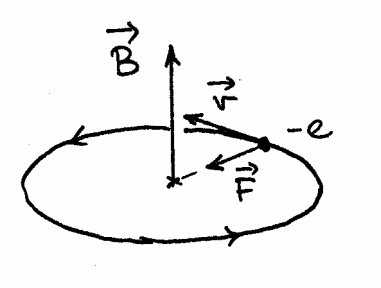
Example. Electron in homogeneous magnetic field. We consider the behaviour of free electron in homogeneous magnetic field $\vec{B}$.

Classical motion is the following. If the velocity is perpenticular to magnetic field ($\vec{v} \perp \vec{B}$), magnetic Lorentz force $\vec{F} = -e\vec{v} \times \vec{B}$ acts as a central force and electron moves on circular orbit. Since $F = evB$, the Newton II law gives the relation between the velocity and orbit radius



$$F = evB = M\frac{v^2}{r} \quad \rightarrow \quad \frac{v}{r} = \frac{eB}{M} \ .$$

Next we find the frequency. Since $v = 2\pi r/T$, where T is period, we get

$$\omega_L = \frac{2\pi}{T} = \frac{v}{r} = \frac{eB}{M} \ ,$$

Which is called the Larmor frequency. Frequency is proportional to magnetic induction.

If the velocity is not perpenticular to magnetic field and has some projection on the direction of magnetic field v_B, trajectory is spiral and particle is moving towards the magnetic field with constant velocity v_B.

Next we treat it using quantum mechanics. Since in microworld there are no trajectories, we must solve the corresponding Schrödinger equation. As we shall see, it reduces to the equation of harmonic oscillator.

We assume that magnetic field is oriented in *z*-axis and homogeneous: $\vec{B} = (0, 0, B)$. Our problem is most easily solved if we take the following vector potential

$$\vec{A} = (0, xB, 0) \ .$$

General equation is

$$\hat{H}\psi = E\psi \ ,$$

where

$$\hat{H} = -\frac{\hbar^2}{2M}\Delta - \frac{ie\hbar}{M}\vec{A}\cdot\nabla + \frac{e^2}{2M}\vec{A}^2 \ ,$$

and which, using our vector potential, turns to

$$\hat{H} = -\frac{\hbar^2}{2M}\Delta - \frac{ie\hbar B}{M}x\frac{\partial}{\partial y} + \frac{e^2B^2}{2M}x^2 \ .$$

Therefore we must solve the following Schrödinger equation

$$-\frac{\hbar^2}{2M}\Delta\psi(x,y,z) - \frac{ie\hbar B}{M}x\frac{\partial\psi(x,y,z)}{\partial y} + \frac{e^2B^2}{2M}x^2\psi(x,y,z) = E\psi(x,y,z) \ .$$

Since the z derivative is only in the kinetic energy operator, it is logical to assume, that z-axis motion is uniform with some momentum $p_z = \hbar k_z$ and energy $E_z = (\hbar k_z)^2 / 2M$ (as in the classical case). Therefore it is described by $\exp(i k_z z)$. Also there are no y variables, and we try to describe the y-axis motion by similar exponent $\exp(i \alpha y)$, where α is some unknown real parameter.

Next we try to find the solution in form

$$\psi(x,y,z) = \psi(x)\, e^{i\alpha y}\, e^{ik_z z} \ .$$

Taking derivatives

$$-\frac{\hbar^2}{2M}\frac{\partial^2 \psi(x,y,z)}{\partial z^2} = \frac{(\hbar k_z)^2}{2M}\psi(x,y,z) = E_z \psi(x,y,z) \ ,$$

$$-\frac{\hbar^2}{2M}\frac{\partial^2 \psi(x,y,z)}{\partial y^2} = \frac{(\hbar \alpha)^2}{2M}\psi(x,y,z) \ , \qquad -\frac{ie\hbar B}{M} x \frac{\partial \psi(x,y,z)}{\partial y} = \frac{\alpha\, e \hbar\, B}{M} x \psi(x,y,z) \ ,$$

we, after substitution, get the following equation for $\psi(x)$

$$-\frac{\hbar^2}{2M}\frac{d^2\psi(x)}{d\,x^2} + \frac{\hbar^2\alpha^2}{2M}\psi(x) + \frac{\hbar e B \alpha}{M} x\psi(x) + \frac{e^2B^2}{2M} x^2 \psi(x) = \varepsilon \psi(x) \ ,$$

where $\varepsilon = E - E_z$ is energy corresponding to the motion on x-y plane.

There are linear and quadratic terms of x, but after the simple change of variables

$$x \ \rightarrow \ x' = x + \delta$$

and proper choice of δ there remains only qyadratic term. Let us take the following three terms from right. After simple algebra we get

$$\frac{\hbar^2\alpha^2}{2M} + \frac{\hbar e B \alpha}{M} x + \frac{e^2B^2}{2M} x^2 = \frac{e^2B^2}{2M}\left(x^2 + 2\frac{\hbar\alpha}{eB}x + \frac{\hbar^2\alpha^2}{e^2B^2}\right) = \frac{e^2B^2}{2M}\left(x + \frac{\hbar\alpha}{eB}\right)^2$$

and therefore one must choose $\delta = \frac{\hbar\alpha}{eB}$. Using the Larmor frequency $\omega_L = \frac{eB}{M}$, we have

$$\frac{\hbar^2\alpha^2}{2M} + \frac{\hbar e B \alpha}{M} x + \frac{e^2B^2}{2M} x^2 = \frac{M\,\omega_L^2}{2} x'^2$$

and our Schrödinger equation reduces to that of harmonic oscillator equation

$$-\frac{\hbar^2}{2M}\frac{d^2\psi(x')}{d\,x'^2} + \frac{M\,\omega_L^2\, x'^2}{2}\psi(x') = \varepsilon \psi(x') \ .$$

(Parameter α finally drops out, and therefore has no physical meaning.)

Finally we obtained the harmonic oscillations on x' axis with the Larmor frequency ω_L . It is logical and corresponds to the classical case, since the projection of circular motion on some axis gives us harmonic oscillations. Energy of oscillations is the following

$$\varepsilon_n = \frac{\hbar\omega_L}{2}(2n+1)\,, \qquad n = 0, 1, 2, \ldots$$

Let us analyse the results. Energy in the homogeneous magnetic field is

$$E_n(k_z) = \frac{e\hbar B}{2M}(2n+1) + \frac{(\hbar k_z)^2}{2M}\ .$$

If we omit the free motion, then on the x-y plane the energy is

$$E_n = \frac{e\hbar B}{2M}(2n+1)\,, \quad n = 0, 1, 2, \ldots$$

We see that the energy is discrete and therefore quantized. It has interesting physical meaning.

