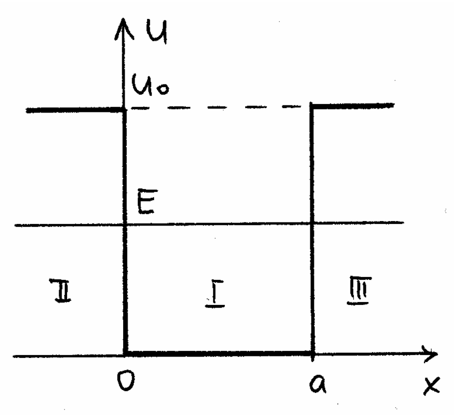
5. Potential well

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



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

where

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

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

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

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

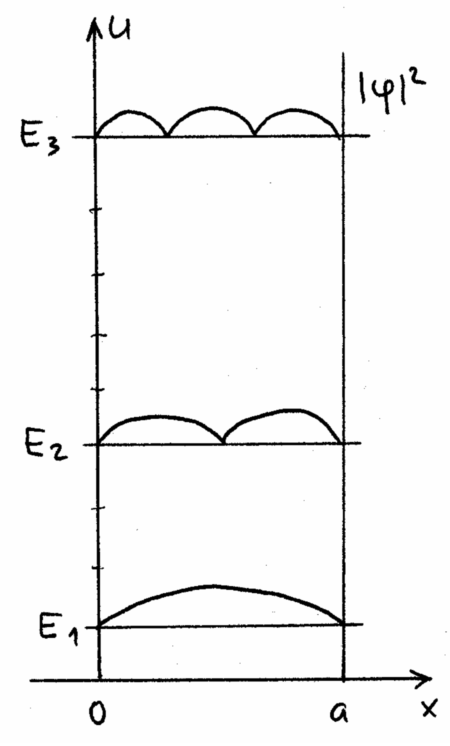
$$A(e^{ika} - e^{-ika}) \equiv 2iA\sin(ka) = 0 \ .$$

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

$$\sin(ka) = 0$$

from which

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



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

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

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

Orthonormed wave functions are

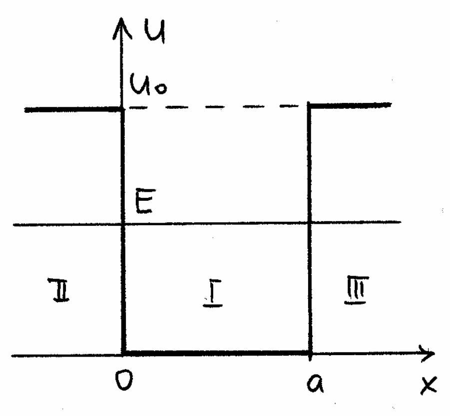
$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} \ .$$

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. 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 coplicated problem, since wave functions in regions II and III are nonzero. It appears that we have no analytical solution at all.

General solutions for different regions are

$$\psi_I(x) = A e^{ikx} + B e^{-ikx} \;, \quad \psi_{II}(x) = C e^{\kappa x} \;, \quad \psi_{III}(x) = D e^{-\kappa x} \;.$$

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

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

$$A e^{ika} + B e^{-ika} = D e^{-\kappa a} \qquad ik(A e^{ika} - B e^{-ika}) = -\kappa D e^{-\kappa a} \;.$$

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

$$\kappa (A + B) = i k (a - B)$$

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

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

$$(\kappa - i k) A + (\kappa + i k) B = 0$$

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

we must demand that

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

whic gives

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

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

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

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 consider how to solve the problem graphically. At first we solve the equation

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

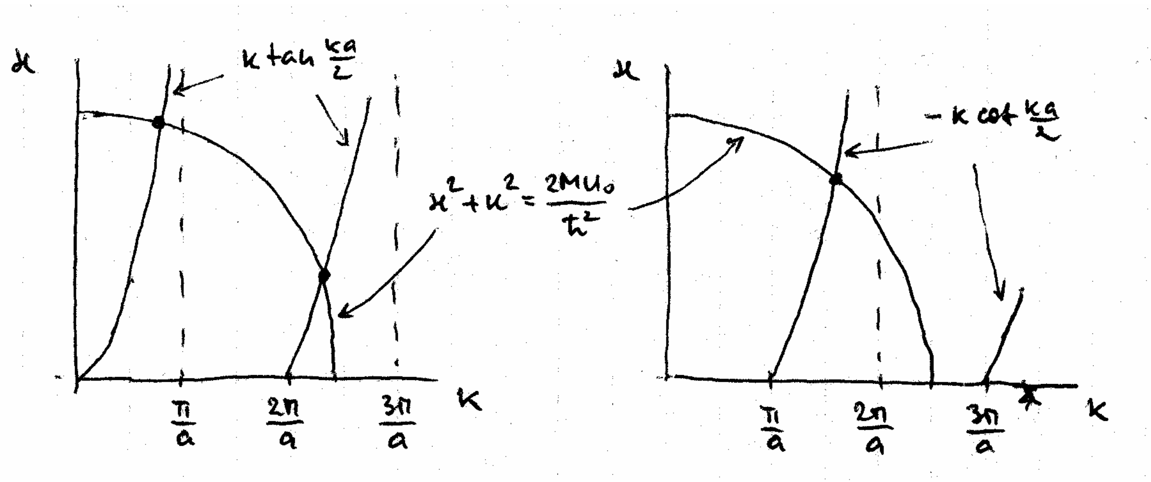
for κ

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

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.

6. Harmonic oscillator

In classical physics if we consider the parabolic potential energy (parabolic potential well) $U = kx^2/2$ (elastic force $F = - kx$) we get harmonic oscillations. Frequency is equal to $\omega = \sqrt{k/M}$, where M is the mass of oscillating body. Energy of oscillations is continuous.

Every body oscillating harmonically is called harmonic oscillator. Harmonic oscillator has several applications (small oscillations in twoatomic molecule, in crystal atoms oscillate and so on). In microworld the behaviour of harmonic oscillator is quite different from the classical one: energy is discrete and the probability disribution is different from the classical one. Next we prove it solving the corresponding Schrödinger equation. As we see, it is quite complicated procedure, since the differential equation we have is different the ones used in classical physics.

Let us consider the following potential energy

$$U(x) = \frac{M\omega^2 x^2}{2} .$$

Next we must solve the following Schrödinger equation

$$-\frac{\hbar^2}{2M}\frac{d^2\psi(x)}{dx^2} + \frac{M\omega^2 x^2}{2}\psi(x) = E\psi(x) .$$

6.1 Change of variables. We give the detailed solution, since it has several steps. The first one is to change variables and write the equation with less constants. In our case we define

$$\xi = \sqrt{\frac{M\,\omega}{\hbar}}\,x , \qquad \lambda = \frac{2E}{\hbar\,\omega}$$

and write our equation as

$$-\frac{d^2\psi(\xi)}{d\xi^2} + \xi^2\psi(\xi) = \lambda\psi(\xi) \quad \text{or} \quad -\psi''(\xi) + \xi^2\psi(\xi) = \lambda\psi(\xi) .$$

6.2 Asymptotical solution. Since the variable is not restricted we must find out whether there exist finite solutions if the variables tend to infinity. If $|\xi| \to \infty$, we demand that $\psi(\xi) \to 0$.

