26. Time dependence of physical quantities, conservation laws

Next we analyse of how physical quantity A changes in time and derive the conditions, when that quantity is conserved. We start with the mean value of A in some possible state $\psi = \psi(\vec{r},t)$ and investigate its time dependence. The mean value of A is calculated as

$$< A >= \int \psi^*(\vec{r},t)\hat{A}\psi(\vec{r},t)\,dV = \langle \psi | \hat{A} | \psi \rangle \ .$$

Time derivative of it is

$$\frac{d}{dt} < A >= \int \psi^* \frac{\partial \hat{A}}{\partial t}\psi\, dV + \int \frac{\partial \psi^*}{\partial t}\hat{A}\psi\, dV + \int \psi^* \hat{A}\frac{\partial \psi}{\partial t} dV$$

(since $\vec{r}$ is variable of integration, all derivatives under the integral become partial derivatives).

Since the wave function $\psi = \psi(\vec{r},t)$ is the solution of Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \ , \qquad -i\hbar \frac{\partial \psi^*}{\partial t} = (\hat{H}\psi)^* \ ,$$

we replace the partial derivatives from wave function and get

$$\frac{d}{dt} < A >= \int \psi^* \frac{\partial \hat{A}}{\partial t}\psi\, dV - \frac{1}{i\hbar}\int (\hat{H}\psi)^* \hat{A}\psi\, dV + \frac{1}{i\hbar}\int \psi^* \hat{A}\hat{H}\psi\, dV \ .$$

Since the Hamilton operator is hermitean, we remove it in the second term to right, and write the result as

$$\frac{d}{dt} < A >= \int \psi^* \frac{\partial \hat{A}}{\partial t}\psi\, dV + \frac{1}{i\hbar}\int \psi^* \left[\hat{A}, \hat{H}\right]\psi\, dV \ .$$

The last expression we write as operator identity

$$\frac{d\hat{A}}{dt} = \frac{\partial \hat{A}}{\partial t} + \frac{1}{i\hbar}\left[\hat{A}, \hat{H}\right] .$$

26.1 Conservation of physical quantity. Next we find conditions when the value of physical quantity is conserved. If A does not change in time then

$$\frac{d}{dt} < A >= 0 \ ,$$

which for operators means

$$\frac{d\hat{A}}{dt} = 0 = \frac{\partial \hat{A}}{\partial t} + \frac{1}{i\hbar}\left[\hat{A}, \hat{H}\right] .$$

When operator does not directly depend on time (i.e. is time independent: $\partial \hat{A} / \partial t = 0$), then A is conserved, if

$$\left[\hat{A}, \hat{H}\right] = 0 \ .$$

Therefore, each physical quantity which does not explicitly depend on time, is conserved, if its operator $\hat{A}$ commutes with the energy operator $\hat{H}$.

Some simple examples.

Example 1. Conservation of energy**.** Now $\hat{A} = \hat{H}$. From here we conclude, that energy is conserved when Hamilton operator does not explicitly depend on time

$$\frac{\partial \hat{H}}{\partial t} = 0 \ .$$

Example 2. Conservation of momentum. Momentum operator $\hat{\vec{p}} = -i\hbar\nabla$ does not depend on time. Momentum is conserved in each system, energy operator of which commutes with momentum operator

$$\left[\hat{\vec{p}}, \hat{H}\right] = 0 \ .$$

The simplest example is free particle. In free particle case

$$\hat{H} = \frac{1}{2M}\hat{\vec{p}}^2 \equiv -\frac{\hbar^2}{2M}\Delta \ .$$

Example 3. Conservation of angular momentum. Angular momentum operator is $\hat{\vec{L}} = \vec{r} \times \hat{\vec{p}}$. Angular momentum is conserved when

$$\left[\hat{\vec{L}}, \hat{H}\right] = 0 \ .$$

Example – particle in central force field.

Nex we demonstrate that the well known conservation laws (energy, momentum and angular momentum) follow from the symmetries of space and time.

26.2 Homogenity of time and energy conservation. As we know the general conservation laws for energy, momentum and angular momentum are valied in macro and microworld, where they are derived from the corresponding fundamental equations. Therefore it is possible to assume that these laws are more general and follow from more general assumtions, rather from physical equations valied in different theories.

Next we demonstrate that from the homogenity of time follows the energy conservation law. Time is homogeneous, since all time moments are equivalent. That concludes from our everyday experience – the results of experiments do not depend when we perform our experiment, important is that all physical conditions in experiments remain the same.

We consider the wave functions at some time moment t and at next moment $t + \delta t$, where δt is infinitesimal time interval (theoretically infinitely small) and find the time shift operator $\hat{T}(\delta t)$

$$\psi(t + \delta t) = \hat{T}(\delta t)\psi(t) \ .$$

Since δt is infinitely small, we may write

$$\psi(t+\delta t)=\psi(t)+\frac{\partial\psi}{\partial t}\delta t=(1+\delta t\frac{\partial}{\partial t})\psi(t)$$

(here is partial derivative, since $\psi=\psi(\vec{r},t)$). Therefore the time shift operator is

$$\hat{T}(\delta t)=1+\delta t\frac{\partial}{\partial t}\ .$$

If we assume that time is homogeneous, then that means that in energy measurements the result does not depend in which order we act: whether we perform the shift of time and them measure energy, of vice versa, measure energy and then perform the shift of time. Mathematically it means that operators $\hat{T}(\delta t)$ and $\hat{H}$ commute

$$\left[\hat{T}(\delta t),\hat{H}\right]=0 \qquad \rightarrow \qquad \hat{T}(\delta t)\hat{H}=\hat{H}\hat{T}(\delta t)\ .$$

From the last expression we conclude the conditions when energy is conserved. We write it as

$$(1+\delta t\frac{\partial}{\partial t})\hat{H}=\hat{H}(1+\delta t\frac{\partial}{\partial t})\ .$$

The latter equality holds, if

$$\frac{\partial\hat{H}}{\partial t}=0\ ,$$

which is the sufficient condition for the energy conservation.

26.3 Homogenity of space and momentum conservation. From the homogenity of space follows consevation of momentum. Space is homogeneous, since all points in space are equivalent. In our everyday experience it is obvious that the result of experiment does not depend on place if all the other physical conditions are the same.

Consider the wave functions in two different points $\vec{r}$ and $\vec{r}+\delta\vec{r}$, where $\delta\vec{r}=(\delta x,\delta y,\delta z)$ is infinitesimal space shift. Next we find the corresponding time shift operator $\hat{T}(\delta\vec{r})$

$$\psi(\vec{r}+\delta\vec{r})=\hat{T}(\delta\vec{r})\psi(\vec{r})\ .$$

Using the series expansion of $\psi(\vec{r}+\delta\vec{r})$, we may write

$$\psi(\vec{r}+\delta\vec{r})=\psi(\vec{r})+\frac{\partial\psi}{\partial x}\delta x+\frac{\partial\psi}{\partial y}\delta y+\frac{\partial\psi}{\partial z}\delta z=(1+\delta\vec{r}\cdot\nabla)\psi(\vec{r})\ .$$

We write it via the momentum operator $\hat{\vec{p}}=-i\hbar\nabla$

$$\psi(\vec{r}+\delta\vec{r})=(1+\frac{i}{\hbar}\delta\vec{r}\cdot\hat{\vec{p}})\psi(\vec{r})\ .$$

The space shift operator herefore is

$$\hat{T}(\delta\vec{r})=1+\frac{i}{\hbar}\delta\vec{r}\cdot\hat{\vec{p}}\ .$$

If we assume that space is homogeneous the space shift operator and Hamilton operator commute (result does not depend on place)

$$\hat{T}(\delta\vec{r})\hat{H} = \hat{H}\hat{T}(\delta\vec{r}) \ .$$

From here it follows that

$$\left[\hat{\vec{p}}, \hat{H}\right] = 0 \ ,$$

which is the momentum conservation law.

26.4 Isotrophy of space and conservation of angular momentum. From the isotrophy of space, which in other words means that all directions in space are equivalent follows the conservation law of angular momentum.