Diamagnetism of electronic gas. Our result explains the new interesting physical phenomenon: electronic gas is diamagnetic and magnetic moment is diamagnetic.

As we know, any object with the magnetic moment M_z has in magnetic field energy

$$E_n = -M_z B\ ,$$

therefore electron itself has magnetic moment

$$M_z = -\frac{e\hbar}{2M}(2n+1) = -\mu_B(2n+1)\ .$$

Since it is opposite to magnetic field, we have diamgnetism. Moreover, magnetic moment is quantized. Magnetical properties of atoms we treat in §25.

14. Gauge invariance

Here we analyse quite interesting problem connected with Schrödinger equation introduced in the last paragraph:

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi\ ,$$

where

$$\hat{H} = \frac{1}{2M}(-i\hbar\nabla - e\vec{A})^2 + e\phi + U\ .$$

We know from electrodynamics that potentials are not determined uniquely. We may always perform gauge transformations and change potentials to the new ones

$$\vec{A} \ \rightarrow\ \vec{A}' = \vec{A} + grad\ f \equiv \vec{A} + \nabla f\ ,$$

$$\phi \quad \rightarrow \quad \phi' = \phi - \frac{\partial f}{\partial t} \ .$$

(These leave the fields $\vec{E}$ *ja* $\vec{B}$ the same). On the other hand, if we choose new potentials, Schrödinger equation is changed and also its solution is changed. What to do to preserve its previous physical meaning?

14.1 Gauge invariance of equation. Next we demonstrate, that by choosing new potentials, we must also change the old wave function Ψ to some bew one Ψ'. That transformation is also called the gauge transformation.

Next we demonstrate that if we perform the following gauge transformation

$$\Psi \quad \rightarrow \quad \Psi' = e^{\frac{ief}{\hbar}} \Psi \ ,$$

we get Schrödinger equation

$$i\hbar \frac{\partial \Psi'}{\partial t} = \hat{H} \Psi' \ ,$$

where in Hamilton operator $\hat{H}'$ there are new potentials $\vec{A}'$ ja ϕ':

$$\hat{H}' = \frac{1}{2M}(-i\hbar\nabla - e\vec{A}')^2 + e\phi' + U \ .$$

Our gauge transformation is complicated, that now it is cot some constant exponent, but it depends on coordinates and time, since $f = f(\vec{r},t)$ depends on coordinates and time. Our calculations are therefore more complicated. At first we calculate derivatives from Ψ'.

$$\frac{\partial \Psi'}{\partial t} = \frac{\partial}{\partial t}(e^{\frac{ie\,f}{\hbar}} \Psi) = \frac{ie}{\hbar}\frac{\partial f}{\partial t} e^{\frac{ie\,f}{\hbar}} \Psi + e^{\frac{ie\,f}{\hbar}} \frac{\partial \Psi}{\partial t} = e^{\frac{ie\,f}{\hbar}} (\frac{ie}{\hbar}\frac{\partial f}{\partial t} \Psi + \frac{\partial \Psi}{\partial t}) \ ,$$

analogically

$$\nabla \Psi' = e^{\frac{ie\,f}{\hbar}} (\frac{ie}{\hbar}(\nabla f)\Psi + \nabla \Psi) = e^{\frac{ie\,f}{\hbar}} (\frac{ie}{\hbar}\nabla f + \nabla)\Psi \ .$$

Next we calcutate $(-i\hbar\nabla - e\vec{A}')\Psi'$:

$$(-i\hbar\nabla - e\vec{A}')\Psi' = e^{\frac{ie\,f}{\hbar}} (-i\hbar\nabla + e(\nabla f) - e\vec{A}')\Psi = e^{\frac{ie\,f}{\hbar}} (-i\hbar\nabla - e\vec{A})\Psi \ .$$

(In the last step we used the transformation of vector potential.) Using the last result it is obvious that

$$(-i\hbar\nabla - e\vec{A}')^2 \Psi' = e^{\frac{ie\,f}{\hbar}} (-i\hbar\nabla - e\vec{A})^2 \Psi \ .$$

Using previous results we from the Schrödinger equation

$$i\hbar \frac{\partial \Psi'}{\partial t} = \frac{1}{2M}(-i\hbar\nabla - e\vec{A}')^2 \Psi' + e\phi' \Psi' + U\Psi'$$

get

$$e^{\frac{ie f}{\hbar}}(i\hbar\frac{\partial\Psi}{\partial t}-e\frac{\partial f}{\partial t}\Psi)=e^{\frac{ie f}{\hbar}}(\frac{1}{2M}(-i\hbar\nabla-e\vec{A})^2\Psi+e(\phi-\frac{\partial f}{\partial t})\Psi+U\Psi)\ ,$$

which after cancelling exponent and $\partial f/\partial t$ gives us the equation we started with

$$i\hbar\frac{\partial\Psi}{\partial t}=\frac{1}{2M}(-i\hbar\nabla-e\vec{A})^2\Psi+e\phi\Psi+U\Psi\ .$$

Therefore, to preserve the invariance of Schrödinger eqation in gauge transformations of potentials

$$\vec{A}\ \rightarrow\ \vec{A}'=\vec{A}+grad\ f\equiv\vec{A}+\nabla f\ ,$$

$$\phi\ \rightarrow\ \phi'=\phi-\frac{\partial f}{\partial t}\ ,$$

one must transforme the wave function in the following way

$$\Psi\ \rightarrow\ \Psi'=e^{\frac{ie f(\vec{r},t)}{\hbar}}\Psi$$

(in all three transformations $f=f(\vec{r},t)$ is the same scalar function). The last transformation is similarly called gauge transformation. Also the physical meaning is preserved, since the probability density and probability current density remain the same

$$|\Psi'|^2=|\Psi|^2\qquad ja\qquad \vec{j}'=\vec{j}\ .$$

14.2 The general gauge invariance. Quantum mechanics is nonrelativistic, space and time are not related with each other. One may always perform tranformations

$$\Psi\ \rightarrow\ \Psi'=e^{i\alpha}\Psi$$

where $\alpha\in R$ is some arbitrary real number, and which are usually called phase transformations (in wave theories it means the chenge of phase). In relativistic world such transformations are not allowed since there exist limiting velocity c (the speed of electromagnetic waves in vacuum) and no information or action cannot move with velocities that exceed c. The constant phase trasformations mean tha we cheage the phase simultaneously in the whole space, which is from the relativistic point of view impossible. In relativistic world we may change phase only locally, in each point in space independently from the other points and also in each moment of time. Therefore in physics generally are allowed only local phase transformations

$$\Psi\ \rightarrow\ \Psi'=e^{i\alpha(\vec{r},t)}\Psi\ ,$$

where

$$\alpha=\alpha(\vec{r},t)$$

is some arbitrary scalar function.