If $|\xi| >> \lambda$, we have $-\psi''(\xi) + \xi^2\psi(\xi) = 0$. It is possible to verify that now the possible approximate solution which tends to zero is

$$\psi(\xi) = e^{-\frac{\xi^2}{2}} .$$

Similarly the solution is also $\exp(\xi^2 / 2)$, but it is unphysical since it infinitely increases.

6.3 Power series. Having asymptotical solution we next try to find the general solution in form

$$\psi(\xi) = v(\xi)e^{-\frac{\xi^2}{2}} ,$$

where $v(\xi)$ is a new function we must find. Substituting the above given solution to our Scrödinger equation we for $v(\xi)$ the following differential equation

$$v'' - 2\xi v' + (\lambda - 1)v = 0 \ .$$

Next we assume, that $v(\xi)$ is expressed as a following power series function

$$v(\xi) = \sum_{r=0} a_r \xi^r \ .$$

Whether the serie is finite or infinite, we analyse later. Calculating derivatives

$$v'(\xi) = \sum_{r=0} r a_r \xi^{r-1}$$

and

$$v''(\xi) = \sum_{r=0} r(r-1) a_r \xi^{r-2} \equiv \sum_{s=0} (s+2)(s+1) a_{s+2} \xi^s \ ,$$

(we changed r to $s = r$-2). After substitution to our differential equation, we get

$$\sum_{r=0} (r+2)(r+1) a_{r+2} \xi^r - 2\sum_{r=0} r a_r \xi^r + (\lambda - 1)\sum_{r=0} a_r \xi^r = 0 \ .$$

Taking the term before ξ^r equal to zero, we have

$$a_{r+2} = \frac{2r + 1 - \lambda}{(r+2)(r+1)} a_r \ .$$

We got the formula to calculate the coefficients a_r. One of the solutions is the even series function

$$a_0 \neq 0 \qquad ja \qquad a_1 = 0 \ ,$$

and other the even series function

$$a_1 \neq 0 \qquad ja \qquad a_0 = 0 \ .$$

Now we analyse the large ξ behaviour of $v(\xi)$. When $\xi \to \infty$ we see that $v(\xi) \to \infty$, since it has identical limiting behavior with e^{ξ^2}. For large ξ we have

$$\frac{a_{r+2}}{a_r} \approx \frac{2}{r} \ ,$$

which is the same as for e^{ξ^2} .

Therefore at large values of ξ

$$v(\xi) \approx e^{\xi^2}$$

and $\psi(\xi) = v(\xi) e^{-\frac{\xi^2}{2}}$ is not finite. Therefore the power series function must be finite. It means that serie terminates on some value n (we have polynomials)

$$a_n \neq 0 \qquad ja \qquad a_{n+2} = 0 \ .$$

From $a_{n+2} = \dfrac{2n+1-\lambda}{(n+2)(n+1)} a_n = 0$ we get that

$$\lambda = 2n+1\,, \quad (n = 0,1,2,...)\,.$$

We got the first important result: to avoid infinities the parameter λ must be discrete and have the above given values.

6.4 Energy. Since the parameter λ was related with energy, we get that the only possible energy values are given as follows

$$E_n = \hbar\omega\,(n + \frac{1}{2})\,, \quad n = 0,1,2,... \ .$$

Therefore the energy of quantum oscillator is discrete, difference between the neighbour levels is equal to $\hbar\omega$. The minimal energy is nonzero

$$E_0 = \frac{\hbar\omega}{2} \ ,$$

therefore the quantum oscillator always „moves“ and cannot be at rest.

6.5 Eigenfunctions. Next we try to find eigenfunctions corresponding to energy E_n. For each $\lambda = 2n+1$ we get certain polynomial which is called Hermite polynomial

$$v_n(\xi) = H_n(\xi) \ .$$

Hermite polynomials are solutions of the following differential equation

$$H_n''(\xi) - 2\xi\, H_n'(\xi) + 2nH_n(\xi) = 0 \ .$$

Eigenfunctions are expressed as

$$\psi_n(\xi) = A_n H_n(\xi) e^{-\frac{\xi^2}{2}} \ ,$$

or using the variable *x*

$$\psi_n(x) = A_n H_n(\sqrt{\frac{M\omega}{\hbar}}\, x) e^{-\frac{M\omega x^2}{2\hbar}} \ .$$

A_n is normalization constant.

6.6 Some properties of Hermite polynomials. Before going to calculations we write down some useful properties of Hermite polynomials. It appears that our calculations simplify if we introduce certain helping function which is called the generating function. It is defined as follows

$$F(s,\xi) = e^{-s^2+2s\xi} \equiv e^{\xi^2-(s-\xi)^2} \ .$$

The use of generating function is that it should be expressed, using Hermite polynomials, as follows

$$F(s,\xi) = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n \quad .$$

In order to prove it we at first give some useful relations for $F(s,\xi)$. Calculating

$$\frac{\partial F}{\partial s} = -2(s-\xi)\, e^{-s^2+2s\xi} \equiv 2(\xi - s)F$$

and

$$\frac{\partial F}{\partial \xi} = 2s\, e^{-s^2+2s\xi} \equiv 2sF$$

we see that $F(s,\xi)$ satisfies the following differential equation

$$\frac{\partial F}{\partial s} + \frac{\partial F}{\partial \xi} = 2\xi\, F \quad .$$

Calculating

$$\frac{\partial^2 F}{\partial \xi^2} = 4s^2 F$$

we see that $F(s,\xi)$ satisfies the following second order differential equation

$$\frac{\partial^2 F}{\partial \xi^2} - 2\xi \frac{\partial F}{\partial \xi} + 2s \frac{\partial F}{\partial s} = 0 \quad .$$

Proof. Now we shall prove that the power series expansion of $F(s,\xi)$ also satisfies the above given differential equation. Calculating derivatives

$$\frac{\partial^2 F}{\partial \xi^2} = \sum_{n=0}^{\infty} \frac{H_n''(\xi)}{n!} s^n \;, \quad \frac{\partial F}{\partial \xi} = \sum_{n=0}^{\infty} \frac{H_n'(\xi)}{n!} s^n \;, \quad \frac{\partial F}{\partial s} = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} n s^{n-1}$$

and substituting them to differential equation, we get

$$\sum_{n=0}^{\infty} \frac{s^n}{n!} (H_n'' - 2\xi\, H_n' + 2nH_n) = 0 \quad .$$

The left side is identically equal to zero, if and only if H_n are Hermite polynomials.

Next we derive the general expression for calculating Hermite polynomials. It is possible to verify that

$$H_n(\xi) = \left[\frac{d^n}{ds^n} F(s,\xi) \right]_{s=0} \equiv \left[\frac{d^n}{ds^n} e^{\xi^2-(s-\xi)^2} \right]_{s=0} =$$

$$= e^{\xi^2} \left[\frac{d^n}{ds^n} e^{-(s-\xi)^2} \right]_{s=0} \equiv (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} (e^{-\xi^2}) \ ,$$

which gives

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} (e^{-\xi^2}) \ .$$

(here the coefficient before ξ^n is always 2^n).