Isotrophy of space means the invariance under the rotations of space. For simplicity we consider the rotations around the z-axis only. On rotation by angle φ, the coordinates of any point transform as follows

$$x' = x\cos\varphi - y\sin\varphi \ ,$$

$$y' = x\sin\varphi + y\cos\varphi \ ,$$

$$z' = z \ .$$

Since z does not change, we consider the transformations of x and y only. In rotations by the infinitesimal angle $\delta\varphi$ we have

$$x' = x - y\,\delta\varphi \ , \quad y' = y + x\,\delta\varphi \ .$$

Next we find the space rotation operator $\hat{T}(\delta\varphi)$ from

$$\psi(x - y\delta\varphi, y + x\delta\varphi, z) = \hat{T}(\delta\varphi)\psi(x, y, z) \ .$$

Using the series expansion of $\psi(x - y\delta\varphi, y + x\delta\varphi, z)$, we get

$$\psi(x - y\delta\varphi, y + x\delta\varphi, z) = \psi(x, y, z) + \frac{\partial\psi}{\partial x}(-y\delta\varphi) + \frac{\partial\psi}{\partial y}(x\delta\varphi) =$$

$$= \psi(x, y, z) + \delta\varphi(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})\psi(x, y, z) \ .$$

Since operator of z-component of angular momentum is

$$\hat{L}_z = -i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}) \ ,$$

we may write

$$\psi(x - y\delta\varphi, y + x\delta\varphi, z) = (1 + \frac{i\delta\varphi}{\hbar}\hat{L}_z)\psi(x, y, z) \ .$$

From here the space rotation operator $\hat{T}(\delta\varphi)$ is

$$\hat{T}(\delta\varphi) = 1 + \frac{i\delta\varphi}{\hbar}\hat{L}_z \ .$$

If we assume the isothrophy of space (in rotations around the z-axis), then

$$\hat{T}(\delta\varphi)\hat{H} = \hat{H}\hat{T}(\delta\varphi) \ .$$

From here follows the conservation of L_z

$$\left[\hat{L}_z\,,\hat{H}\right] = 0 \ .$$

If we analyse similar rotations around the x- and y-axis, we get the conservations of L_x and L_y

$$\left[\hat{L}_x\,,\hat{H}\right] = \left[\hat{L}_y\,,\hat{H}\right] = 0 \ .$$

Of course, from these three it follows $\left[\ \hat{\vec{L}}^2\,,\hat{H}\ \right] = 0$.

26.5 Parity and parity conservation. In addition to the "classical" conservation laws, we treated above, in microworld there are conservation laws connected with discrete transformations, such as space reflection $\vec{r} \to -\vec{r}$, time rflection $t \to -t$ and charge conjugation $q \to -q$, which are called as P, T and C transformations.

As an example we analyse here only space reflection symmetry, which introduces the new conservative quantity, called <u>parity.</u> We define the following space reflection operator $\hat{P}$, which in transformations

$$\vec{r} = (x,y,z) \quad \to \quad -\vec{r} = (-x,-y,-z)$$

gives

$$\hat{P}\psi(\vec{r}) = \psi(-\vec{r}) \ ,$$

therefore for each function $\psi(\vec{r})$ makes the coordinates of each point opposite.

Let us solve the eigenvalue problem

$$\hat{P}\psi(\vec{r}) = \lambda\psi(\vec{r}) \ ,$$

where eigenvalues λ are called parity. Next we demonstrate, that $\lambda = \pm 1$.

First we take the eigenvalue problem and apply once more operator $\hat{P}$ from left. Then using the same eigenvalue problem, we get

$$\hat{P}^2\psi(\vec{r}) = \hat{P}(\hat{P}\psi(\vec{r})) = \lambda\,\hat{P}\psi(\vec{r}) = \lambda^2\,\psi(\vec{r}) \ .$$

Next we perform similar calculations using the definition of parity operator $\hat{P}$

$$\hat{P}^2\psi(\vec{r}) = \hat{P}(\hat{P}\psi(\vec{r})) = \hat{P}\psi(-\vec{r}) = \psi(\vec{r}) \ .$$

Comparing these two results, we conclude tha $\lambda^2 = 1$, and therefore $\lambda = \pm 1$.

The states with $\lambda = 1$ are called positive parity states. These states satisfy

$$\psi(\vec{r}) = \psi(-\vec{r}) \ .$$

States with $\lambda = -1$ are called negative parity states. These satisfy

$$\psi(\vec{r}) = -\psi(-\vec{r}) \ .$$

When parity operator commutes with the hamiltonian operator

$$\left[\hat{P}, \hat{H}\right] = 0,$$

parity is conserved, which means that all states have definite parity. If the hamiltonian describes also spectral transitions then there are allowed only transitions between the same parity.

Example 4. Electron in central symmetric field. In central symmetric field

$$\hat{H} = -\frac{\hbar^2}{2M}\Delta + U(r) \ .$$

Since in reflections $\vec{r} \to -\vec{r}$ Laplace operator $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ and potential energy $U(r)$ do not change, parity is conserved quantity. We usually use spherical coordinates (r, θ, φ) and there Hamiltonian operator is written as

$$\hat{H} = -\frac{\hbar^2}{2M}\Delta_r + \frac{1}{2Mr^2}\hat{\vec{L}}^2 + U(r)$$

and it has solutions in form

$$\psi_{nlm}(r, \theta, \varphi) = R_{nl}(r) Y_{lm}(\theta, \varphi) \ .$$

Since $\left[\hat{P}, \hat{H}\right] = 0$, then it also follows that

$$\left[\hat{P}, \hat{\vec{L}}^2\right] = 0 \ ,$$

moreover, it is possible to demonstrate that $\left[\hat{P}, \hat{L}_x\right] = \left[\hat{P}, \hat{L}_y\right] = \left[\hat{P}, \hat{L}_z\right] = 0$.

The above given means that solutions

$$\psi_{nlm}(r, \theta, \varphi) = R_{nl}(r) Y_{lm}(\theta, \varphi),$$

corresponding to energy E_{nl}, must have certain fixed parity. On space reflections the spherical coordinates change, as follows

$$(r, \theta, \varphi) \quad \to \quad (r, \pi - \theta, \varphi + \pi) \ ,$$

therefore all reduces to the parity of spherical functions.

Spherical functions are usually defined to satisfy

$$Y_{lm}(\pi - \theta, \varphi + \pi) = (-1)^l Y_{lm}(\theta, \varphi) \ ,$$

which gives that these have parities

$$\lambda = (-1)^l \ .$$

In our course we do not analyse discrete symmetries more thoroughly, but in particle physics they are very important. Parity is connected with the left-right symmetry. When there is total parity concervation the world is symmteric and it is not important whether we use the right hand coordinate system, or the left hand coordinate system (some physics quantities change their directions, but physical laws do not change). Up to 1956 physicists believed that parity

conservation is universal, but unfortunately it is not so, in weak processes (as β-decay, as an example) parity is not conserved. In other processes it is conserved. For that reason the parity conservation, which is alo calles as P-invariance, is not universal. After the violation of parity conservation, it was found, that if we add to space reflections charge conjugation, i.e. change the electrical charges of all particles to opposite (change particles to its antiparticles), the physics remains the same. That was called the CP-invariance. In 1964 it appears that there exist some particles (neutral K-mesons), which violate the CP-invariance. There is also the third important discrete symmetry, symmetry under the time reflection $t \to -t$, which is called T-invariance. Some processes are T-invariant, which means that if it is possible to proceed opposite in time, the processes remain the same. But T-invariance is also not universal. In modern physics it is proved that the universal invariance is the CPT-invariance, which means that if we go from the right hand world to the left hand one, change particles to corresponding antiparticles and also turn the time arrow to opposite, all physical laws remain the same.

Appendix.

In quantum mechanics the relations between operators are the same that the similar relations between the same quantities in classical physics.

First example: relation between the velocity and momentum $\vec{v} = (\dot{\vec{r}}) = \vec{p}/M$ in quantum mechanics turns to the same relation between the corresponding operators (prove it)

$$\dot{\hat{r}} = \frac{\hat{\vec{p}}}{M} \ .$$

Second example: the fundamental law of classical meshanics is the Newton second law

$$\frac{d\vec{p}}{dt} = \vec{F} \equiv -gradU \ .$$

Prove that the same relation in quantum mechanics is

$$\frac{d\hat{\vec{p}}}{dt} = -gradU \ .$$

27. Klein-Gordon equation

Next we consider the first relativistic generalization of Schrödinger equation.

27.1 Formal derivation of Schrödinger equation. Here we give the „derivation“ of Schrödingeri equation for free particle. The total energy (now it is kinetic energy) is

$$E = \frac{Mv^2}{2} = \frac{p^2}{2M} \ .$$

If we replace the physical quantities by corresponding operators

$$E \ \rightarrow \ i\hbar\frac{\partial}{\partial t}, \qquad \vec{p} \ \rightarrow \ -i\hbar\nabla$$

and apply the result to function ψ, we get Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2M}\Delta\psi \ .$$

(If we add potential energy, then it is general Schrödinger equation we started our course.)

27.2 Klein-Gordon equation. Here we „derive“ analogically new equation, but start from the relativistic relation between energy and momenyum $E = \sqrt{p^2c^2 + m_0^2c^4}$. Since here appears square root, which for operators is not defined, we take the square of energy

$$E^2 = p^2c^2 + m_0^2c^4 \ .$$

Making analogical replacements we get the following equation

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2} = -\hbar^2c^2\Delta\psi + m_0^2c^4\psi \ .$$

We rewrite it as

$$\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \Delta\psi + \frac{m_0^2c^2}{\hbar^2}\psi = 0 \ .$$

The given equation is called Klein-Gordon equation. It differs from the classial wave equation

$$\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \Delta\psi = 0$$

by the mass term added and therefore describes some massive particle.