In relativistic physics, especially in particle physics (relativistic quantum field theory), it is the general principle that any acceptable physical theory must be invariant under local phase transformations, which ususally are called gauge transformations:

$$\Psi \quad \rightarrow \quad \Psi' = e^{i\alpha(\vec{r},t)}\,\Psi$$

and the field equations which describe some microparticlessuhtes must remain invariant under the above given trasformations.

It is interesting to note that there are no invariant equation for the field Ψ only, i.e. equations

$$W\Psi = 0 \ ,$$

where W is some function of derivatives. It appears, that these equations are somewhat specific, because we in addition to Ψ must introduce one (or more) vector fields ($\vec{A}, \phi$), which are analogical to the electromagnetic fields, treated previously. Therefore the equations for physical fields are in form

$$W(\vec{A},\phi)\,\Psi = 0 \ .$$

If Ψ describes fundamental particles, for example quarks, then additional vector fields (totally 8 fields) describe particles which describe interactions between quarks. Thay are called gluons.

15. Basics of representations theorie

The formalism of quantum mechanics may be built up using matrices and matrix calculus. The first formulation of quantum of mechanics (W. Heisenberg, 1925) as we know based on matrices and is sometimes called the matrix mechanics, after that E. Schrödinger (1926) introdused wave function and corresponding wave equation (Schrödinger equation) and treated quantum mechnanics as eigenvalue problem (Schrödinger version was called wave mechanics). At first glance these theories were so different that it was problematical, whether these two theories describe the same physics. When E. Schrödinger proves that both theories are equivalent, it turns out that the Heisenberg quantum mechanics is the mayrix version of Schrödinger's "wave" mechanics. Nowadays is Schrödinger version the mostly used one, but solving problems it is useful to know, how the physical quatities are represented in the matrix form.

15.1 *F*-representation. Let us consider some Hermitean operator $\hat{F}$ and let us assume that we have solved its eigenvalue problem

$$\hat{F}\varphi_n = f_n\varphi_n \ .$$

The matrix repsesentation built up using eigenfuctions of operator $\hat{F}$ we call the *F*-representation.

To simplify the further calculations we assume that the eigenvalues of $\hat{F}$ are discrete and there are infinite number of eigenvalues and eigenfunctions (we also assume that to each eigenvalue there is only one eigenfunction)

$$\varphi_1, \varphi_2, \ldots, \varphi_n \ .$$

(The generalization to other cases is in principal simple and needs no special mathematical tricks.)

Since eigenfunctions of $\hat{F}$ form a full set of functions, all the functions ψ from the same class of functions may be represented as an expansion

$$\psi = \sum_{i=1}^{n} c_i \varphi_i \ ,$$

in Dirac notation

$$|\psi\rangle = \sum_{i=1}^{n} c_i |\varphi_i\rangle \ ,$$

where $c_i = \langle \varphi_i | \psi \rangle$.

It is obvious, that the coefficients $c_1, c_2, \ldots, c_n$ of the series expansion determine function ψ uniquely. And vice versa, for each ψ the coefficients are determined uniquely.

Therefore, proceeding from eigenfunctions of some Hermite operator all functions are representated by series of coefficients $c_1, c_2, \ldots, c_n$. We represent functions by one column matrices

$$\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = ((c_i)) \ ,$$

where $((c_i))$ is its symbolic writing. Therefore

$$\psi \quad \leftrightarrow \quad \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} ,$$

We call it a *F*-representation of ψ.

15.2 Bilinear form. Next we find the matrix representation of two function's χ and ψ bilinear form. Assuming that

$$\chi = \sum_{i=1}^{n} d_i \varphi_i \ , \quad \text{or} \quad |\chi\rangle = \sum_{i=1}^{n} d_i |\varphi_i\rangle \ ,$$

we get the matrix form $((d_j))$ of χ. Since $\langle \chi | = \sum_{i=1}^{n} d_i^* \langle \varphi_i |$, we get

$$\langle \chi | \psi \rangle = \sum_{i,j=1}^{n} d_i^* c_j \langle \varphi_i | \varphi_j \rangle = \sum_{i=1}^{n} d_i^* c_i \ .$$

If we introduce $\langle \chi | = \chi^*$ as a one row matrix

$$(d_1^* \quad d_2^* \quad \dots \quad d_n^*) \ ,$$

the matrix product

$$(d_1^* \quad d_2^* \quad \dots \quad d_n^*) \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = \sum_{i=1}^{n} d_i^* c_i$$

gives a bilinear form $\langle \chi | \psi \rangle$.

As each function $\psi = |\psi\rangle$ is represented as a matrix

$$\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} ,$$

its complex conjugate $\psi^* = \langle \psi |$ is represented as a comjugated matrix $((c_i))^+$, which is previous matrix transposed and then each c_i is replaced by its complex conjugated

$$((c_i))^+ = ((c_i^*))^T = (c_1^* \quad c_2^* \quad \cdots \quad c_n^*)$$

Bilinear form is

$$\langle \chi | \psi \rangle = ((d_i))^+ ((c_i)) \ .$$

Therefore we have

$$\langle \chi | \psi \rangle = \int \chi^* \psi \, dV \qquad and \qquad \langle \psi | \chi \rangle = \int \psi^* \chi \, dV = \left(\langle \chi | \psi \rangle \right)^* \ ,$$

and also

$$\left(((d_i))^+ ((c_i)) \right)^+ = ((c_i))^+ ((d_i)) \ .$$

15.3 Matrix form of operators. Consider some operator $\hat{A}$, which transforms each function ψ to some fixed function χ

$$\chi = \hat{A} \psi \ .$$

We demonstrate that it is represented as a matrix product

$$\begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix},$$

where $\hat{A}$ is represented as a square matrix $((a_{ij}))$ with matrix elements

$$a_{ij} = \langle \varphi_i | \hat{A} | \varphi_j \rangle = \int \varphi_i^* \hat{A} \varphi_j \, dV \ .$$