Some examples

$$H_0(\xi) = 1 , \quad H_1(\xi) = 2\xi , \quad H_2(\xi) = 4\xi^2 - 2 ,$$

$$H_3(\xi) = 8\xi^3 - 12\xi , \quad H_4(\xi) = 16\xi^4 - 48\xi^2 + 12 \ .$$

Some useful relations

$$H_n'(\xi) = 2nH_{n-1}(\xi) , \quad \xi H_n(\xi) = \frac{1}{2} H_{n+1}(\xi) + nH_{n-1}(\xi) \ .$$

6.7 Normalization of eigenfunctions. Let us prove that eigenfunctions are orthonormal and find normalization coefficient A_n. Consider the integral

$$\int_{-\infty}^{+\infty} \psi_m{}^*(x) \psi_n(x) dx \ .$$

Going to variable ξ and using the general expressions of eigenfunctions via Hermite polynomials, we get

$$\int_{-\infty}^{+\infty} \psi_m{}^*(x) \psi_n(x) dx = A_m{}^* A_n \sqrt{\frac{\hbar}{M\omega}} \int_{-\infty}^{+\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi \ .$$

In the next paragraph we prove that

$$\int_{-\infty}^{+\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi = \begin{cases} \sqrt{\pi}\, 2^n n! , & kui \quad m = n , \\ 0 \quad , & kui \quad m \neq n . \end{cases}$$

If $m \neq n$, the integraal is zero, therefore the different eigenfunctions are orthogonal.

If $m = n$ we normalize the function to 1. We have

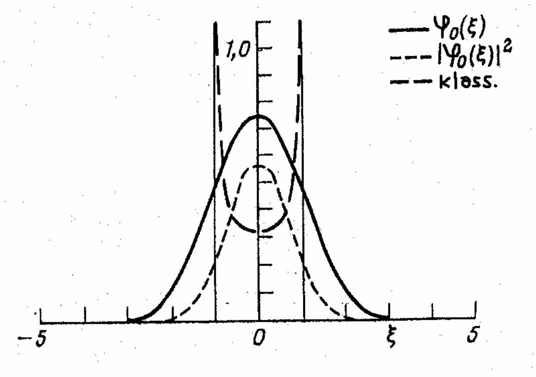
$$|A_n|^2 \sqrt{\frac{\hbar}{M\omega}} \sqrt{\pi}\, 2^n n! = 1 \ ,$$

which gives (we choose A_n to be real)

$$A_n = \sqrt{\frac{\sqrt{M\omega}}{\sqrt{\pi\hbar}2^n n!}} \equiv (\frac{M\omega}{\hbar})^{1/4} \frac{1}{\sqrt{\sqrt{\pi}2^n n!}} \ .$$

Eigenfunctions in a final form are

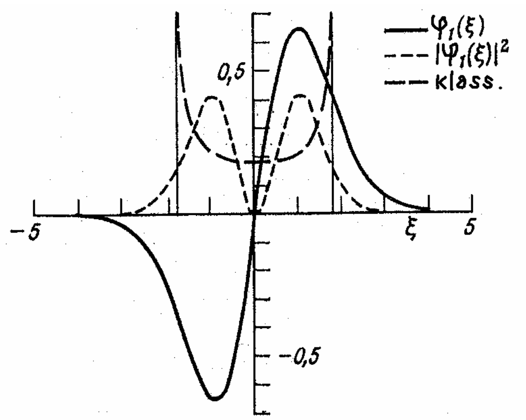
$$\psi_n(x) = (\frac{M\omega}{\hbar})^{1/4} \frac{1}{\sqrt{\sqrt{\pi}\, 2^n n!}} H_n(\sqrt{\frac{M\omega}{\hbar}}\, x) e^{-\frac{M\omega x^2}{2\hbar}} \ .$$



Some special cases. Ground state.

$$E_0 = \hbar\omega/2\,, \quad \psi_0(x) = (\frac{M\omega}{\pi\hbar})^{1/4} e^{-\frac{M\omega x^2}{2\hbar}} \ .$$

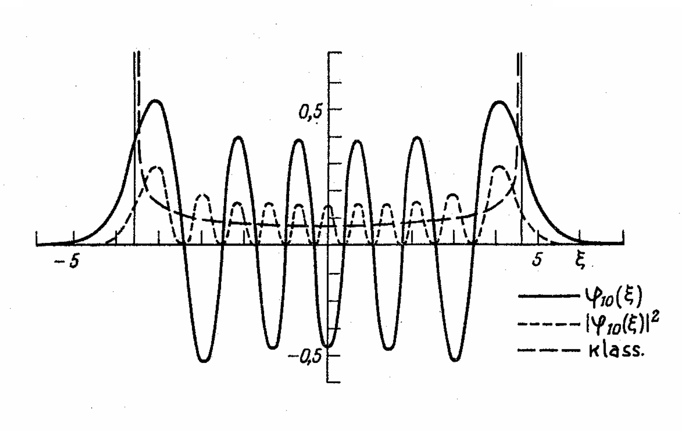
Behaviour of quantum oscillator is different from the classical one. Probability density is maximal in centre (equilibrium point) and is nonzero outside the classsical region.



First exited state. $E_1 = 3\hbar\omega/2$ and

$$\psi_1(x) = (\frac{M\omega}{\hbar})^{3/4} (\frac{4}{\pi})^{1/4} x e^{-\frac{M\omega x^2}{2\hbar}} \ .$$

Behaviour of quantum and classical oscillators are also different.



n = 10. The classical and quantum oscillators behave differently, but in the case of large n we see that the average of quantum probability distribution is practically equal to the probability of classical oscillator. That is the general result, since in the limit of large quantum numbers we have the same results as in classical physics.

7. Harmonic oscillator (integrals)

Here we discuss how to calculate integrals. For each special case there are certain rules and procedures how to do it.

In the previous paragraph we used the integral

$$\int_{-\infty}^{+\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi = \begin{cases} \sqrt{\pi}\, 2^n n!\,, & if \quad m = n\,, \\ 0 \quad, & if \quad m \neq n\,. \end{cases}$$

Here we prove how it is calculated. The general principle is that using the generating function we try to find such a integral, which is expressed through above given integrals. In our case it is integral

$$\int_{-\infty}^{+\infty} F(s,\xi) F(t,\xi) e^{-\xi^2} \, d\xi \ .$$

We write it down using the direct expression of generating function (left side of the following equality) and next using the expression via the Hermite polynomials (right side of the following equality)

$$\int_{-\infty}^{+\infty} e^{-s^2+2s\xi-t^2+2t\xi-\xi^2} \, d\xi = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \int_{-\infty}^{+\infty} \frac{H_m(\xi) H_n(\xi)}{m!\,n!} s^m t^n e^{-\xi^2} \, d\xi \ .$$

As we see, on the right side there are just the integrals we try to calculate. We now must calculate the integral on the right side (which in principle simple, since we must integrate exponents) and then expand the result as series on s and t.

The left side integraal gives us

$$\int_{-\infty}^{+\infty} e^{-s^2+2s\xi-t^2+2t\xi-\xi^2} \, d\xi = e^{2st} \int_{-\infty}^{+\infty} e^{-(\xi-s-t)^2} \, d\xi = e^{2st} \int_{-\infty}^{+\infty} e^{-u^2} \, du = \sqrt{\pi}\, e^{2st} \quad .$$

(In the last step we changed the variable: $u = \xi - s - t$ and used the table integraal

$$\int_{0}^{\infty} e^{-r^2 x^2} \, dx = \frac{\sqrt{\pi}}{2r}\,, \qquad r > 0 \ .)$$

Expanding the result as series on *s* and *t*, and demanding that it is equal to the right side, we get

$$\sqrt{\pi}\, e^{2st} \equiv \sqrt{\pi} \sum_{m=0}^{\infty} \frac{2^m s^m t^m}{m!} = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{s^m t^n}{m!\,n!} \int_{-\infty}^{+\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} \, d\xi \ .$$

Comparing the expressions on the left and right side we obtain the integrals we have used in the previous paragraph.