Since it is a free particle equation, we try find the solutions in form of de'Broglie waves

$$\psi(\vec{r},t) = \psi_0\, e^{-\frac{i}{\hbar}(Et - \vec{p}\cdot\vec{r})} \ .$$

If we calculate derivatives

$$\frac{\partial^2\psi}{\partial t^2} = -\frac{E^2}{\hbar^2}\psi \ , \qquad \Delta\psi = -\frac{p^2}{\hbar^2}\psi \ ,$$

we after repalcement get the following relation

$$(-\frac{E^2}{\hbar^2 c^2} + \frac{p^2}{\hbar^2} + \frac{m_0^2 c^2}{\hbar^2})\psi_0 = 0 \ ,$$

which is valied if $E^2 = p^2c^2 + m_0^2c^4$. Therefore the Klein-Gordon equation is indeed relativistic generalization of Schrödinger equation, since it gives the right relativistic expression for energy and momentum.

27.3 Continuity equation. Next we derive the continuity equation

$$\frac{\partial\rho}{\partial t} + div\vec{j} = 0$$

and demonstrate that ρ is not a probability density, as it is in quantum mechanics we treated before.

Equation for the complex conjugated wave function is

$$\frac{1}{c^2}\frac{\partial^2\psi^*}{\partial t^2} - \Delta\psi^* + \frac{m_0^2c^2}{\hbar^2}\psi^* = 0 \ .$$

We multiply the ordinary equation from left to ψ^* and the complex conjugated equation from right to ψ. After subtracting the results, we have

$$\frac{1}{c^2}(\psi^*\frac{\partial^2\psi}{\partial t^2} - \frac{\partial^2\psi^*}{\partial t^2}\psi) - \psi^*(\Delta\psi) + (\Delta\psi^*)\psi = 0 \, .$$

The result is also written as

$$\frac{1}{c^2}\frac{\partial}{\partial t}(\psi^*\frac{\partial\psi}{\partial t} - \frac{\partial\psi^*}{\partial t}\psi) + \nabla\cdot((\nabla\psi^*)\psi - \psi^*(\nabla\psi)) = 0 \ ,$$

whic is the continuity equation, where

$$\rho = \psi^*\frac{\partial\psi}{\partial t} - \frac{\partial\psi^*}{\partial t}\psi \ ,$$

and

$$\vec{j} = c^2((\nabla\psi^*)\psi - \psi^*(\nabla\psi)) \ .$$

From the above expressions it is obvious that we cannot interprete ρ as the probability density, since it is not positively determined (there exists no negative probability!).

Since ρ is not always positive, is a serious problem from quantum mechanical point of view and it was the main reason why the Klein-Gordon equation was not taken seriously after it was derived. Moreover, it has in addition to positive energy solutions $E = +\sqrt{p^2c^2 + m_0^2c^4}$ always

negative energy solutions $E = -\sqrt{p^2c^2 + m_0^2c^4}$, which is also problematical in quantum mechanics.

It should be mentioned, that there are indeed problems if we try to use Klein-Gordon equation in ordinary quantum mechanics, but it is normal relativistic equation and is used in quantum field theory (relativistic particle physics) and it describes spinnless (s = 0) massive particles.

27.4 Nonrelativistic limit. As it is known, classical relativity theory (special relativity) goes in small velocities limit over to Newtonian mechanics. That is called nonrelativistic limit. Similarly Klein-Gordon equation has nonrelativistic limit and it is Schrödinger equation. Next we shall demonstrate it for the Klein-Gordon particle in an external electromagnetic field. After the substitution

$$E \rightarrow i\hbar\frac{\partial}{\partial t} - e\phi\,, \quad \vec{p} \rightarrow -i\hbar\nabla - e\vec{A}$$

and using $E^2 = p^2c^2 + m_0^2c^4$ we get the equation

$$(i\hbar\frac{\partial}{\partial t} - e\phi)^2\psi = c^2(-ih\nabla - e\vec{A})^2\psi + m_0^2c^4\psi \ .$$

In nonrelativistic case the rest energy of a particle $E_0 = m_0c^2$ is of some orders of magnitude greater that its nonrelativistic energy E', we separate it from our equation using the following transformation

$$\psi(\vec{r},t) = \psi'(\vec{r},t)\,e^{-\frac{i}{\hbar}m_0c^2t} \ .$$

Also we in next calsutaions use the fact that the rest energy $E_0 = m_0c^2$ is large and all other energies are small, and for that reason also $|e\phi| << m_0c^2$. It means that all terms which do not contain the rest energy, are omitted.

We start from the left side of our equation

$$(i\hbar\frac{\partial}{\partial t} - e\phi)\,e^{-\frac{i}{\hbar}m_0c^2t}\psi' = e^{-\frac{i}{\hbar}m_0c^2t}(i\hbar\frac{\partial\psi'}{\partial t} + m_0c^2\psi' - e\phi\psi') \ ,$$

$$(i\hbar\frac{\partial}{\partial t} - e\phi)^2\,e^{-\frac{i}{\hbar}m_0c^2t}\psi' = e^{-\frac{i}{\hbar}m_0c^2t}m_0c^2(2i\hbar\frac{\partial\psi'}{\partial t} - 2e\phi\psi' + m_0c^2\psi') \ ,$$

where in the last expression all terms without m_0c^2 were omitted.

Similarly the right side of our eqution gives

$$e^{-\frac{i}{\hbar}m_0c^2t}(\,c^2(-i\hbar\nabla - e\vec{A})^2\psi' + m_0^2c^4\psi') \ .$$

As a final result, after cancelling exponent and dividing by $2m_0c^2$, we get

$$i\hbar\frac{\partial\psi'}{\partial t}-e\phi\psi'+\frac{m_0c^2}{2}\psi'=\frac{1}{2m_0}(-i\hbar\nabla-e\vec{A})^2\psi'+\frac{m_0c^2}{2}\psi' \ ,$$

which after some simple transformations gives us Schrödinger equation

$$i\hbar\frac{\partial\psi'}{\partial t}=\frac{1}{2m_0}(-i\hbar\nabla-e\vec{A})^2\psi'+e\phi\psi' \ .$$

28. Dirac equation

In the previous paragraph we noted that the relativistic Klein-Gordoni equation was not satisfactory, since there are no quantity which should be treated as probability density. The main reason for it is, that there is the second order derivative of time. That was the main reason why Dirac starts to look for some new relativistic equation which has a normal probability interpretation. At first he decided that it must be a first order equation (in relativistic equation all derivatives must be of the same order due to the relation between energy and momentum). If we try to start from the classical relation $E=\sqrt{p^2c^2+m_0^2c^4}$, as before, then it gives nothing normal, since we are not able to go directly to operators, since roots of operators are not defined mathematically.

28.1 General form of Dirac equation. We try to find our new equation in form

$$i\hbar\frac{\partial\Psi}{\partial t}=c(\alpha_z\hat{p}_x+\alpha_y\hat{p}_y+\alpha_z\hat{p}_z+m_0c\beta)\Psi \ ,$$

where $\alpha_x,\alpha_y,\alpha_z$ and β are some new operators which commute with the momentum operator (for simplicity we omit the operator mark, since as we soon see, these are some matrices).

We write it in standard form

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

where the haniltonian operator is

$$\hat{H}=c(\alpha_z\hat{p}_x+\alpha_y\hat{p}_y+\alpha_z\hat{p}_z+m_0c\beta) \ .$$

Next we calcuate the square of $\hat{H}$. If $\hat{H}$ is indeed energy operator, the we must get the operator form of $E^2=p^2c^2+m_0^2c^4$, that is $\hat{H}^2=\hat{\vec{p}}^2c^2+m_0^2c^4$, or

$$\hat{H}^2=c^2(\hat{p}_x^2+\hat{p}_y^2+\hat{p}_z^2)+m_0^2c^4 \ .$$

In calculating the square of $\hat{H}$, we take into consideration that $\alpha_x,\alpha_y,\alpha_z$ and β are operators and for that reason its order in products is important. The result is

$$\hat{H}^2 = c^2(\alpha_x^2\hat{p}_x^2 + \alpha_y^2\hat{p}_y^2 + \alpha_z^2\hat{p}_z^2) + m_0^2c^4\beta^2 +$$

$$+ c^2((\alpha_x\alpha_y + \alpha_y\alpha_x)\hat{p}_x\hat{p}_y + (\alpha_y\alpha_z + \alpha_z\alpha_y)\hat{p}_y\hat{p}_z + (\alpha_z\alpha_x + \alpha_x\alpha_z)\hat{p}_z\hat{p}_x +$$

$$+ m_0c\hat{p}_x(\alpha_x\beta + \beta\alpha_x) + m_0c\hat{p}_y(\alpha_y\beta + \beta\alpha_y) + m_0c\hat{p}_z(\alpha_z\beta + \beta\alpha_z)) \ .$$

Comapring it with the previous expression of $\hat{H}^2$, we get the following relations for $\alpha_x, \alpha_y, \alpha_z$ and β

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = I \ ,$$

$$\alpha_x\alpha_y + \alpha_y\alpha_x = 0 \ , \quad \alpha_y\alpha_z + \alpha_z\alpha_y = 0 \ , \quad \alpha_z\alpha_x + \alpha_x\alpha_z = 0 \ ,$$

$$\alpha_x\beta + \beta\alpha_x = 0 \ , \quad \alpha_y\beta + \beta\alpha_y = 0 \ , \quad \alpha_z\beta + \beta\alpha_z = 0$$

must be valid. First we see that operators $\alpha_x, \alpha_y, \alpha_z$ and β are not numbers, since numbers commute, but our quantities do not commute, they anticommute, for example $\alpha_x\alpha_y = -\alpha_y\alpha_x$. For that reason we try to search them in matrix form, and for that reason, must assume that the wave function Ψ is also some n-component matrix. We therefore must find 4 anticommuting matrices whch squares are equal to unit matrix.