We start from $\chi = \hat{A}\psi$, i.e.

$$| \chi \rangle = \hat{A} | \psi \rangle$$

and represent χ and ψ by corresponding series

$$\sum_{k=1}^{n} d_k | \varphi_k \rangle = \sum_{j=1}^{n} c_j \hat{A} | \varphi_j \rangle \ .$$

Multiplying from left with $\langle \varphi_i |$ and using orthonormality, we may express the matrix elements of $| \chi \rangle$: d_i $(i = 1, 2, \dots n)$, as

$$d_i = \sum_{j=1}^{n} c_j \langle \varphi_i | \hat{A} | \varphi_j \rangle \equiv \sum_{j=1}^{n} a_{ij} \, c_j \ .$$

Since it may be written as a matrix product $((d_i)) = ((a_{ij}))((c_j))$, where operator $\hat{A}$ is represented as a square matrix

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix},$$

with elements

$$a_{ij} = \langle \varphi_i | \hat{A} | \varphi_j \rangle = \int \varphi_i^* \hat{A} \varphi_j \, dV \ .$$

It is obvious that the product of matrices $\hat{A}$ ja $\hat{B}$ is represented as a product of corresponding matrices (prove).

If we have the matrix form of some operator $\hat{A}$, its conjugated operator has matrix elements a_{ij}^+ (prove):

$$a_{ij}^+ = a^*_{ji} = (a^*_{ij})^T \ .$$

In quantum mechanics the physical quantities are represented with Hermitean matrices. Hermitean operators satisfy

$$\hat{A}^+ = \hat{A} \ ,$$

which means that the elements of corresponding operator satisfy

$$a_{ij}^{+} = a_{ij} = a_{ji}\,*$$

Diagonal elements are real (if $i = j$)

$$a_{ii} = a_{ii}\,* \ ,$$

elements on secondary diagonal ($i \neq j$) satisfy

$$a_{ij} = a_{ji}\,* \ .$$

Example 1. 2x2 matrix is Hermitean, if $a_{11}, a_{22} \in R$ and $a_{12} = a_{21}\,*$

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{12}\,* & a_{22} \end{pmatrix} .$$

15.4 Eigenvalue problem. Eigenvalue problem is to solve the equation

$$\hat{A}\psi = a\psi \ .$$

Replacing ψ by its expansion, we have

$$(\hat{A} - a)\psi = \sum_{k=1}^{n} c_k (\hat{A} - a)\left|\varphi_k\right\rangle = 0 \ .$$

Multiplying from left to $\left\langle \varphi_i \right|$

$$\sum_{k=1}^{n} c_k \left\langle \varphi_i \right|(\hat{A} - a)\left|\varphi_k\right\rangle = \sum_{k=1}^{n} c_k (a_{ik} - a\delta_{ik}) = 0 \ ,$$

we write it as

$$\sum_{k=1}^{n} (a_{ik} - a\delta_{ik})\, c_k = 0 \ .$$

It is the linear homogeneous system for c_k

$$\begin{pmatrix} a_{11} - a & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} - a & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} - a \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = 0 \ .$$

That system has nontrivial solutions iff the determinant is equal to zero

$$\begin{vmatrix} a_{11}-a & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22}-a & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn}-a \end{vmatrix} = 0 \ ,$$

(the shorthand of it is $\det((a_{ij} - a\delta_{ij})) = 0$).

Determinant gives us the following n-th degree equation

$$(-1)^n a^n + \alpha_1 a^{n-1} + \ldots + \alpha_n = 0 \ ,$$

where $\alpha_1, \alpha_2, \ldots, \alpha_n$ are some numerical coefficients. In general such equations have n solutions

$$a_1, a_2, \ldots, a_n \ ,$$

which now are the eigenvalues of operator $\hat{A}$.

In order to calculate eigenfunctions of $\hat{A}$ we must replace a_i and solve the equation finding coefficients $c_1^i, c_2^i, \ldots, c_n^i$.

Example 2. Operator given by arbitrary 2x2 matrix:

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} .$$

Eigenvalue problem gives a system

$$\begin{pmatrix} a_{11}-a & a_{12} \\ a_{21} & a_{22}-a \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0 \ .$$

Eigenvalues are calculated fron equation

$$\begin{vmatrix} a_{11}-a & a_{12} \\ a_{21} & a_{22}-a \end{vmatrix} = (a_{11}-a)(a_{22}-a) - a_{12}a_{21} = 0 \ .$$

Since it is a quadratic equation

$$a^2 - (a_{11} + a_{22})\, a + (a_{11}a_{22} - a_{12}a_{21}) = 0 \ ,$$

it gives two solutions

$$a_{1,2} = \frac{a_{11} + a_{22}}{2} \pm \sqrt{\left(\frac{a_{11} + a_{22}}{2}\right)^2 - (a_{11}a_{22} - a_{12}a_{21})} =$$

$$= \frac{a_{11} + a_{22}}{2} \pm \frac{\sqrt{(a_{11} - a_{22})^2 + 4a_{12}a_{21}}}{2} .$$

To find eigenfunctions we replace a_1 and then a_2, and find the corresponding c_i. Replacing, for example a_1, we must solve the system

$$(a_{11} - a_1)c_1 + a_{12}c_2 = 0 ,$$

$$a_{21}c_1 + (a_{22} - a_1)c_2 = 0 .$$

(In such systems one of coefficients is always arbitrary. If we take c_1 as known, c_2 is represented as

$$c_2 = -\frac{a_{11} - a_1}{a_{12}} c_1 .$$

Example 3. 2x2 Hermitean matrix. Now the matrix is

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{12}* & a_{22} \end{pmatrix},$$

where $a_{11}, a_{22} \in R$. Solutions of corresponding quadratic equation are

$$a_{1,2} = \frac{a_{11} + a_{22}}{2} \pm \frac{\sqrt{(a_{11} - a_{22})^2 + 4|a_{12}|^2}}{2} .$$

As we see, eigenvalues are real numbers.