Next we give three more useful integrals (proofs are given in Appendix).

First integral.

$$\int_{-\infty}^{+\infty} \psi_n \frac{d\psi_m}{dx} dx = \begin{cases} \sqrt{\frac{M\omega}{\hbar}}\sqrt{\frac{n+1}{2}}, & if \quad m = n+1, \\ -\sqrt{\frac{M\omega}{\hbar}}\sqrt{\frac{n}{2}}, & if \quad m = n-1, \\ 0, & if \quad m \neq n \pm 1. \end{cases}$$

Second integral.

$$\int_{-\infty}^{+\infty} \psi_n x \psi_m \, dx = \begin{cases} \sqrt{\frac{\hbar}{M\omega}}\sqrt{\frac{n+1}{2}}, & if \quad m = n+1, \\ \sqrt{\frac{\hbar}{M\omega}}\sqrt{\frac{n}{2}}, & if \quad m = n-1, \\ 0, & if \quad m \neq n \pm 1. \end{cases}$$

Third integral.

$$\int_{-\infty}^{+\infty} \psi_n x^2 \psi_m \, dx = \begin{cases} \frac{\hbar}{2M\omega}(2n+1), & if \quad m = n, \\ \frac{\hbar}{2M\omega}\sqrt{(n+1)(n+2)}, & if \quad m = n+2, \\ \frac{\hbar}{2M\omega}\sqrt{n(n-1)}, & if \quad m = n-2, \\ 0, & if \quad m \neq n \; and \; m \neq n \pm 2. \end{cases}$$

Example 1. Mean value of energy. Mean value of potential energy for state $\psi_n(x)$. Using the third integral, we get

$$< U >_n = \int_{-\infty}^{+\infty} \psi_n(x) \frac{M\omega^2 x^2}{2} \psi_n(x) dx = \frac{M\omega^2}{2} \int_{-\infty}^{+\infty} x^2 \psi_n^2(x) dx = \frac{\hbar\omega}{4}(2n+1) \equiv \frac{E_n}{2} \; .$$

The result is the same as in the classical case.

Since the energy operator is a sum of operators of kinetic and potential energy

$$\hat{H} = \hat{T} + U \; ,$$

we without calculations can say that also

$$< T >_n = \frac{E_n}{2} \; .$$

(Always $< \hat{H} >= E_n$).

Since $\hat{T} = -\frac{\hbar^2}{2M}\frac{d^2}{dx^2} = \frac{\hat{p}^2}{2M}$, we find the mean value of momentum square.

$$< T >_n = \frac{1}{2M} < p^2 >_n = \frac{E_n}{2} \ ,$$

therefore

$$< p^2 >_n = M\, E_n = \frac{M\,\hbar\omega}{2}(2n+1) \ .$$

Example 2. Uncertainty relations for oscillator. At first we demonstrate that

$$< x >_n = \int_{-\infty}^{+\infty} \psi_n(x)\, x\, \psi_n(x)\, dx = 0 \ ,$$

$$< p >_n = -i\hbar \int_{-\infty}^{+\infty} \psi_n(x) \frac{d\psi_n(x)}{dx} dx = 0 \ .$$

First result follows from tha fact that under the first integraal there is always an odd function, the second follows from our first integral.

Next we deal with root mean square deviation

$$(\Delta x)^2 \equiv < (x - < x >)^2 > = < x^2 > - < 2x < x >> + << x >^2 > \equiv < x^2 > -2 < x >^2 + < x >^2 =$$

$$= < x^2 > - < x >^2 \ .$$

Since $< x >_n = 0$ and using the third integral, we get

$$(\Delta x)_n^2 = < x^2 >_n = \int_{-\infty}^{+\infty} x^2 \psi_n^2(x)\, dx = \frac{\hbar}{2M\omega}(2n+1) \ .$$

Above we find that

$$< p^2 >_n = M\, E_n = \frac{M\,\hbar\omega}{2}(2n+1) \ .$$

Therefore we have

$$(\Delta x)_n^2 (\Delta p)_n^2 = \frac{\hbar^2}{4}(2n+1)^2 \ ,$$

and the standard form of uncertainty relation is

$$\Delta x_n \cdot \Delta p_n = \frac{\hbar}{2}(2n+1) \ .$$

For the ground state $n = 0$ it is minimal

$$\Delta x \cdot \Delta p = \frac{\hbar}{2} \ ,$$

for other states it increases linearly on *n*. Here we see that the minimal value of products of uncertinties is indeed $\hbar/2$, but mostly it is greater.

Näide 3. Dipole transitions. Next we see see that the selection rules for electromagnetic transitions for dipole radiation are determined by the integral $\int_{-\infty}^{+\infty}\psi_n(x)\,x\,\psi_m(x)\,dx$. Only these transitions are allowed when that integraal is nonzero. From the above given we have

$$\int_{-\infty}^{+\infty}\psi_n(x)\,x\,\psi_m(x)\,dx \neq 0, \quad if \quad m = n \pm 1 \ .$$

Transitions are allowed between the neighbouring levels and oscillator always radiates or absorbs energy equal to $\pm\hbar\omega$.

Appendix:

1. First integral. Expressing it with the help of Hermite polynomials we have

$$\int_{-\infty}^{+\infty}\psi_n(x)\frac{d\psi_m(x)}{dx}dx = \int_{-\infty}^{+\infty}\psi_n(\xi)\frac{d\psi_m(\xi)}{d\xi}d\xi =$$

$$= A_n A_m \int_{-\infty}^{+\infty} H_n(\xi)\,e^{-\frac{\xi^2}{2}}\frac{d}{d\xi}\left(H_m(\xi)\,e^{-\frac{\xi^2}{2}}\right)d\xi$$

We calculate the next integral using the following combination of generating function.

$$\int_{-\infty}^{+\infty} F(s,\xi)\,e^{-\frac{\xi^2}{2}}\frac{\partial}{\partial\xi}\left(F(t,\xi)\,e^{-\frac{\xi^2}{2}}\right)d\xi = \int_{-\infty}^{+\infty} e^{-s^2+2s\xi-\frac{\xi^2}{2}}\frac{\partial}{\partial\xi}\left(e^{-t^2+2t\xi-\frac{\xi^2}{2}}\right)d\xi =$$

$$= \int_{-\infty}^{+\infty} e^{-s^2-t^2-\xi^2+2s\xi+2t\xi}(-\xi+2t)\,d\xi = e^{2st}\int_{-\infty}^{+\infty} e^{-(\xi-s-t)^2}\left[-(\xi-s-t)+t-s\right]d\xi =$$

$$= (t-s)\,e^{2st}\int_{-\infty}^{+\infty} e^{-(\xi-s-t)^2}\,d\xi = \sqrt{\pi}\,(t-s)\,e^{2st} \ .$$

Next we express these integrals using Hermite polynomials

$$\int_{-\infty}^{+\infty} F(s,\xi)\,e^{-\frac{\xi^2}{2}}\frac{\partial}{\partial\xi}\left(F(t,\xi)\,e^{-\frac{\xi^2}{2}}\right)d\xi = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{s^n t^m}{n!\,m!}\int H_n(\xi)e^{-\frac{\xi^2}{2}}\frac{d}{d\xi}\left[H_m(\xi)e^{-\frac{\xi^2}{2}}\right]d\xi =$$

$$= \sqrt{\pi}\,(t-s)\,e^{2st} = \sqrt{\pi}\,(t-s)\sum_{n=0}^{\infty}\frac{(2st)^n}{n!} = \sqrt{\pi}\sum_{n=0}^{\infty}\frac{2^n\left(s^n t^{n+1} - s^{n+1}t^n\right)}{n!} \ .$$

Comparing the expressions of both series, we get as a final result

$$\int_{-\infty}^{+\infty} H_n(\xi) e^{-\frac{\xi^2}{2}} \frac{d}{d\xi}\left[H_m(\xi) e^{-\frac{\xi^2}{2}} \right] d\xi = \begin{cases} \sqrt{\pi}\, 2^n (n+1)!, & m = n+1 \\ -\sqrt{\pi}\, 2^{n-1} n!, & m = n-1 \\ 0, & other\ cases \end{cases}$$

Substituting the normalisation coefficient, we get the first integral.