First we see that these matrices have an even number of rows and columns. As an example, we take the following relation

$$\alpha_x\beta = -\beta\alpha_x \equiv -I\beta\alpha_x$$

(in the last equality we added unit matrix). We take dterminants from both sides and use the fact that determinant from the product of matrices is the product of its determinants

$$\det\alpha_x \det\beta = \det(-I)\det\beta\det\alpha_x \ .$$

From here it follows that

$$\det(-I) = (-1)^n = 1 \ ,$$

and therefore the possible values of n are n = 2, 4, 6, ...

It is easy to verify that there are no four 2x2 matrices. There are four independent 2x2 matrices $I, \sigma_x, \sigma_y, \sigma_z$, but only three anticommuting ones (Pauli matrices).

The next possibility is to use 4x4 matrices. It appears that we indeed find 4 matrices which satisfy all above given relations. There exist of course different sets of matrices to use, but here we give one of them which is mostly used. These are expressed via the Pauli matrices and have the following form

$$\alpha_x = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}, \quad \alpha_y = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix}, \quad \alpha_z = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} .$$

As we see that it is the representation via 2x2 matrices and is mostly used form of them, but in reality they are the following 4x4 matrices

$$\alpha_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \alpha_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \alpha_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

By direct calculation it is easy to verify that all the above given relation are satisfied (the square of matrices equals to 4x4 unit matrix).

Since operators $\alpha_x, \alpha_y, \alpha_z$ and β are 4x4 matrices, our wave function Ψ has four components

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}.$$

Since we mostly use the so-called two component representation (using 2x2 Pauli matrices), we present also Ψ in "two component" form, as

$$\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix},$$

where

$$\varphi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

and

$$\chi = \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix}.$$

They are frequently called upper and lower components.

Similarly, as Pauli matrices, we treat matrices $\alpha_x, \alpha_y, \alpha_z$ as matrix vector $\vec{\alpha} = (\alpha_x, \alpha_y, \alpha_z)$ components and it allows to write the Dirac equation in more compact form

$$i\hbar \frac{\partial \Psi}{\partial t} = c(\hat{\vec{p}} \cdot \vec{\alpha} + m_0 c\beta)\Psi \ .$$

First we derive the continuity equation and show that now we got the nonnegative quantity ρ which is interpreted as the probability density. We start from the Dirac equation in the following form

$$i\hbar \frac{\partial \Psi}{\partial t} = c(-i\hbar \nabla \cdot \vec{\alpha} + m_0 c\beta)\Psi \ .$$

Since it is a matrix equation we derive the equation for the conjugated wave function Ψ^+ (which is four component one row matrix). The result is

$$-i\hbar \frac{\partial \Psi^+}{\partial t} = c(i\hbar(\nabla \Psi^+) \cdot \vec{\alpha}^+ + m_0 c\Psi^+ \beta^+) \ .$$

Since $\vec{\alpha}^+ = \vec{\alpha}$ and $\beta^+ = \beta$, then

$$-i\hbar\frac{\partial\Psi^+}{\partial t} = c\,(i\hbar(\nabla\Psi^+)\cdot\vec{\alpha} + m_0 c\Psi^+\beta) \ .$$

Next we multiply the first equation from the left to Ψ^+ and the latter one from the right to Ψ and subtract the second one from the first one, we get the following result

$$\Psi^+\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^+}{\partial t}\Psi = -c\,(\Psi^+\vec{\alpha}\cdot(\nabla\Psi) + (\nabla\Psi^+)\cdot\vec{\alpha}\,\Psi) \ ,$$

which we rewrite as

$$\frac{\partial}{\partial t}(\Psi^+\Psi) + c\nabla\cdot(\Psi^+\vec{\alpha}\,\Psi) = 0 \ .$$

We therefore got the continuity equation

$$\frac{\partial\rho}{\partial t} + div\vec{j} = 0 \ ,$$

where

$$\rho = \Psi^+\Psi \ , \qquad \vec{j} = c\Psi^+\vec{\alpha}\,\Psi \ .$$

From it it is easy to verify that the quantity

$$\rho = \Psi^+\Psi = \psi_1{}^*\psi_1 + \psi_2{}^*\psi_2 + \psi_3{}^*\psi_3 + \psi_4{}^*\psi_4$$

is nonnegative and therefore may be treated as probability density.

28.2 Solutions of Dirac equation. Next we analyse the solutions of Diraci equation. Since it is a free particle equation, we try to find solutions in the form of de'Broglie waves

$$\Psi = \Psi_0 e^{-\frac{i}{\hbar}(Et - \vec{p}\cdot\vec{r})} \ ,$$

where Ψ_0 is some four component constant

$$\Psi_0 = \begin{pmatrix}\varphi_0\\ \chi_0\end{pmatrix} \ .$$

Calculating derivatives

$$\frac{\partial\Psi}{\partial t} = -\frac{iE}{\hbar}\Psi \ , \quad \frac{\partial\Psi}{\partial x} = \frac{ip_x}{\hbar}\Psi \ , \quad \frac{\partial\Psi}{\partial y} = \frac{ip_y}{\hbar}\Psi \ , \quad \frac{\partial\Psi}{\partial z} = \frac{ip_z}{\hbar}\Psi \ ,$$

and substituting to the Dirac equation, we get equation for Ψ_0

$$E\Psi_0 = c(\vec{p}\cdot\vec{\alpha} + m_0 c\beta)\Psi_0 \ .$$

Its two-component form is (we omit the index 0)

$$E\begin{pmatrix}\varphi\\ \chi\end{pmatrix} = (\,c\begin{pmatrix}0 & \vec{p}\cdot\vec{\sigma}\\ \vec{p}\cdot\vec{\sigma} & 0\end{pmatrix} + m_0 c^2\begin{pmatrix}I & 0\\ 0 & -I\end{pmatrix})\begin{pmatrix}\varphi\\ \chi\end{pmatrix} \ ,$$

and gives us two equations

$$E\varphi = c(\vec{p}\cdot\vec{\sigma})\chi + m_0c^2\varphi \ ,$$

$$E\chi = c(\vec{p}\cdot\vec{\sigma})\varphi - m_0c^2\chi \ .$$

We also write them as

$$(E - m_0c^2)\varphi = c(\vec{p}\cdot\vec{\sigma})\chi \ ,$$

$$(E + m_0c^2)\chi = c(\vec{p}\cdot\vec{\sigma})\varphi \ .$$

Next we find the conditions which give us nontrivial solutions for φ and χ. If we write these equations as one matrix equation

$$\begin{pmatrix} E - m_0c^2 & c\vec{p}\cdot\vec{\sigma} \\ c\vec{p}\cdot\vec{\sigma} & E + m_0c^2 \end{pmatrix}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = 0 \ ,$$

it is easy to see, that nontrivial solutions exists if the determinant of a given system equals to zero

$$\begin{vmatrix} E - m_0c^2 & c\vec{p}\cdot\vec{\sigma} \\ c\vec{p}\cdot\vec{\sigma} & E + m_0c^2 \end{vmatrix} = 0 \ .$$

Since it is 4x4 determinant

$$\begin{vmatrix} E - m_0c^2 & 0 & cp_z & cp_x - icp_y \\ 0 & E - m_0c^2 & cp_x + icp_y & -cp_z \\ cp_z & cp_x - icp_y & E + m_0c^2 & 0 \\ cp_x + icp_y & -cp_z & 0 & E + m_0c^2 \end{vmatrix} = 0 \ .$$

our calculations give the following result

$$((E - m_0c^2)(E + m_0c^2) - c^2p^2)^2 = (E^2 - c^2p^2 - m_0^2c^4)^2 = 0 \ .$$

Now it is obvious that we have nontrivial solutions if energy and momentum are related by the above given relativistic relation (and we have particle with the rest mass m_0.

Of course there are two types of solutions: solutions with positive energy and solutions with the negative energy:

$$E = \sqrt{p^2c^2 + m_0^2c^4} \quad , \quad E = -\sqrt{p^2c^2 + m_0^2c^4} \ .$$

In the Klein-Gordon equation case there were similarly positive and negative energy solutions. That is the common property of all relativistic wave equations (about the physical meaning of negative energy solutions we talk later).

Next we analyse solutions more closely. From the equations

$$(E - m_0c^2)\varphi = c(\vec{p}\cdot\vec{\sigma})\chi \ ,$$

$$(E + m_0c^2)\chi = c(\vec{p}\cdot\vec{\sigma})\varphi \ ,$$

we see, that there is possible to express the lower components via the upper ones, and vice versa.