Example 4. Pauli matrix σ_y

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} .$$

Now $a_{11} = a_{22} = 0$, $a_{12} = -i$, $a_{12}* = i$, therefore eigenvalues are

$$a_{1,2} = \pm \frac{\sqrt{4|a_{12}|^2}}{2} = \pm 1 .$$

Nxt we find eigenfunctions. For $a_1 = +1$ we must solve equation

$$\begin{pmatrix} -1 & -i \\ i & -1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0$$

or

$$-c_1 - ic_2 = 0 ,$$

$$ic_1 - c_2 = 0 .$$

We have only one independent equation. If we take $c_1 = 1$, we get $c_2 = i$ and therefore the corresponding eigenfunction is

$$\psi_1 = \begin{pmatrix} 1 \\ i \end{pmatrix} .$$

Similarly we for $a_2 = -1$ get

$$\psi_2 = \begin{pmatrix} 1 \\ -i \end{pmatrix} .$$

15.5 Operator $\hat{F}$ in F-representation. Operator $\hat{F}$ itself is represented as a diaginal mtarix and its diagonal elements are its eigenvalues. Indeed

$$f_{ij} = \langle \varphi_i | \hat{F} | \varphi_j \rangle = f_j \langle \varphi_i | \varphi_j \rangle = f_j \delta_{ij} .$$

15.6 Connection between different representations. If we use *F*-repsesentation, we use as basis eigenfunctions $\varphi_1, \varphi_2, \ldots, \varphi_n$ ($\hat{F}\varphi_i = f_i \varphi_i$) of operator $\hat{F}$. In the G-representation we similarly use eigenfunctions

$$\psi_1, \psi_2, \ldots, \psi_n$$

of operator $\hat{G}$. Let us take some arbitrary function χ. Its F- and G-representations are

$$\chi = \sum_{i=1}^{n} c_i \varphi_i \quad \rightarrow \quad |\chi\rangle = \sum_{i=1}^{n} c_i |\varphi_i\rangle ,$$

$$\chi = \sum_{i=1}^{n} d_i \psi_i \quad \rightarrow \quad |\chi\rangle = \sum_{i=1}^{n} d_i |\psi_i\rangle .$$

Since

$$\sum_{j=1}^{n} d_j |\psi_j\rangle = \sum_{k=1}^{n} c_k |\varphi_k\rangle .$$

Multiplying from left to $\langle \psi_i |$ and using orthonormality, we get the relation between the coefficients in different representations

$$d_i = \sum_{k=1}^{n} \langle \psi_i | \varphi_k \rangle c_k .$$

In the matrix form

$$((d_i)) = ((U_{ij}))((c_j)),$$

where the matrix elements of transition matrix U are

$$U_{ij} = \langle \psi_i | \varphi_j \rangle = \int \psi_i^* \varphi_j \, dV .$$

It is easy to prove (prove it) that matrix U is unitary:

$$U^+ = U^{-1} \qquad ehk \qquad U^+ U = I .$$

Example 5. Harmonic oscillator in *E*-representation. *E*-representation means that we use eigenfunctions of Hamilton operator $\hat{H}$. We have

$$E_n = \hbar\omega(n+1/2) \ ,$$

and

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

n = 0, 1, 2, ... Using integrals, calculated previously we write down some operators in matrix form.

Since n = 0, 1, 2, ... we label the matrix elements of operator $\hat{A}$ as follows (matrices are infinite square matrices)

$$((a_{mn})) = \begin{pmatrix} a_{00} & a_{01} & a_{02} & \cdots \\ a_{10} & a_{11} & a_{12} & \cdots \\ a_{20} & a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} .$$

Hamilton operator $\hat{H}$ is diagonal, matrix elements are energy eigenvalues, therefore

$$h_{mn} = E_n \delta_{mn} = \hbar\omega(n+1/2)\delta_{mn} \ ,$$

or in matrix form

$$((h_{mn})) = \frac{\hbar\omega}{2} \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 3 & 0 & \cdots \\ 0 & 0 & 5 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} .$$

Next the coordinate operator $\hat{x} = x$. Its matrix elements are

$$x_{mn} = \langle \psi_m | x | \psi_n \rangle = \int_{-\infty}^{+\infty} \psi_m x \psi_n \, dx \, .$$

Using the corresponding integrals (see §7), we obtain

$$x_{mn} = \sqrt{\frac{\hbar}{2M\omega}} \, (\sqrt{n+1}\, \delta_{mn+1} + \sqrt{n}\, \delta_{mn-1}) \, ,$$

or in matrix form

$$((x_{mn})) = \sqrt{\frac{\hbar}{2M\omega}} \begin{pmatrix} 0 & \sqrt{1} & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & \cdots \\ 0 & \sqrt{2} & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} .$$

Momentum operator $\hat{p} = -i\hbar \frac{d}{dx}$. Its matrix elements are

$$p_{mn} = -i\hbar \langle \psi_m | \frac{d}{dx} | \psi_n \rangle = -i\hbar \int_{-\infty}^{+\infty} \psi_m \frac{d\psi_n}{dx} dx \ .$$

Using integrals, we obtain

$$p_{mn} = i\hbar \sqrt{\frac{M\omega}{2\hbar}} (\sqrt{n+1}\,\delta_{mn+1} - \sqrt{n}\,\delta_{mn-1}) ,$$

or in matrix form

$$((p_{mn})) = i\sqrt{\frac{M\omega\hbar}{2}} \begin{pmatrix} 0 & -\sqrt{1} & 0 & \cdots \\ \sqrt{1} & 0 & -\sqrt{2} & \cdots \\ 0 & \sqrt{2} & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} .$$

Using matrices it is possible to perform calsulations. For example, if it is needed to prove that $[x, \hat{p}] = i\hbar$, we first calculate $(x\hat{p})_{mn}$ and $(\hat{p}x)_{mn}$, using the above given matrices and that gives us the final result

$$(x\hat{p} - \hat{p}x)_{mn} = i\hbar\,\delta_{mn} \ .$$

Some results are more easily calculated using matrices. If we, for example try to find matrix elements of x^2, it means calculation of matrix elements $(x^2)_{mn}$, which in turn means that one must multiply two x-matrices

$$(x^2)_{mn} = \sum_r x_{mr} x_{rn} \ .$$

Since x_{mn} has nonzero elements when $n = m \pm 1$, we conclusion obtain

$$(x^2)_{mn} = \frac{\hbar}{2M\,\omega} \left((2m+1)\delta_{nm} + \sqrt{m(m-1)}\,\delta_{nm-2} + \sqrt{(m+1)(m+2)}\,\delta_{nm+2} \right) .$$

(Compare it with the results of §7, obtained by integration.)