2. <u>Second integral.</u> That integral is calculated without the generating function. We use the properties of Hermite polynomials and express $\xi H_n(\xi)$ as a superposition of other polynomials

$$\int_{-\infty}^{+\infty} \psi_n(x)\, x \psi_m(x)\, dx = \frac{\hbar}{M\omega} A_n A_m \int_{-\infty}^{+\infty} H_n(\xi) \xi H_m(\xi) e^{-\xi^2} d\xi =$$

$$= \frac{\hbar A_n A_m}{M\omega} \int_{-\infty}^{+\infty} H_n(\xi) (\frac{1}{2} H_{m+1}(\xi) + m H_{m-1}(\xi)) e^{-\xi^2} d\xi =$$

$$= \frac{\hbar A_n A_m}{M\omega} \left\{ \frac{1}{2} \int_{-\infty}^{+\infty} H_n(\xi) H_{m+1}(\xi) e^{-\xi^2} d\xi + m \int_{-\infty}^{+\infty} H_n(\xi) H_{m-1}(\xi) e^{-\xi^2} d\xi \right\} .$$

To obtain the final result we must use integrals we calculated at first.

3. <u>Third integral.</u> Third integral

$$\int_{-\infty}^{+\infty} \psi_n(x)\, x^2 \psi_m(x)\, dx = (\frac{\hbar}{M\omega})^{\frac{3}{2}} A_n A_m \int_{-\infty}^{+\infty} H_n(\xi) \xi^2 H_m(\xi) e^{-\xi^2} d\xi$$

is calculated with the help of generating function. We start with the integral

$$\int_{-\infty}^{+\infty} F(s,\xi) F(t,\xi) \xi^2 e^{-\xi^2} d\xi = e^{2st} \int_{-\infty}^{+\infty} e^{-(\xi - s - t)^2} \xi^2 d\xi = \sqrt{\pi}\, e^{2st} \left[\frac{1}{2} + (s+t)^2 \right] =$$

$$= \sqrt{\pi} \left\{ \sum_{n=0}^{\infty} \frac{2^n (s^{n+2} t^n + s^n t^{n+2})}{n!} + \sum_{n=0}^{\infty} \frac{2^{n-1} s^n t^n (2n+1)}{n!} \right\} .$$

On the other hand

$$\int_{-\infty}^{+\infty} F(s,\xi) F(t,\xi) \xi^2 e^{-\xi^2} d\xi = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{s^n t^m}{n! m!} \int_{-\infty}^{+\infty} H_n(\xi) H_m(\xi) \xi^2 e^{-\xi^2} d\xi ,$$

which finally gets

$$\int_{-\infty}^{+\infty} H_n(\xi)H_m(\xi)\xi^2 e^{-\xi^2}d\xi = \begin{cases} \sqrt{\pi}\,2^{n-1}n!(2n+1), & m=n \\ \sqrt{\pi}\,2^{n}(n+2)!, & m=n+2 \\ \sqrt{\pi}\,2^{n-2}n!, & m=n-2 \\ 0, & other\ cases \end{cases}$$

and leads to third integral.

8. Harmonic oscillator (representation of filling numbers)

1. Harmonic oscillator. Next we shortly discuss the representation of harmonic oscillator using raising and lowering operators. That method is used in quantum field theory where the quantum field is interpreted as some set of microparticles.

We had the following Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + \frac{M\,\omega^2 x^2}{2} \ .$$

Let us define two new operators

$$\hat{a} = \sqrt{\frac{M\omega}{2\hbar}}\,x + \frac{i}{\sqrt{2M\,\hbar\,\omega}}\,\hat{p} \equiv \sqrt{\frac{M\omega}{2\hbar}}\,x + \sqrt{\frac{\hbar}{2M\omega}}\frac{d}{dx} \ ,$$

$$\hat{a}^+ = \sqrt{\frac{M\omega}{2\hbar}}\,x - \frac{i}{\sqrt{2M\,\hbar\,\omega}}\,\hat{p} \equiv \sqrt{\frac{M\omega}{2\hbar}}\,x - \sqrt{\frac{\hbar}{2M\omega}}\frac{d}{dx} \ .$$

Direct calculation gives (prove!) that $\hat{a}$ and $\hat{a}^+$ satisfy the following commutation relation

$$\left[\hat{a}\,,\hat{a}^+\right] = 1 \ .$$

Operators $\hat{a}$ and $\hat{a}^+$ are not Hermitean, but are conjugated to each other.

Direct calculations demonstrate that applying them to eigenfunctions, the results are

$$\hat{a}\,\psi_n(x) = \sqrt{n}\,\psi_{n-1}(x) \ ,$$

$$\hat{a}^+\psi_n(x) = \sqrt{n+1}\,\psi_{n+1}(x) \ .$$

Here we see that operator $\hat{a}$ acting on state $\psi_n(x)$ with energy E_n leads to state $\psi_{n-1}(x)$ with energy $E_{n-1} = E_n - \hbar\omega$ and operator $\hat{a}^+$ similarly to state $\psi_{n+1}(x)$ with energy $E_{n+1} = E_n + \hbar\omega$. Therefore they are lowering and raising operators (in quantum field theory these operators are called annihilation and creation operators). In the first case energy $\hbar\omega$ is absorbed, in the second case energy $\hbar\omega$ is radiated.

Using operators $\hat{a}$ and $\hat{a}^+$ the Hamiltonia operator is expressed as

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{a}\hat{a}^+ + \hat{a}^+\hat{a}) \ .$$

Using commutation relations ($\hat{a}\hat{a}^+ = \hat{a}^+\hat{a} + 1$) it is also expressed as

$$\hat{H} = \hbar\omega(\hat{a}^+\hat{a} + \frac{1}{2})$$

Since $(\hat{a}^+\hat{a})\psi_n = \sqrt{n}\,\hat{a}^+\psi_{n-1} = n\psi_n$, it is easy to verify that $\hat{H}\psi_n = \hbar\omega(n + 1/2)\psi_n$. If we treat the radiation as a systems of particles (similarly, as A. Einstein interpreted electromagnetic radiation as a set of photons), we may interprete *n* as a number of particles or filling number and then the operator

$$\hat{N} = \hat{a}^+\hat{a}$$

as a particle number operator, since $\hat{N}\psi_n = n\psi_n$.

