowest energies and corresponding probability distribution:

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

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

5.2 Finite potential well. Now we deal with the following potential energy



$$U = \begin{cases} 0 & , 0 \le x\ a\ , \\ U_0\ , & x < 0\ ,\ x > a\,. \end{cases}$$

and assume that $E < U_0$.

Comparing with $U_0 \to \infty$ case, we are faced with more complicated problem, since wave functions in regions II and III are nonzero. As we see, we have no analytic solution at all.

General solutions for different regions are

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \ , \quad \psi_{II}(x) = C e^{\kappa x}\ , \quad \psi_{III}(x) = De^{-\kappa x} \ .$$

Continuity conditions for $x = 0$ and $x = a$ give

$$A + B = C \qquad\qquad ik(A - B) = \kappa C$$

$$Ae^{ika} + Be^{-ika} = De^{-\kappa a} \qquad ik(Ae^{ika} - Be^{-ika}) = -\kappa De^{-\kappa a} \ .$$

We eliminate C and D, then it reduces to the system for A and B

$$\kappa(A + B) = ik(A - B)$$

$$-\kappa(Ae^{ika} + Be^{-ika}) = ik\,(Ae^{ika} - Be^{-ika}) \ .$$

That system has nontrivial solution if the determinant is equal to zero. Writing it as

$$(\kappa - ik)A + (\kappa + ik)B = 0$$

$$e^{ika}(\kappa + ik)A + e^{-ika}(\kappa - ik)B = 0 \ ,$$

we must demand that

$$\begin{vmatrix} \kappa - ik & \kappa + ik \\ e^{ika}(\kappa + ik) & e^{-ika}(\kappa - ik) \end{vmatrix} = 0\,,$$

which gives

$$(\kappa - i k)^2 e^{-ika} - (\kappa + i k)^2 e^{ika} = 0 \ .$$

Real part of above given relation is automatically zero. For the imaginary part we have

$$(\kappa^2 - k^2)\sin ka + 2k\kappa\cos ka = 0 \ ,$$

which is written as

$$(\kappa^2 - k^2) + 2k\kappa\cot ka = 0$$

or

$$\tan ka = \frac{2k\kappa}{k^2 - \kappa^2} \ .$$

Using the expressions of k and κ it may be written as

$$\tan\left(\frac{a\sqrt{2ME}}{\hbar}\right) = \frac{2\sqrt{E(U_0 - E)}}{2E - U_0} \ .$$

It is obvious, that the last equation is not solvable analytically. It can be solved numerically or graphically.

We shortly show how to solve it graphically. At first we solve the equation

$$(\kappa^2 - k^2) + 2k\kappa\cot ka = 0$$

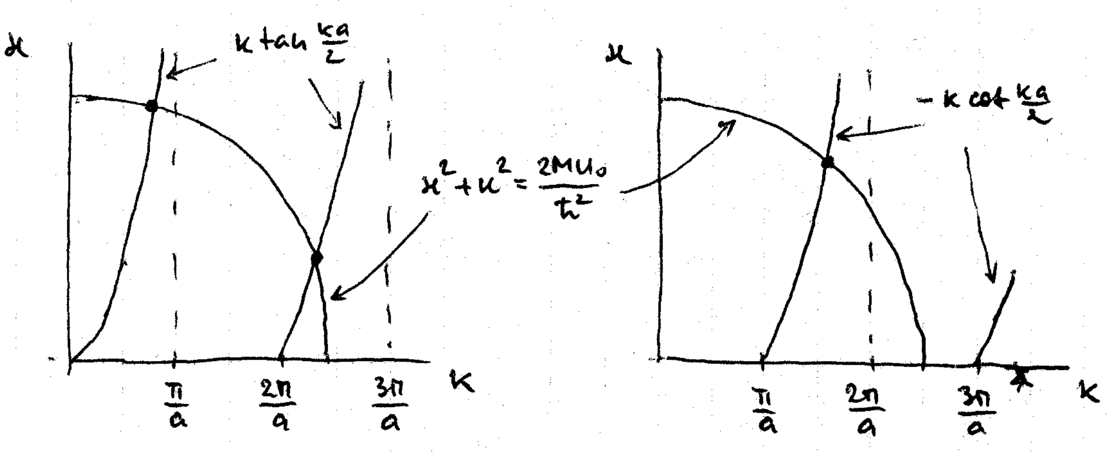
for κ

$$\kappa = k\tan\frac{ka}{2}, \quad \kappa = -k\cot\frac{ka}{2} \ .$$

Next we draw the graphs of both functions using $\kappa - k$ coordinate frame and use the relation between κ and k

$$\kappa^2 + k^2 = \frac{2MU_0}{\hbar^2} \ .$$

It is a circle in $\kappa - k$ frame with radius $r = \sqrt{2MU_0}/\hbar$. The common points correspond to possible energy values: we find the values of k (or κ) and calculate E.



On figures we see that inside the well there is always finite number of possible energy states (minimum is 1 state) and it depends how large U_0 is. In our case thare is three energy levels.