We give also the natrix elements of x^3 . It is product of x^2 and x, therefore

$$(x^3)_{mn} = \sum_p (x^2)_{mp} x_{pn} \ .$$

Nex we give only nonzero elements

$$(x^3)_{nn-1} = (x^2)_{nn}(x)_{nn-1} + (x^2)_{nn-2}(x)_{n-2n-1} = 3\sqrt{(\frac{\hbar}{M\omega})^3}\sqrt{(\frac{n}{2})^3} \ ,$$

$$(x^3)_{nn-3} = (x^2)_{nn-2}(x)_{n-2n-3} = \sqrt{(\frac{\hbar}{M\omega})^3}\sqrt{\frac{n(n-1)(n-2)}{8}} \ ,$$

$$(x^3)_{nn+1} = (x^2)_{nn}(x)_{nn+1} + (x^2)_{nn+2}(x)_{n+2n+1} = 3\sqrt{(\frac{\hbar}{M\omega})^3}\sqrt{(\frac{n+1}{2})^3} \ ,$$

$$(x^3)_{nn+3} = (x^2)_{nn+2}(x)_{n+2n+3} = \sqrt{(\frac{\hbar}{M\omega})^3}\sqrt{\frac{(n+3)(n+2)(n+1)}{8}} \ .$$

(x^3 is symmetrical matrix, for example $(x^3)_{nn-1} = (x^3)_{n-1n}$ and so on.)

16. Matrix representation of angular momentum

Assume that we have three Hermitean operators

$$\hat{J}_x \ , \hat{J}_y \ , \hat{J}_z \ ,$$

which satisfy similar commutation relations as operators of orbital angular momentum $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$ (see §9)

$$\left[\hat{J}_x \ , \hat{J}_y \ \right] = ih\hat{J}_z \quad , \quad \left[\hat{J}_y \ , \hat{J}_z \ \right] = ih\hat{J}_x \quad , \quad \left[\hat{J}_z \ , \hat{J}_x \ \right] = ih\hat{J}_y \ .$$

We inroduce one more operator

$$\hat{\hat{J}}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \ .$$

It is easy to verity (prove), that

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

16.1 Eigenvalue problem. Similarly as for orbital angular momentum we may find the square and one projection (we choose again the z-projection). Therefore we start to solve eigenvalue problems

$$\hat{\hat{J}}^2 \left| jm \right\rangle = \hbar^2 J^2 \left| jm \right\rangle , \qquad \hat{J}_z \left| jm \right\rangle = \hbar m \left| jm \right\rangle \ .$$

and try to find J and m, and also the matrix form of operators $\hat{J}_x \ , \hat{J}_y \ , \hat{J}_z$. $\left| jm \right\rangle$ are matrix elements of corresponding states.

It is natural to use the representation where operators $\hat{\hat{J}}^2$ and $\hat{J}_z$ are diagonal matrices (the *J*-representation or angular momentum representation). We assume similarly to the orbital angular momentum that in the sub-space where J^2 is fixed the only variable is eigenvalue *m* of operator $\hat{J}_z$. Then the matrix elements of $\hat{\hat{J}}^2$ are

$$(\hat{J}^2)_{m'm} = \langle jm' | \hat{\vec{J}}^2 | jm \rangle = \hbar^2 J^2 \delta_{m'm}$$

and similarly for $\hat{J}_z$

$$(\hat{J}_z)_{m'm} = \langle jm' | \hat{J}_z | jm \rangle = \hbar\, m\, \delta_{m'm} \ .$$

Matrixelements of $\hat{J}_z$ are labelled by m and we assume that the possible values of m are

$$m_1 , m_2 , \ldots , m_r \ ,$$

where $m_1 = \max(m_i)$ is maximal and $m_r = \min(m_i)$ the lowest one.

16.2 Restrictions to projections of $\hat{J}_z$. Proceeding from

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

we calculate diagonal element of both sides

$$\langle jm | \hat{\vec{J}}^2 | jm \rangle = \langle jm | \hat{J}_x^2 | jm \rangle + \langle jm | \hat{J}_y^2 | jm \rangle + \langle jm | \hat{J}_z^2 | jm \rangle ,$$

which is expressed as

$$\hbar^2 J^2 = (\hat{J}_x^2)_{mm} + (\hat{J}_y^2)_{mm} + \hbar^2 m^2 \ .$$

From the above given it follows that

$$\hbar^2 J^2 \geq \hbar^2 m^2 \qquad or \qquad J^2 \geq m^2 \ .$$

(Qunatities $(\hat{J}_x^2)_{mm}$ and $(\hat{J}_y^2)_{mm}$ are nonnegative. For example

$$(\hat{J}_x^2)_{mm} = \langle jm | \hat{J}_x^2 | jm \rangle = \sum_{m'} \langle jm | \hat{J}_x | jm' \rangle \langle jm' | \hat{J}_x | jm \rangle = \sum_{m'} (\hat{J}_x)_{mm'} (\hat{J}_x)_{m'm} = \sum_{m'} \left| (\hat{J}_x)_{m'm} \right|^2$$

In the last step we used that $\hat{J}_x$ is Hermitean.)

From unequality $J^2 \geq m^2$ we get the following restrictions to *m*:

$$J \geq m_1 , m_2 , \ldots , m_r \geq -J \ .$$

16.3 Rising and lowering operators. Next we introduse operators which rise or lower eigenvalues of $\hat{J}_z$. For that we instead of $\hat{J}_x$ ja $\hat{J}_y$ the following operators

$$\hat{J}_+ = \hat{J}_x + i\hat{J}_y \ , \quad \hat{J}_- = \hat{J}_x - i\hat{J}_y \ ,$$

which satisfy $(\hat{J}_+)^+ = \hat{J}_-$, $(\hat{J}_-)^+ = \hat{J}_+$.