2. Model example. Next we consider the following problem. Assume that we know nothing about the harmonic oscillator representation, but we have the following Hamiltonian operator

$$\hat{H} = \hbar\omega(\hat{a}^+\hat{a} + \frac{1}{2})$$

and nonhermitean operators $\hat{a}$ and $\hat{a}^+$ satisfy

$$\left[\hat{a}, \hat{a}^+\right] = 1 \ .$$

Next we analyse properties of a given system, using the commutation relations and in addition assume that the system has a minimal energy state.

At fist we find the commutation relation for $\hat{H}$ and operators $\hat{a}$ and $\hat{a}^+$. These are

$$\left[\hat{H}, \hat{a}\right] = -\hbar\omega\hat{a} \ , \quad \left[\hat{H}, \hat{a}^+\right] = \hbar\omega\hat{a}^+ \ .$$

We prove here the first one, using $\hat{a}\hat{a}^+ = \hat{a}^+\hat{a} + 1$:

$$\left[\hat{H}, \hat{a}\right] = \frac{\hbar\omega}{2}\left[\hat{a}\hat{a}^+ + \hat{a}^+\hat{a}, \hat{a}\right] = \frac{\hbar\omega}{2}(\hat{a}^+\hat{a}\hat{a} - \hat{a}\hat{a}\hat{a}^+) = \frac{\hbar\omega}{2}(\hat{a}^+\hat{a}\hat{a} - \hat{a}\hat{a}^+\hat{a} - \hat{a}) =$$

$$= \frac{\hbar\omega}{2}(\hat{a}^+\hat{a}\hat{a} - \hat{a}^+\hat{a}\hat{a} - 2\hat{a}) = -\hbar\omega\hat{a} \ .$$

Similarly one can prove the second relation.

Operators $\hat{a}$ and $\hat{a}^+$ correspondingly lower and rise eigenvalue E_n of operator $\hat{H}$ by $\hbar\omega$.

Let us consider the eigenfunction $|n\rangle$ of $\hat{H}$ having energy E_n. We apply $\hat{a}$ and show that $\hat{a}|n\rangle$ ~ $|n-1\rangle$. Using

$$\hat{H}\,\hat{a}-\hat{a}\,\hat{H}=-\hbar\,\omega\,\hat{a}$$

and applying to $|n\rangle$, we get

$$\hat{H}\,(\hat{a}|n\rangle)-\hat{a}\,(E_n|n\rangle)=-\hbar\,\omega\,(\,\hat{a}|n\rangle)\ .$$

It may be written as

$$\hat{H}\,(\hat{a}|n\rangle)=(E_n-\hbar\,\omega)(\,\hat{a}\,|n\rangle)\ ,$$

which shows that $\hat{a}|n\rangle \sim |n-1\rangle$.

Using analogically

$$\hat{H}\,\hat{a}^{\,+}-\hat{a}^+\,\hat{H}=\hbar\,\omega\,\hat{a}^+$$

and applying to $|n\rangle$, we get

$$\hat{H}\,(\hat{a}^+|n\rangle)=(E_n+\hbar\,\omega)(\,\hat{a}^{\,+}|n\rangle)\ ,$$

which shows that $\hat{a}^+|n\rangle \sim |n+1\rangle$.

Therefore $\hat{a}^+$ and $\hat{a}$ are indeed rising and lowering operators (in quantum field theory radiation and annigilation operators).

Now we assume that there exists the state with minimal energy. We denote it $|0\rangle$. Since there are no states below it, that sate satisfies

$$\hat{a}|0\rangle=0\ .$$

Other states we get applying step by step operator $\hat{a}^+$

$$|1\rangle=\alpha_1\,\hat{a}^+|0\rangle\,,\quad |2\rangle=\alpha_2\,\hat{a}^+\hat{a}^+|0\rangle\,,\qquad \textit{and so on}\ ,$$

α_i are normalization coefficients.

Our Hamiltonian operator was

$$\hat{H}=\hbar\,\omega(\hat{a}^+\,\hat{a}+\frac{1}{2})\ .$$

Applying to state $|0\rangle$ and using $\hat{a}|0\rangle=0$ we get

$$\hat{H}|0\rangle = \frac{\hbar\omega}{2}|0\rangle \ .$$

Therefore minimal energy is $E_0 = \hbar\,\omega/2$.

For $|1\rangle$ we at first write

$$\hat{H}|1\rangle = \alpha_1\,\hbar\omega(\hat{a}^+\hat{a} + \frac{1}{2})\hat{a}^+|0\rangle \ .$$

In similar expressions we use $\hat{a}\,\hat{a}^+ = \hat{a}^+\hat{a} + 1$ one, two, or more times to move operators $\hat{a}^+$ left from operators $\hat{a}$ and then use $\hat{a}|0\rangle = 0$. For a given case the above given relation is used once, writing $\hat{a}^+\,\hat{a}\,\hat{a}^+ = \hat{a}^+\hat{a}^+\,\hat{a} + \hat{a}^+$, which gives

$$\hat{H}|1\rangle = \frac{3\hbar\omega}{2}\alpha_1\,\hat{a}^+|0\rangle \equiv \frac{3\hbar\omega}{2}|1\rangle \ .$$

Therefore the energy of $|1\rangle$ is $E_1 = 3\hbar\omega/2 = (1+1/2)\hbar\omega$.

Using operators $\hat{a}^+$ we can generate states

$$|n\rangle = \alpha_n(\hat{a}^+)^n|0\rangle$$

wiht energy $E_n = (n+1/2)\hbar\omega$. The number n is called filling number (interpreting it as particle system it is number of particles) for a given state. Operator

$$\hat{N} = \hat{a}^+\hat{a}$$

is called filling nymber (particle number) operator

$$\hat{N}|n\rangle = n|n\rangle \ .$$

Our model system was interesting, since we derived important physical results, basing only on commutation relations and some general assumptions (minimal energy).

9. Angular momentum in quantum mechanisc

9.1 Angular momentum operator. In classical physics angular momentum is defined as

$$\vec{L} = \vec{r} \times \vec{p} \ ,$$

the corresponding operator in quantum mechanics is

$$\hat{\vec{L}} = \vec{r} \times \hat{\vec{p}} \ .$$

In rectangular coordinates it has components

$$\hat{L}_x = -i\hbar\,(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}) \ , \quad \hat{L}_y = -i\hbar\,(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}) \ , \quad \hat{L}_z = -i\hbar\,(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}) \ .$$

Direct calculation gives the following commutation relations

$$\left[\hat{L}_x , \hat{L}_y\right] = i\hbar\,\hat{L}_z \ , \quad \left[\hat{L}_y , \hat{L}_z\right] = i\hbar\,\hat{L}_x \ , \quad \left[\hat{L}_z , \hat{L}_x\right] = i\hbar\,\hat{L}_y \ .$$

The components do not commute and are not simultaneously measureable. If we want exact values, then only one component is exatly measureable (other components are then arbitrary).