Before doing it, we use the simplest way and at first take the rest system (coordinate system where particle is at rest), therefore we take $\vec{p} = 0$. In that case

$$(E - m_0c^2)\varphi = 0 \ ,$$

$$(E + m_0c^2)\chi = 0 \ .$$

In the positive energy case ($E = m_0c^2$) we have: $\varphi \neq 0$ and $\chi = 0$, therefore our particle is described with the help of two upper components

$$\Psi_0 = \begin{pmatrix} \varphi \\ 0 \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ 0 \\ 0 \end{pmatrix} .$$

In the negative energy case ($E = -m_0c^2$) we have: $\varphi = 0$ and $\chi \neq 0$, therefore our particle is described with the help of two lower components

$$\Psi_0 = \begin{pmatrix} 0 \\ \chi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \psi_3 \\ \psi_4 \end{pmatrix} .$$

In other reference frames the solutions have more complicated form, since $\vec{p} \neq 0$, and all four components are usually nonzero. The solutions are usually written in form where one pair of components is expressed via anotger pair of components. In the positive energy case $E + m_0c^2 \neq 0$, and therefore we may express χ as

$$\chi = \frac{c\vec{p} \cdot \vec{\sigma}}{E + m_0c^2} \varphi$$

and write the corresponding general solution as

$$\Psi_0 = \begin{pmatrix} \varphi \\ \dfrac{c\vec{p} \cdot \vec{\sigma}}{E + m_0c^2} \varphi \end{pmatrix} .$$

We see that the solution is determined by two upper components.

In the negative energy case $E - m_0c^2 \neq 0$ we may express analogically φ and express the corresponding general solution as

$$\Psi_0 = \begin{pmatrix} \dfrac{c\vec{p} \cdot \vec{\sigma}}{E - m_0c^2} \chi \\ \chi \end{pmatrix} .$$

28.3 Spin of Dirac particle. Next we prove that Dirac equation describes particles with spin 1/2. Therefore it is the equation which must be used, as an example, for electrons. The easiest way to prove it is using the rest system of a particle: $\vec{p} = 0$. The Hamilton operator is

$$\hat{H} = m_0 c^2 \beta \ .$$

It is easy to verify that it commutes with the spin operator

$$\vec{s} \equiv \vec{\Sigma} = \frac{\hbar}{2}\begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} .$$

(These are spin 1/2 matrices correspondingly for upper and lowe components.)

Since $\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$ is diagonal, then it is obvious that

$$\left[\hat{H}, \vec{\Sigma}\right] = 0 \ .$$

It means that Dirac equation has solutions with certain spin (1/2) and spin-projection.

Simple calculation gives that

$$\vec{\Sigma}^2 = \frac{3\hbar^2}{4} I \ ,$$

therefore all components correspond to spin 1/2 . Spin projection operator is

$$\Sigma_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} .$$

From here: spin projection $\sigma = +1/2$ corresponds to solutions

$$\Psi_0^1 = \begin{pmatrix} \psi_1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad \Psi_0^3 = \begin{pmatrix} 0 \\ 0 \\ \psi_3 \\ 0 \end{pmatrix},$$

spin projection $\sigma = -1/2$ corresponds to solutions

$$\Psi_0^2 = \begin{pmatrix} 0 \\ \psi_2 \\ 0 \\ 0 \end{pmatrix}, \qquad \Psi_0^4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \psi_4 \end{pmatrix} .$$

In mathematics two component quatities, which described spin 1/2 are called spinors, the four component quantities corresponding to the solutions of Dirac equation are called bispinors.

We do not give here the general proof that Dirac equation describes spin 1/2. In order to prove it one must use the general free particle equation

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

where

$$\hat{H}=c(\vec{\alpha}\cdot\hat{\vec{p}}+m_0c\beta)\,.$$

Now it is possible to demonstrate that the conserved quantity is the total momentum

$$\vec{J}=\vec{L}+\vec{s}\ .$$

(Prove it!)

Which concerns the negative energy solutions, one may ask what is the physical meaning of such solutions. In 1928 when Dirac write down his famous equation only electron and proton were the two known elementary particles and at first Dirac proposed that the negative energy solution describes proton (if positine energy solution is used for electron) since negative energy solutions for charged particles always describe the opposite charge described by the positive energy solutions. Since both solutions must describe particles with the same rest mass that was not true, because the masses of electrons and protons are different. For that reason Dirac assumed that negative energy particles must describe antiparticles (particles with the same rest mass but different electrical charge and magnetic moments orientations. Therefore in addition to electron there must exist particle with the same mass, but with positive elementary charge. That particle was called positron. It was experimentally discovered in cosmic radiation in 1932. Now we know that all microparticles have its antiparticle, there are also some neutral particles (photon, neutral π-meson, ...) but these particles are identical with its antiparticle.

29. Approximations of Dirac equation

In previous paragraph we demostrated that the Dirac equation is a relativistic wave equation for particles with spin 1/2 . Therefore it must be used for electrons, moreover it also gives the right connection between spin and magnetic moment of electron. However Dirac equation is quite complicated and for that reason it is mainly used in quantum field theory (theory of elementary particles). But also in quantum mechanics (which is nonrelativistic theory) it describes some important physical effects. Next we analyse two different approximations: the first one is nonrelativistic approximation and gives us the well known Pauli equation, the second one is the first relativistic approximation, it explains the fine structure of hydrogen atom's energy levels.

29.1 Pauli equation. First we demonstrate that the nonrelatvistic approximation of Dirac equation is the two component Pauli equation.

We start with free particle equation, which for spinors φ ja χ is written as

$$(E-m_0c^2)\varphi=c(\vec{p}\cdot\vec{\sigma})\chi\ ,$$

$$(E+m_0c^2)\chi=c(\vec{p}\cdot\vec{\sigma})\varphi\ .$$

Since in quantum mechanics we operate only with positive energy solutions, we express χ via φ

$$\chi = \frac{c\vec{p}\cdot\vec{\sigma}}{E + m_0c^2}\varphi \ .$$

Now it is possible to verify, that in nonrelativistic limit the latter components are so small that we may neglect them. Indeed, the nonrelativistic energy E' is much smaller that the rest energy of our particle, therefore

$$E = m_0c^2 + E', \quad where \quad E' << m_0c^2 \ ,$$

and

$$\chi = \frac{c\vec{p}\cdot\vec{\sigma}}{2m_0c^2 + E'}\varphi \approx \frac{c\vec{p}\cdot\vec{\sigma}}{2m_0c^2}\varphi << \varphi \ .$$

Next we introduce the external electromagnetic field and treat the electron in external field. We use the standard minimal substitution

$$i\hbar\frac{\partial}{\partial t} \ \rightarrow \ i\hbar\frac{\partial}{\partial t} + e\phi \ , \quad \hat{\vec{p}} \ \rightarrow \hat{\vec{p}} + e\vec{A}$$

and get the following Dirac equation

$$i\hbar\frac{\partial\Psi}{\partial t} + e\phi\,\Psi = c\vec{\alpha}\cdot(\hat{\vec{p}} + e\vec{A})\,\Psi + m_0c\beta\,\Psi \ .$$

Suppose that external field does not depend on time, we search the solutions in the following form

$$\Psi(\vec{r},t) = e^{-\frac{i}{\hbar}Et}\Psi_0(\vec{r}) \ .$$

It gives for the $\Psi_0(\vec{r})$ components φ and χ the following equations

$$(E + e\phi - m_0c^2)\varphi = c\,\vec{\sigma}\cdot(\hat{\vec{p}} + e\vec{A})\,\chi \ ,$$

$$(E + e\phi + m_0c^2)\chi = c\,\vec{\sigma}\cdot(\hat{\vec{p}} + e\vec{A})\,\varphi \ .$$

Next we assume that in nonrelativistic limit $E = m_0c^2 + E'$ and also the electrons potential energy is small, i.e. $\left|E' + e\phi\right| << m_0c^2$.

From the first equation

$$(E' + e\phi)\varphi = c\,\vec{\sigma}\cdot(\hat{\vec{p}} + e\vec{A})\,\chi \ ,$$

from the second one we express χ as

$$\chi = \frac{c\vec{\sigma}\cdot(\hat{\vec{p}} + e\vec{A})}{E' + e\phi + 2m_0c^2}\varphi \approx \frac{1}{2m_0c}\vec{\sigma}\cdot(\hat{\vec{p}} + e\vec{A}) \ .$$

After replacing χ to the first equation we may write

$$E'\varphi = \frac{1}{2m_0 c}(\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A}))(\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A}))\varphi - e\phi\varphi \ .$$

The equation, obtained, is the Pauli equation. To write it in the standard form we must calculate $(\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A}))(\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A}))$. Using $(\vec{\sigma}\cdot\vec{a})(\vec{\sigma}\cdot\vec{b}) = \vec{a}\cdot\vec{b} + i\vec{\sigma}\cdot(\vec{a}\times\vec{b})$, we get

$$(\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A}))(\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A})) = (\hat{\vec{p}}+e\vec{A})^2 + i\vec{\sigma}\cdot((\hat{\vec{p}}+e\vec{A})\times(\hat{\vec{p}}+e\vec{A})) \ .$$

The last term takes the form

$$(\hat{\vec{p}}+e\vec{A})\times(\hat{\vec{p}}+e\vec{A}) = e\hat{\vec{p}}\times\vec{A} = -i\hbar e\nabla\times\vec{A} \equiv -i\hbar e\, rot\vec{A} = -i\hbar e\vec{B} \ ,$$

and in total

$$(\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A}))(\vec{\sigma}\cdot(\hat{\vec{p}}+e\vec{A})) = (\hat{\vec{p}}+e\vec{A})^2 + e\hbar\vec{\sigma}\cdot\vec{B} \ .$$

After substituting the results of our calculations we get the Pauli equation

$$E'\varphi = \frac{1}{2m_0}(\hat{\vec{p}}+e\vec{A})^2\varphi + \frac{e\hbar}{2m_0}\vec{\sigma}\cdot\vec{B}\varphi - e\phi\varphi \ ,$$

from which the known relation between electron's spin $\vec{s}$ and its magnetic moment follows

$$\vec{\mu}_s = -\frac{e}{m_0}\vec{s}$$

(here m_0 denotes the rest mass of electron, in previous paragraphs it was denoted by M).