Now we find the following commutation relations

$$\left[\hat{J}_z\,,\,\hat{J}_+\right]=\hbar\hat{J}_+\quad,\qquad\left[\hat{J}_z\,,\,\hat{J}_-\right]=-\hbar\hat{J}_-$$

It is easy to verify that operator $\hat{J}_+$ rises eigenvalues of $\hat{J}_z$ by +1

$$\hat{J}_+\left|jm\right\rangle\ \sim\ \left|jm+1\right\rangle$$

and operator $\hat{J}_-$ lowers eigenvalues of $\hat{J}_z$ by -1

$$\hat{J}_-\left|jm\right\rangle\ \sim\ \left|jm-1\right\rangle\ .$$

We prove only the first relation. Using $\left[\hat{J}_z\,,\,\hat{J}_+\right]=\hbar\hat{J}_+$, which we write as

$$\hat{J}_z\hat{J}_+=\hat{J}_+\hat{J}_z+\hbar\hat{J}_+$$

and applying it to $\left|jm\right\rangle$, we get

$$\hat{J}_z(\hat{J}_+\left|jm\right\rangle)=\hat{J}_+(\hat{J}_z\left|jm\right\rangle)+\hbar(\hat{J}_+\left|jm\right\rangle)=\hbar\,(m+1)(\hat{J}_+\left|jm\right\rangle)\ .$$

We see that indeed $\hat{J}_+\left|jm\right\rangle$ is the eigenfuntion of $\hat{J}_z$ with eigenvalue $\hbar(m+1)$.

16.4 Eigenvalues. Next we analyse the general structure of eigenvalues *m*. Let proceed from the state with maximal projection

$$\left|jm_1\right\rangle\ .$$

Since the other values of *m* are smaller, we have

$$\hat{J}_+\left|jm_1\right\rangle=0\ .$$

Applying step by step the lowering operator, we get

$$\hat{J}_-\left|jm_1\right\rangle\ \sim\ \left|jm_1-1\right\rangle$$

$$(\hat{J}_-)^2\left|jm_1\right\rangle\ \sim\ \left|jm_1-2\right\rangle$$

$$\ldots$$

$$(\hat{J}_-)^{r-1}\left|jm_1\right\rangle\ \sim\ \left|jm_1-(r-1)\right\rangle\ .$$

Therefore the possible values of m are

$$m_1\,,\,m_1-1,\,m_1-2,\ldots,m_1-(r-1)\ .$$

Taking on the other hand the state with minimal projection

$$\left|jm_r\right\rangle\ ,$$

we have $\hat{J}_-\left|jm_r\right\rangle = 0$. Applying step by step the rising operator, we get

$$\hat{J}_+\left|jm_r\right\rangle \sim \left|jm_r+1\right\rangle$$

$$(\hat{J}_+)^2\left|jm_r\right\rangle \sim \left|jm_r+2\right\rangle$$

$$\ldots$$

$$(\hat{J}_+)^{r-1}\left|jm_r\right\rangle \sim \left|jm_r+(r-1)\right\rangle .$$

It means that the possible values of m are

$$m_r+(r-1),\ldots,m_r+2,m_r+1,m_r .$$

We see that $m_1 = m_r+(r-1)$, but in ordes to determine eigenvalues we must separately find m_1 or m_r .

Next we derive the relation between m_1 or m_r from which the exact eigenvalues are calculated. We start from

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

and express it in the following two different ways. Using the products of rising and lowering operators $\hat{J}_+\hat{J}_- = \hat{J}_x^2+\hat{J}_y^2+\hbar\hat{J}_z$ and $\hat{J}_-\hat{J}_+ = \hat{J}_x^2+\hat{J}_y^2-\hbar\hat{J}_z$, we have

$$\hat{\vec{J}}^2 = \hat{J}_-\hat{J}_+ + \hat{J}_z^2+\hbar\hat{J}_z ,$$

$$\hat{\vec{J}}^2 = \hat{J}_+\hat{J}_- + \hat{J}_z^2-\hbar\hat{J}_z .$$

At first we apply the first relation to the state with maximal projection $\left|jm_1\right\rangle$

$$\hat{\vec{J}}^2\left|jm_1\right\rangle = \hat{J}_-\hat{J}_+\left|jm_1\right\rangle + \hat{J}_z^2\left|jm_1\right\rangle + \hbar\hat{J}_z\left|jm_1\right\rangle .$$

Since $\hat{J}_+\left|jm_1\right\rangle = 0$ and $\hat{J}_z\left|jm_1\right\rangle = \hbar m_1\left|jm_1\right\rangle$, we get

$$\hat{\vec{J}}^2\left|jm_1\right\rangle = \hbar^2 m_1(m_1+1)\left|jm_1\right\rangle ,$$

from which

$$J^2 = m_1(m_1+1) .$$

Applying similarly the second expression to the state with the lowest projection$\left|jm_r\right\rangle$ and using $\hat{J}_-\left|jm_r\right\rangle = 0$, we get

$$J^2 = m_r(m_r-1) .$$

Since both give the same result, we have

$$J^2 = m_1(m_1+1) = m_r(m_r-1) \ .$$

If we solve our quadratic equation for m_1 , we get

$$m_1 = m_r - 1 \quad ja \quad m_1 = -m_r$$

The first solution do not match, since m_r was the lowest one, therefore we have

$$m_r = -m_1 \ .$$

Finally we fing the general solution to our eigenvalue problems. Denoting

$$m_1 = j \ ,$$

we get

$$J^2 = j(j+1)$$

and the following values of m

$$j\,,\ j-1,\ldots,j-(r-1) = -j \ .$$

From these we see that the only possible values of j are

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$$

(after *n* steps we must from j reach to $-j$, which means that $j-n=-j$ and $j=n/2$).

In conclusion the values of j are integers or half odd integers. The projection quantum number m has for given j $r = 2j+1$ possible values

$$m = j\,,\ j-1,\ldots,-(j-1),-j \ .$$

Our eigenvalue problems, we started, are now written as

$$\hat{\vec{J}}^2\left|jm\right\rangle = \hbar^2 j(j+1)\left|jm\right\rangle, \qquad \hat{J}_z\left|jm\right\rangle = \hbar m\left|jm\right\rangle \ .$$

Since our proof was general, since we used only general commutation relations of operators, our result is also general. It means that the only allowed values for *j* are

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots \ .$$

For angular momentum there were only integer values $l = j = 0, 1, 2, \ldots$ allowed, but in physics there are physical objects, which angular momentum is equal to some half odd integer. Next we see that electron has intrinsic angular momentum, called spin, which has value $s = j = 1/2$).