In addition to one component the square of angular momentum is simultaneously measureable. Indeed, the root is

$$\hat{\vec{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \ ,$$

and it is possible to verify that

$$\left[\hat{\vec{L}}^2 , \hat{L}_x\right] = 0 \ , \quad \left[\hat{\vec{L}}^2 , \hat{L}_y\right] = 0 \ , \quad \left[\hat{\vec{L}}^2 , \hat{L}_z\right] = 0 \ .$$

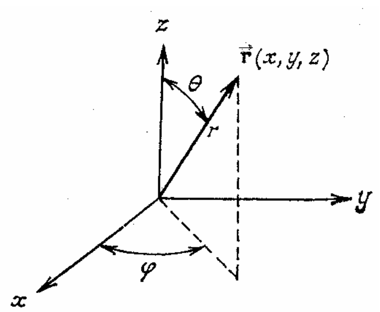
Next we choose the following measurable: square of angular momentum and z-component

$$\hat{\vec{L}}^2 \quad , \quad \hat{L}_z$$

and shall solve two eigenvalue problems

$$\hat{\vec{L}}^2\, Y = L^2\, Y \ , \quad \hat{L}_z\, Y = l_z\, Y \ .$$

9.2 Angular momentum in spherical coordinates. Since angular momentum is important in the case of central symmetric fields, it is useful to go to spherical coordinates.



$$x = r\sin\theta\cos\varphi \ ,$$

$$y = r\sin\theta\sin\varphi \ ,$$

$$z = r\cos\theta \ .$$

Since the calculation of components is quite tedious, we give only results.

$$\hat{L}_x = i\hbar(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}) \ ,$$

$$\hat{L}_y = i\hbar(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}) \ ,$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi} \ ,$$

$$\hat{\vec{L}}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] .$$

9.3. Eigenvalue problem of $\hat{L}_z$. We start from the z-component and its eigenvalue problem

$$\hat{L}_z\,\phi(\varphi) = l_z\phi(\varphi) ,$$

which gives

$$-i\hbar\frac{\partial\phi}{\partial\varphi} = l_z\phi \ .$$

The general solution is

$$\phi(\varphi) = e^{\frac{il_z}{\hbar}\varphi} \ .$$

The continuity condition

$$\phi(\varphi) = \phi(\varphi + 2\pi) \ ,$$

gives that

$$e^{\frac{il_z 2\pi}{\hbar}} = 1 \ .$$

That is possible, if

$$l_z = m\hbar \ , \quad kus\ m = 0, \pm 1, \pm 2, \ldots \ .$$

Therefore the eigenvalue problem we started with, is

$$\hat{L}_z\,\phi(\varphi) = m\hbar\phi(\varphi), \quad m = 0, \pm 1, \pm 2, \ldots \ ,$$

where the quatum number *m* is historically called the magnetic quantum number. In reality, it gives projections of angular momentum. Differently from classical physics the projections of angular momentum in quantum mechanics are discrete, not continuous.

Since we shall use the eigenfunctions of angular momentum projection in some cases separately we normed them separately. Writing

$$\phi(\varphi) = A\,e^{im\varphi} \ ,$$

where *A* is normalization factor, we from

$$\int_0^{2\pi} \phi^* \phi \, d\varphi = |A|^2 \int_0^{2\pi} e^{-im\varphi} e^{im\varphi} d\varphi = |A|^2 \, 2\pi = 1$$

have $A = 1/\sqrt{2\pi}$ (if possible, we always choose the normalization factors to be real numbers).

The final expression of eigenfunctions is

$$\phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} \ .$$

9.4 Eigenvalue problem of $\hat{\vec{L}}^2$. Next we consider the more complicated eigenvalue problem. We write it as

$$\hat{\vec{L}}^2 \, Y_\beta(\theta,\varphi) = \hbar^2 \beta \, Y_\beta(\theta,\varphi) \ ,$$

where the eigenvalue we try to find is denoted as β . Since $Y_\beta(\theta,\varphi)$ is at the same time the eigenfunction of $\hat{L}_z$ and we just find them, we represent $Y_\beta(\theta,\varphi)$ in form

$$Y_\beta(\theta,\varphi) = \frac{1}{\sqrt{2\pi}} P_{\beta m}(\theta) \, e^{im\varphi} \ .$$

If we use the direct expression of $\hat{\vec{L}}^2$, we have

$$-\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (\sin\theta \frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \right] Y_\beta(\theta,\varphi) = \hbar^2 \beta \, Y_\beta(\theta,\varphi) \ ,$$

and after substitution we get for $P_{\beta m}(\theta)$

$$\left[\frac{1}{\sin\theta} \frac{d}{d\theta} (\sin\theta \frac{d}{d\theta}) - \frac{m^2}{\sin^2\theta} \right] P_{\beta m}(\theta) = -\beta \, P_{\beta m}(\theta) \ .$$

The last problem is solved using the same general principles as in the harmonic oscillator case. Therefore we do not give here the exact derivation (you may find it in textbooks, if needed), but give some general remarks of how to do it.

9.5 New variable. It is useful to change the variable and take

$$w = \cos\theta \ ,$$

which has its values between –1 and +1. It gives differential equation

$$\frac{d}{dw} \left[(1-w^2) \frac{dP_{\beta m}}{dw} \right] + (\beta - \frac{m^2}{1-w^2}) P_{\beta m} = 0 \ ,$$

or the same as

$$P''_{\beta m} - \frac{2w}{1-w^2}P'_{\beta m} + (\frac{\beta}{1-w^2} - \frac{m^2}{(1-w^2)^2})P_{\beta m} = 0 \ .$$

9.6 Singular points. Since $-1 \le w \le 1$, we must analyse behaviour in singular points ± 1.

Near $w = 1$ the equation reduces to

$$P''_{\beta m} - \frac{1}{1-w}P'_{\beta m} - \frac{m^2}{4(1-w)^2}P_{\beta m} = 0$$

If we try to find solution in form

$$P_{\beta m}(w) = (1-w)^{\alpha}\left[a_0 + a_1(1-w) + ...\right] ,$$

where $a_0 \neq 0$, we get, demanding that the term before $\alpha - 2$ is zero, the condition

$$a_0(\alpha(\alpha-1) + \alpha - \frac{m^2}{4}) = a_0(\alpha^2 - \frac{m^2}{4}) = 0 \ .$$

It has two solutions

$$\alpha = \pm\frac{|m|}{2} \ .$$

It is obvious, that negative degree is unphysical, since if $w \to 1$, then $P \to \infty$. Therefore, if it is positive, there are no problems when $w \to 1$ and we choose

$$\alpha = \frac{|m|}{2} \ .$$

Analogically, for $w = -1$ we try to find solution in form

$$P_{\beta m}(w) = (1+w)^{\alpha}\left[b_0 + b_1(1+w) + ...\right]$$

and similarly find that

$$\alpha = \frac{|m|}{2} \ .$$

9.7 The general form of solution. Using the above given analysis, we try to find solution in the following form

$$P_{\beta m}(w) = (1-w)^{\frac{|m|}{2}}(1+w)^{\frac{|m|}{2}}Z_{\beta m}(w) \equiv (1-w^2)^{\frac{|m|}{2}}Z_{\beta m}(w) \ ,$$

where $Z_{\beta m}$ must satisfy differential equation

$$(1-w^2)Z''_{\beta m} - 2(|m|+1)wZ'_{\beta m} + \left[\beta - |m|(|m|+1)\right]Z_{\beta m} = 0 \ .$$

Since here are no singularities, we choose $Z_{\beta m}$ to be the following power series expansion

$$Z_{\beta m}(w) = \sum_{k=0} a_k w^k \quad .$$

The equation dives the following reccurrent expression for coefficients

$$(k+2)(k+1)\ a_{k+2} = ((k+|m|)(k+|m|+1)-\beta)\ a_k \quad .$$

9.8 Finite power series function. Here also the power series function must be finite (if infinite, then in points $|w|=1$ function $Z_{\beta m}$ is infinite). Demanding that

$$a_k \neq 0, \quad and \quad a_{k+2} = 0 \ ,$$

we obtain that

$$\beta = l(l+1) \ ,$$

where we denoted

$$l = k + |m| \ .$$

l has values

$$l = 0, 1, 2, ... \ .$$

That new quantum number *l*, which gives us square on angular momentum, is called the orbital quantum number.