As we told before, Pauli introduced the magnetmoment term to its equation using common sense and general physical considerations. In the Dirac equation case it follows directly from equation and proves that Dirac equation describes electron with its real magnetic moment.

29.2 First relativistic approximation. Next we go to the following approximation and take into account also the v^2/c^2 terms. Since the general analysis is very complicated we treat only the fine structure of hydrogen atom. That is, we next treat the case where the magnetic field (vector potential) is absent and there exists only electrical field which is due to the proton (nucleus): $\vec{A} = 0$, $\phi(r) \neq 0$. The equations, we started with, taking $E = m_0c^2 + E'$ are the following

$$(E' + e\phi)\varphi = c\vec{\sigma}\cdot\hat{\vec{p}}\,\chi \ ,$$

$$(E' + e\phi + 2m_0c^2)\chi = c\vec{\sigma}\cdot\hat{\vec{p}}\,\varphi \ .$$

In next analyse we also want to go to two component equation, as we did in the nonrelativistic approximation case. However, it cannot be done simply by direct replacement, since the direct replacement changes the probability density. Therefore we first analyse the problem with probability density and find the possibility to go over to two component equation which preserves the probability. Probability density in the four component case is

$$\Psi^+\Psi = \varphi^+\varphi + \chi^+\chi \ .$$

In the nonrelativistic case lower components are small

$$\chi = \frac{\vec{p}\cdot\vec{\sigma}}{2m_0 c}\varphi << \varphi$$

and since v/c is also very small, we get $\chi^+\chi = 0$. Therefore in that approximation

$$\Psi^+\Psi = \varphi^+\varphi \ .$$

But now, if we take into account terms with v^2/c^2 , the product of lower components is nonzero $\chi^+\chi \neq 0$. For that reason we define a new two component quantity ψ

$$\varphi = N\psi$$

and find such N, which gives

$$\Psi^+\Psi = \psi^+\psi \ .$$

In other words it means, that if we replace χ using the second equation, we also must perform the change $\varphi = N\psi$. If we write it symbolically as $\chi = \hat{V}\varphi$, we after the replacement have

$$\chi = \hat{V}N\psi$$

and the problem is to find N which preserves the probability density

$$\Psi^+\Psi = \varphi^+\varphi + \chi^+\chi = \psi^+N^+N\psi + \psi^+N^+V^+VN\psi \equiv \psi^+\psi \ .$$

Next we start with direct calculations to find the "renorming" factor N. At first we find χ from the second equation

$$\chi = \frac{c}{2m_0c^2 + E' + e\phi}\hat{\vec{p}}\cdot\vec{\sigma}\varphi \ .$$

We rewrite it assuming that $(E'+e\phi)/2m_0c^2$ is of the same order of magnitude as v^2/c^2 ($(E'-U) \approx p^2/2m_0$), and get

$$\chi = \frac{1}{2m_0c}(1+\frac{E'+e\phi}{2m_0c^2})^{-1}(\hat{\vec{p}}\cdot\vec{\sigma})\varphi = \frac{1}{2m_0c}(1-\frac{E'+e\phi}{2m_0c^2})(\hat{\vec{p}}\cdot\vec{\sigma})\varphi \ .$$

We use it soon to replace it to equation. Since we take the terms up to v^2/c^2, then calculating $\chi^+\chi$ up to v^2/c^2 terms, we may take

$$\chi = \frac{\hat{\vec{p}}\cdot\vec{\sigma}}{2m_0c}N\psi \ ,$$

which must give us

$$\Psi^+\Psi = \psi^+(N^+N + N^+\frac{\hat{\vec{p}}^2}{4m_0^2c^2}N)\psi \equiv \psi^+\psi \ .$$

Taking N as $N = 1+\alpha\frac{\hat{\vec{p}}^2}{c^2}$, we get $\alpha = -\frac{1}{8m_0^2c^2}$ and it gives the following renorming factor

$$N = 1 - \frac{\hat{\vec{p}}^2}{8m_0^2c^2} \ .$$

Going back to our equation, we must perform the following change on the right side of the first equation

$$\chi = \frac{1}{2m_0 c}(1-\frac{E'+e\phi}{2m_0c^2})(\hat{\vec{p}}\cdot\vec{\sigma})(1-\frac{\hat{\vec{p}}^2}{8m_0^2c^2})\psi = \frac{1}{2m_0 c}(1-\frac{E'+e\phi}{2m_0c^2}-\frac{\hat{\vec{p}}^2}{8m_0^2c^2})(\hat{\vec{p}}\cdot\vec{\sigma})\psi \ .$$

If we also express the left hand side via ψ, we have

$$(E'+e\phi)(1-\frac{\hat{\vec{p}}^2}{8m_0^2c^2})\psi = (E'+e\phi-\frac{(E'+e\phi)\,\hat{\vec{p}}^2}{8m_0^2c^2})\psi \ ,$$

which in total gives us the equation

$$(E'+e\phi-\frac{(E'+e\phi)\hat{\vec{p}}^2}{8m_0^2c^2})\psi = \frac{1}{2m_0}(\hat{\vec{p}}\cdot\vec{\sigma})(1-\frac{E'+e\phi}{2m_0c^2}-\frac{\hat{\vec{p}}^2}{8m_0^2c^2})(\hat{\vec{p}}\cdot\vec{\sigma})\psi \ ,$$

which after some simple calculations gives

$$(E'+e\phi-\frac{(E'+e\phi)\hat{\vec{p}}^2}{8m_0^2c^2})\psi = \frac{1}{2m_0}\,(\hat{\vec{p}}^2-\frac{(\hat{\vec{p}}\cdot\vec{\sigma})(E'+e\phi)(\hat{\vec{p}}\cdot\vec{\sigma})}{2m_0c^2}-\frac{\hat{\vec{p}}^4}{8m_0^2c^2})\,\psi \ .$$

Before starting further calculations we once more rewrite the above given equation. In the left side there remains Schrödinger equation without any perturbations, all the higher order terms (perturbations) are written on the right side. After that we treat the right side as some small perturbation to the ordinary Schrödinger equation

$$(E'-\frac{\hat{\vec{p}}^2}{2m_0}+e\phi)\,\psi = \frac{1}{8m_0^2c^2}\,((E'+e\phi)\,\hat{\vec{p}}^2-(\hat{\vec{p}}\cdot\vec{\sigma})(E'+e\phi)(\hat{\vec{p}}\cdot\vec{\sigma})-\frac{\hat{\vec{p}}^4}{2m_0})\,\psi \ .$$

Next we tranform the right side in order to eliminate the $E'+e\phi$ term and terms connected with it. We start from the middle term, which using the properties of Pauli matrices gives

$$(\hat{\vec{p}}\cdot\vec{\sigma})(E'+e\phi)(\hat{\vec{p}}\cdot\vec{\sigma}) = (E'+e\phi)\hat{\vec{p}}^2+(e\hat{\vec{p}}\phi\cdot\sigma)(\hat{\vec{p}}\cdot\vec{\sigma}) \ .$$

Further, the second term here, using $\hat{\vec{p}}\phi = -i\hbar\nabla\phi = i\hbar\vec{\mathrm{E}}$, where $\vec{\mathrm{E}}$ is the electric field strength connected with potential $\phi(\vec{r})$, gives

$$e(\hat{\vec{p}}\phi\cdot\vec{\sigma})(\hat{\vec{p}}\cdot\vec{\sigma}) = ie\hbar(\vec{\mathrm{E}}\cdot\vec{\sigma})(\hat{\vec{p}}\cdot\vec{\sigma}) = ie\hbar\vec{\mathrm{E}}\cdot\hat{\vec{p}}-e\hbar\vec{\sigma}\cdot(\vec{\mathrm{E}}\times\hat{\vec{p}}) \ .$$

In conclusion the middle term is

$$(\hat{\vec{p}}\cdot\vec{\sigma})(E'+e\phi)(\hat{\vec{p}}\cdot\vec{\sigma}) = (E'+e\phi)\hat{\vec{p}}^2+ie\hbar\vec{\mathrm{E}}\cdot\hat{\vec{p}}-e\hbar\vec{\sigma}\cdot(\vec{\mathrm{E}}\times\hat{\vec{p}}) \ .$$