16.5 Matrix form of operators. Next we derive tha matrix form of $\hat{J}_x$ and $\hat{J}_y$. Since $\hat{\vec{J}}^2$ and $\hat{J}_z$ were diagonal $(2j+1)\times(2j+1)$ square matrices, matrices $\hat{J}_x$ and $\hat{J}_y$ are not diagonal.

At first we derive matrix elements of $\hat{J}_+$ ja $\hat{J}_-$, since it is simpler. We start from

$$\hat{\vec{J}}^2 = \hat{J}_+\hat{J}_- + \hat{J}_z^2 - \hbar\hat{J}_z$$

and calculate the following matrix element $\langle jm'|\hat{\vec{J}}^2|jm\rangle$ for $\hat{\vec{J}}^2$

$$\langle jm'|\hat{\vec{J}}^2|jm\rangle = \langle jm'|\hat{J}_+\hat{J}_-|jm\rangle + \hbar^2 m(m-1)\langle jm'|jm\rangle \ ,$$

which is written as

$$\hbar^2 j(j+1)\,\delta_{m'm} = \langle jm'|\hat{J}_+\hat{J}_-|jm\rangle + \hbar^2 m(m-1)\,\delta_{m'm} \ .$$

At first we see, that in the case of $m' \neq m$ we have

$$\langle jm'|\hat{J}_+\hat{J}_-|jm\rangle = 0 \ ,$$

and for that reason we consider the case $m' = m$

$$\hbar^2 j(j+1) = \langle jm|\hat{J}_+\hat{J}_-|jm\rangle + \hbar^2 m(m-1) \ .$$

It gives

$$\langle jm|\hat{J}_+\hat{J}_-|jm\rangle = \hbar^2\,(j(j+1) - m(m-1)) = \hbar^2\,(j+m)(j+1-m) \ .$$

Next we analyse the matrix element on left more closely, taking into account that $\hat{J}_+$ and $\hat{J}_-$ are rising and lowering operators, and use the fullness condition of states $|jm\rangle$. After some simple algebra we get

$$\langle jm|\hat{J}_+\hat{J}_-|jm\rangle = \sum_{m'}\langle jm|\hat{J}_+|jm'\rangle\langle jm'|\hat{J}_-|jm\rangle = \langle jm|\hat{J}_+|jm-1\rangle\langle jm-1|\hat{J}_-|jm\rangle$$

($\hat{J}_-|jm\rangle \sim |jm-1\rangle$ and $\hat{J}_+|jm-1\rangle \sim |jm\rangle$). Since $\hat{J}_+$ and $\hat{J}_-$ are conjugated to each other, we have

$$(\hat{J}_+)_{mm-1} = (\hat{J}_-)^*{}_{m-1m} \ ,$$

or

$$\langle jm|\hat{J}_+|jm-1\rangle = (\langle jm-1|\hat{J}_-|jm\rangle)^* \ .$$

Therefore

$$\langle jm|\hat{J}_+\hat{J}_-|jm\rangle = \left|(\hat{J}_-)_{m-1m}\right|^2 ,$$

which on other hand equals

$$\left|(\hat{J}_-)_{m-1m}\right|^2 = \hbar^2\,(j+m)(j+1-m) \ ,$$

we get for $\hat{J}_-$ the following nonzero matrix elements (we choose them to be the real numbers)

$$(\hat{J}_-)_{m-1m} = \hbar\sqrt{(j+m)(j+1-m)} \ .$$

The nonzero matrix elements of $\hat{J}_+$ we find using the relation $(\hat{J}_+)_{mm-1} = (\hat{J}_-)^*_{m-1m}$

$$(\hat{J}_+)_{mm-1} = \hbar\sqrt{(j+m)(j+1-m)} \ ,$$

or after changing indices

$$(\hat{J}_+)_{m+1m} = \hbar\sqrt{(j+m+1)(j-m)} \ .$$

Matrix elements of $\hat{J}_x$ and $\hat{J}_y$ are calculated from relations

$$\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-) \ , \qquad \hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-) \ .$$

Järgmistes näidetes tuletame operaatorite ilmse maatrikskuju $j = 1/2$ ja $j = 1$ jaoks.

Example 1. *j* = 1/2. Now $m = +1/2, -1/2$. All matrices are 2x2 square matrices with matrix elements labelled as follows

$$\begin{pmatrix} a_{1/21/2} & a_{1/2-1/2} \\ a_{-1/21/2} & a_{-1/2-1/2} \end{pmatrix} .$$

$\hat{\vec{J}}^2$ and $\hat{J}_z$ were diagonal

$$\hat{J}^2 = \hbar^2 \frac{1}{2}(\frac{1}{2}+1)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{3\hbar^2}{4} I \ , \qquad J_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

To find matrix elements of $\hat{J}_x$ and $\hat{J}_y$ we first calculate nonzero matrix elements of $\hat{J}_+$ and $\hat{J}_-$, which are

$$(\hat{J}_+)_{1/2-1/2} = \hbar \ , \qquad (\hat{J}_-)_{-1/21/2} = \hbar \ ,$$

and therefore

$$J_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad J_y = \frac{\hbar}{2i}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} .$$

In next paragraphs we use these matrices to describe spin 1/2 (electron, for example). We introduce a set of matrices $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, called Pauli matrices, as follows

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

Now

$$\vec{J} = \frac{\hbar}{2}\vec{\sigma} \ .$$

Example 2. $j = 1$. Now $m = +1, 0, -1$. All matrices are 3x3 matrices

$$\begin{pmatrix} a_{11} & a_{10} & a_{1-1} \\ a_{01} & a_{00} & a_{0-1} \\ a_{-11} & a_{-10} & a_{-1-1} \end{pmatrix}.$$

$\hat{\hat{J}}^2$ and $\hat{J}_z$ are

$$\hat{J}^2 = \hbar^2 1(1+1)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = 2\hbar^2 I\,, \qquad J_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Nonzero matrix elements of $\hat{J}_+$ and $\hat{J}_-$ are

$$(\hat{J}_+)_{10} = \hbar\sqrt{2} \quad , \qquad (\hat{J}_+)_{0-1} = \hbar\sqrt{2}\ ,$$

$$(\hat{J}_-)_{01} = \hbar\sqrt{2} \quad , \qquad (\hat{J}_-)_{-10} = \hbar\sqrt{2}\ .$$

Therefore

$$J_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad , \qquad J_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$