From $l = k + |m|$, where k = 0, 1, 2, ... , we have the following restriction to the magnetic quantum number *m*

$$|m| \leq l \ .$$

For each orbital quantum number *l* there is 2*l*+1 possible values for magnetic quantum number *m* (possible projections for angular momentum)

$$m = +l, l-1, ..., 0, ..., -(l-1), -l \ .$$

9.9 The result. The eigenvalue problem has the following solution

$$\hat{L}^2\ Y_{lm} = \hbar^2 l(l+1)\, Y_{lm} \ ,$$

where

$$l = 0, 1, 2, ...$$

and

$$m = +l, l-1, ..., 0, ..., -(l-1), -l \ .$$

Eigenfunctions are

$$Y_{lm}(\theta,\varphi) = \frac{N_{lm}}{\sqrt{2\pi}} P_{lm}(\theta)\, e^{im\varphi} \ ,$$

where the polynumials $P_{lm}(\theta)$ are called associated Legendre' polynomials (if m = 0, then Legendre' polynomials) and N_{lm} is normalization constant. Eigenfunctions $Y_{lm}(\theta,\varphi)$ are called spherical functions.

For spherical functions there is also developed the mathemacical formalism for calculating integrals, which is also based on generating function. Since one can find them in textbooks, we here give one example to demonstrate the problems we face using Legendre' polynomials.

If we want to normalize spherical functions, we must calculate integrals

$$\int |Y_{lm}(\theta,\varphi)|^2 \, d\Omega = 1$$

over whole solid angle. $d\Omega$ is

$$d\Omega = \sin\theta \, d\theta \, d\varphi \ .$$

More detailly

$$\frac{N_{lm}^2}{2\pi} \int_0^{\pi} \int_0^{2\pi} (P_{lm}(\theta))^2 \sin\theta \, d\theta \, d\varphi = 1 \ .$$

Integrating over φ we get 2π . Going further to $w = \cos\theta$, we must calculate the following integral

$$|N_{lm}|^2 \int_{-1}^{+1} [P_{lm}(w)]^2 \, dw = 1 \ .$$

Here we need integrals over associated Legendre'i polynomials. Here we use

$$\int_{-1}^{+1} P_{lm}(w) P_{l'm}(w) \, dw = \begin{cases} \dfrac{2}{(2l+1)} \dfrac{(l+|m|)!}{(l-|m|)!}, & l = l' \\ 0 \, , & l \neq l' \end{cases} \ .$$

From the above given we may choose the following normalization coefficient for spherical functions

$$N_{lm} = (-1)^m \left[\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!} \right]^{1/2} \ .$$

In conclusion, some spherical functions for lower l values ($l = 0, 1, 2$)

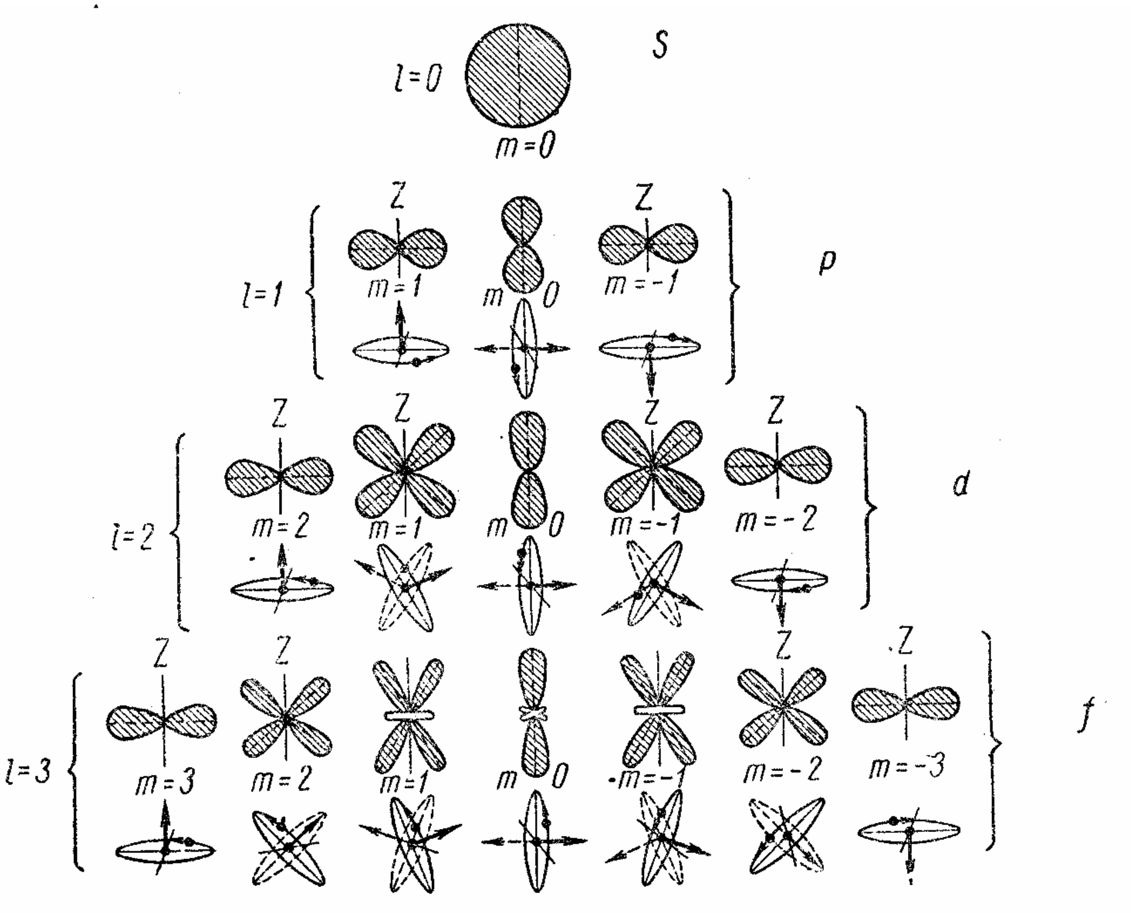
$$Y_{00} = \frac{1}{2\sqrt{\pi}} \ ,$$

$$Y_{11} = -\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{i\varphi} \ , \quad Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta \ , \quad Y_{1-1} = \sqrt{\frac{3}{8\pi}} \sin\theta \, e^{-i\varphi} \ .$$

$$Y_{22} = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \sin^2\theta e^{2i\varphi} \ , \quad Y_{21} = -\frac{1}{2}\sqrt{\frac{15}{2\pi}} \sin\theta \cos\theta \, e^{i\varphi} \ , \quad Y_{20} = \frac{1}{2}\sqrt{\frac{5}{4\pi}} (3\cos^2\theta - 1) \ ,$$

$$Y_{2-1} = \frac{1}{2}\sqrt{\frac{15}{2\pi}} \sin\theta \cos\theta \, e^{-i\varphi} \ , \quad Y_{2-2} = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \sin^2\theta \, e^{-2i\varphi}$$

The following figure gives graphical illustration of spherical functions (below is the classical orbital motion,corresponding to the same angular momentum and its projection).



In quantum world (microworld) angular momentum and its projection are discrete.