If we denote the right side term as $\hat{H}'\psi$, our perturbation Hamiltonian after replacements is

$$\hat{H}' = -\frac{1}{8m_0^2c^2}((E'+e\phi)\hat{\vec{p}}^2+\frac{\hat{\vec{p}}^4}{2m_0}+2ie\hbar\vec{\mathrm{E}}\cdot\hat{\vec{p}}-2e\hbar\vec{\sigma}\cdot(\vec{\mathrm{E}}\times\hat{\vec{p}})) \ .$$

Next we express $(E'+e\phi)\hat{\vec{p}}^2$ in another way. Since without perturbation ($\hat{H}'=0$) we have equation

$$(E' - \frac{\hat{\vec{p}}^2}{2m_0} + e\phi)\,\psi = 0 \ ,$$

we from it take

$$E' + e\phi = \frac{\hat{\vec{p}}^2}{2m_0}$$

and write $\hat{\vec{p}}^4 / 2m_0$ as

$$\frac{\hat{\vec{p}}^4}{2m_0} = \hat{\vec{p}}^2 (E' + e\phi) \ .$$

Transforming the right side, we get

$$\hat{\vec{p}}^2 (E' + e\phi) = (E' + e\phi)\hat{\vec{p}}^2 + e\hat{\vec{p}}^2\phi \ .$$

The last term here gives

$$\hat{\vec{p}} \cdot \hat{\vec{p}}\phi = \hat{\vec{p}} \cdot (\hat{\vec{p}}\phi) + \hat{\vec{p}} \cdot (\phi\,\hat{\vec{p}}) = (\hat{\vec{p}}^2\phi) + 2i\hbar\,\vec{\mathrm{E}} \cdot \hat{\vec{p}} \ .$$

In conclusion we write

$$\frac{\hat{\vec{p}}^4}{2m_0} = (E' + e\phi)\hat{\vec{p}}^2 + e(\hat{\vec{p}}^2\phi) + 2ie\hbar\,\vec{\mathrm{E}} \cdot \hat{\vec{p}}$$

and from here express $(E' + e\phi)\hat{\vec{p}}^2$ as

$$(E' + e\phi)\hat{\vec{p}}^2 = \frac{\hat{\vec{p}}^4}{2m_0} - e(\hat{\vec{p}}^2\phi) - 2ie\hbar\,\vec{\mathrm{E}} \cdot \hat{\vec{p}} \ .$$

In conclusion, our parturbation operator has the following final form

$$\hat{H}' = \frac{e\hbar}{4m_0^2c^2}\vec{\sigma} \cdot (\vec{\mathrm{E}} \times \hat{\vec{p}}) - \frac{\hat{\vec{p}}^4}{8m_0^3c^2} + \frac{e(\hat{\vec{p}}^2\phi)}{8m_0^2c^2} \ .$$

We denote the summands here as $\hat{H}_1'$, $\hat{H}_2'$ and $\hat{H}_3'$ and start to analyse their physical meaning.

29.3 Spin-orbital coupling. The first summand

$$\hat{H}_1' = \frac{e\hbar}{4m_0^2c^2}\vec{\sigma} \cdot (\vec{\mathrm{E}} \times \hat{\vec{p}})$$

is the spin-orbital coupling. In order to demonstrate it, we use the general central symmetric potential $\phi = \phi(r)$ jaoks. Electrical field strength $\vec{\mathrm{E}} = -grad\phi(r)$ is written as

$$\vec{\mathrm{E}} = -\frac{d\phi}{dr}\frac{\vec{r}}{r} \ .$$

Therefore

$$\hat{H}_1' = -\frac{d\phi}{dr}\frac{e\hbar}{4m_0^2c^2r}\vec{\sigma} \cdot (\vec{r} \times \hat{\vec{p}}) = -\frac{d\phi}{dr}\frac{e\hbar}{4m_0^2c^2r}\vec{\sigma} \cdot \hat{\vec{L}} \ .$$

Using the spin operator $\vec{s} = \hbar\vec{\sigma}/2$ it gives

$$\hat{H}_1' = -\frac{d\phi}{dr}\frac{e}{2m_0^2c^2r}\vec{s}\cdot\hat{\vec{L}} \ .$$

For the Coulomb field $\phi(r) = be/r$ and $d\phi/dr = -be/r^2$ (we next apply it in the case of hydrogen atom), we get

$$\hat{H}_1' = \frac{be^2}{2m_0^2c^2r^3}\vec{s}\cdot\hat{\vec{L}} = \frac{be^2\hbar}{4m_0^2c^2r^3}\vec{\sigma}\cdot\hat{\vec{L}} \ .$$

It is interesting to note that our derivation gives the exast value for the coefficient before $\vec{\sigma}\cdot\vec{L}$ and it is different from that, we obtain from classical physics.

29.4 Mass dependence from velocity. The second summand in perturbation is

$$\hat{H}_2' = -\frac{\hat{\vec{p}}^4}{8m_0^3c^2} \ .$$

The given term gives us correction to the kinetic energy due to the mass dependence from velocity (up to v^2/c^2). Indeed, relativistic kinetic energy is

$$T_{kin} = E - E_0 = \sqrt{p^2c^2 + m_0^2c^4} - m_0c^2 = m_0c^2\left(\sqrt{1+\frac{p^2}{m_0^2c^2}} - 1\right)$$

In series expansion the first three terms are

$$\sqrt{1+\frac{p^2}{m_0^2c^2}} = 1 + \frac{p^2}{2m_0^2c^2} - \frac{p^4}{8m_0^4c^4}$$

and after replacement gives for kinetic energy

$$T_{kin} = \frac{p^2}{2m_0} - \frac{p^4}{8m_0^3c^2} \ .$$

The first term is the classical kinetic energy, the second one takes into account that the mass increases with velocity. Comparing it with our perturbation operator, we see, that it indeed takes into account the mass dependence from velocity.

29.5 Contact interaction. The third summand

$$\hat{H}_3' = \frac{e(\hat{\vec{p}}^2\phi)}{8m_0^2c^2}$$

has no classical analogy and is connected with the charge density of nucleus. If we rewrite $\hat{\vec{p}}^2\phi$ as

$$\hat{\vec{p}}^2\phi = -\hbar^2\nabla^2\phi = -\hbar^2 div\, grad\phi = \hbar^2 div\vec{\mathrm{E}} = \frac{\hbar^2\rho}{\varepsilon_0} \ ,$$

where ρ is charge which generates the electrical field acting on electron (we used the Gauss theorem).

In Coulomb field $\phi(r) = be/r$ the charge density is $\rho(\vec{r}) = e\delta(\vec{r})$, therefore in our case

$$\hat{H}_3' = \frac{\hbar^2 e^2}{8m_0^2c^2\varepsilon_0}\delta(\vec{r}) = \frac{\hbar^2\pi\, be^2}{2m_0^2c^2}\delta(\vec{r}) \ .$$

Since the corresponding operator is nonzero only on one point $\vec{r} = 0$, it is called contact-interation and it acts only to these states which in $\vec{r} = 0$ have nonzero values for wave functions $\psi(0) \neq 0$. In hydrogen atom these are s-states ($l = 0$).

29.6 Fine structure of H-atom. Next we analyse the change of hydrogen energy levels due to perturbations treated before. Our starting equation was

$$(E' - \frac{\hat{\vec{p}}^2}{2m_0} + \frac{be^2}{r})\psi = \hat{H}'\psi \ ,$$

where

$$\hat{H}' = \hat{H}_1' + \hat{H}_2' + \hat{H}_3'$$

and

$$\hat{H}_1' = \frac{be^2}{2m_0^2c^2r^3}(\vec{s}\cdot\hat{\vec{L}}) \ , \quad \hat{H}_2' = -\frac{\hat{\vec{p}}^4}{8m_0^3c^2} \ , \quad \hat{H}_3' = \frac{\hbar^2\pi\, be^2}{2m_0^2c^2}\delta(\vec{r}) \ .$$

In the absence of perturbation (nonrelativistic limit), we have energy

$$E_n' = -\frac{R\hbar}{n^2} \ .$$

Next the energy corrections due to the added perturbations are equal to the diagonal matrix elements $\Delta E_i = \langle\psi_{nlm}|\hat{H}_i'|\psi_{nlm}\rangle$.

Spin orbital coupling. We have to calculate

$$\Delta E_1 = \frac{be^2}{2m_0^2c^2}\langle\psi_{nlm}|\frac{(\vec{s}\cdot\vec{L})}{r^3}|\psi_{nlm}\rangle \ .$$

Since $(\vec{s}\cdot\vec{L}) = \hbar^2 q/2$, where $q = l$ if $j = l + 1/2$ and $q = -(l+1)$ if $j = l - 1/2$ (see §23), then all reduces to the mean value of r^{-3}

$$\Delta E_1 = \frac{be^2 q}{2m_0^2c^2}\langle\psi_{nlm}|\frac{1}{r^3}|\psi_{nlm}\rangle = \frac{be^2 q}{2m_0^2c^2} < r^{-3} > \ .$$

Mean value of r^{-3} is (see §10)

$$< r^{-3} >= \frac{1}{r_0^3 n^3 \, l(l+1/2)(l+1)} \ .$$

Before we write down the energy correction, we use the following expresiions for the Rydberg constant, Bohr's radius and fine structure constant

$$R = \frac{m_0 b^2 e^4}{2\hbar^3} \ , \quad r_0 = \frac{\hbar^2}{m_0 b e^2} \ , \quad \alpha = \frac{be^2}{\hbar c} \ .$$

The final result is therefore

$$\Delta E_1 = \frac{R\hbar\alpha^2 q}{n^3 \, l(l+1/2)(l+1)} \ .$$

Since it is nonzero for states with $l \neq 0$ (if $l = 0$ then $\Delta E_1 = 0$), we write it the following general form, valid for each l

$$\Delta E_1 = \frac{R\hbar\alpha^2 q}{n^3 \, l(l+1/2)(l+1)} (1 - \delta_{l0}) \ .$$

Relativistic mass correction. Calculating matrix elements of $\hat{H}_2'$ we assume that in nonrelativistic limit

$$\frac{\hat{\vec{p}}^2}{2m_0} = E' + \frac{be^2}{r}$$

and write $\hat{H}_2'$ as

$$\hat{H}_2' = -\frac{1}{2m_0 c^2} (E' + \frac{be^2}{r})^2 = -\frac{1}{2m_0 c^2} (E'^2 + \frac{2E' be^2}{r} + \frac{b^2 e^4}{r^2})$$

The corresponding energy correstion reduces to the mean values of r^{-1} and r^{-2}, which are

$$< r^{-1} >= \frac{1}{r_0 n^2} \ , \quad < r^{-2} >= \frac{1}{r_0^2 n^3 (l+1/2)} \ .$$

After some simple calculations the final result is

$$\Delta E_2 = -\frac{1}{2m_0 c} (\frac{R^2\hbar^2}{n^4} - 2R\hbar be^2 < r^{-1} > + b^2 e^4 < r^{-2} >) = -\frac{R\hbar\alpha^2}{n^4} (\frac{2n}{2l+1} - \frac{3}{4})$$

(valid for each possible values of l).

Contact interaction. Calculatin matrix elements of $\hat{H}_3'$ we must take into account that $\delta(\vec{r})$ is nonzero in one point $\vec{r} = 0$, therefore

$$\langle \psi_{nlm} | \delta(\vec{r}) | \psi_{nlm} \rangle = |\psi_{nlm}(0)|^2 \ ,$$

The only wave functions which are nonero at $r = 0$ are the s-state functions. Since

$$\psi_{n00}(0) = \frac{1}{n\sqrt{n\pi r_0^3}} \ ,$$

then

$$|\psi_{n00}(0)|^2 = \frac{1}{n^3 \pi r_0^3} \ .$$

Therefore the corresponding energy correction is

$$\Delta E_3 = \frac{\hbar^2 \pi b e^2}{2 m_0^2 c^2} |\psi_{n00}(0)|^2 = \frac{R\hbar\alpha^2}{n^3} \ .$$

Since it is valid for $l = 0$ only, we write it as

$$\Delta E_3 = \frac{R\hbar\alpha^2}{n^3} \delta_{l0} \ .$$

Fine structure of hydrogen atom. The final result, adding all energy corrections give

$$\Delta E = -\frac{R\hbar\alpha^2}{n^4} \left(-\frac{nq(1-\delta_{l0})}{l(2l+1)(l+1)} + \frac{2n}{2l+1} - \frac{3}{4} - n\delta_{l0} \right) \ .$$

If we express it via the total angular momentum (if $l \neq 0$ total angular momentum is $j = l \pm 1/2$, if $l = 0$ $j = 1/2$), and taking into account the corresponding values of q , the total energy correction is

$$\Delta E = -\frac{R\hbar\alpha^2}{n^4} \left(\frac{2n}{2j+1} - \frac{3}{4} \right) \ .$$

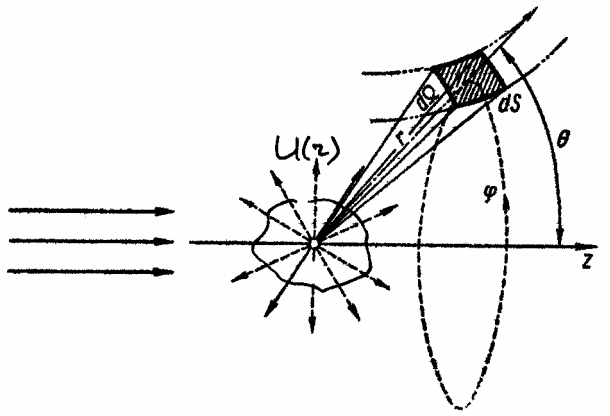
In conclusion we derived the result, we already analysed in §23, from the relativistic Dirac equation.

30. Basics of scattering theory

Under the scattering process we mean the inclination of particles from its previous direction due to the interaction with some other paticle or system. Scattering processes are the main experimental basic in particle physics. So the Rutherford experiments with α-particle scattering lead to tha discovery of atomic nucleus. Nowadays the scattering of particles in modern particle colliders is basic in investigations of particles and their characterics. For that reason the scattering theory is very important, but unfortunaly one of the most complicated chapters of physics.

30.1 Cross-section, scattering amplitude. Consider the scattering of particle flux on some scatterer. Incoming particles are characterised by flux density j_l, scattered particles in every element of solid angle $d\Omega$ are characterised by the number of particles dN_h per unit time. If we take z-axis along the flux of incoming particles and take the initial point of our coordinate system in scattering center (see figure), the number of scattered particles depends on angles θ and φ, i.e. $dN_h(\theta, \varphi)$. Differential cross section is defined as

$$d\sigma(\theta, \varphi) = \frac{dN_h(\theta, \varphi)}{j_l} \ .$$



In scattering processes we assume that incoming particles are "flying" from infinity and are therefore free particles, after scattering we register particles also far from scatterer, therefore they may also be treated as free particles.

Before we start more thorough analysis of scattering processes we express the differential cross section in another form. We express the number of scattered particles $dN_h(\theta, \varphi)$ via the flux of scattered particles, as

$$dN_h(\theta, \varphi) = j_h(\theta, \varphi)\, dS \ ,$$

where dS is the area, determined by solid angle

$$dS = r^2\, d\Omega \ .$$

In conclusion the diferential cross section is given, as follows

$$d\sigma(\theta, \varphi) = \frac{j_h(\theta, \varphi)}{j_l} dS \ , \qquad \text{or shorthand} \qquad d\sigma = \frac{j_h}{j_l} dS \ .$$

Here we see, that the dimension of differential cross section is the same as that of area. In microworld there is the corresponding special unit called barn ($1\ \text{b} = 10^{-28}\ \text{m}^2$).

The classical analog of scattering processes is collisions of particles. At the beginning the particles are free, at close distances there start to act forces which change their directions (sometimes also the number of particles is changed) and in the final stage particles also move freely. For that reason we are able to use certain conservation laws, which give us a lot of useful information about collisions. The main problems in scattering theory is to find what interactions lead to the results, obtained from scattering experiments. In quantum mechanics we usually from the known potential energy calculate the properties of particles (its energies and wave functions), in the scattering theory the prolems, we must solve, are opposite – to find the corresponding potential energy which leads to certain scattering.

As in classical scattering it is useful to analyse separately the processes of elastic scattering and nonelastic scattering. In elastic scattering the states of incoming particle and scattering centre do not change, in nonelastic scattering it changes. If we, for example consider the scattering of electrons on atoms (Franck-Hertz experiment), then in elastic scattering the electron's energy and atom's energy do not change, only the electon's direction changes, in unelastic scattering electron gives some of its energy to atom and atom goes to some of its exited states (electrons direction is also changed).

Since the mathematical theory of nonelastic processes is rather complicated, we restrict ourselves to the case of elastic scattering. In elastic scattering the inner state of scattering centre is unimportant and for that reason we charactrize it by some time independent potential energy

$$U = U(\vec{r})$$

which gives the interaction between particles and scattering centre (in classical interpretation – it gives the force which acts on particles).

In that case the problem reduses to the corresponding Schrödinger equation for stationary states

$$-\frac{\hbar^2}{2M}\Delta\psi + U\psi = E\psi \ .$$

Energy E is here the energy of incoming particle, therefore it is positive. We define

$$k^2 = \frac{2ME}{\hbar^2}$$

and rewrite the Schrödinger equation for scattering processes in the following form

$$(\Delta + k^2)\psi = \frac{2MU}{\hbar^2}\psi \ .$$

In scattering processes we must assume that the potential energy is nonzero only in limited distances from scattering centre. All forces in nature quite rapidly decrease and therefore that restriction is not quite important.

We are interested in specific solutions which desribes both – incoming particles and outcoming particles. Incoming particles are described (we choose the flux in the direction of z-axis) by the plane wave

$$e^{ikz} \ .$$

The outcoming particles far from scattering centre are described by spherical wave, moving away from scattering centre and depending on direction

$$f(\theta,\varphi)\,\frac{e^{ikr}}{r}\ .$$

For that reason we search the general solution in form

$$\psi(r,\theta,\varphi)=e^{ikz}+f(\theta,\varphi)\frac{e^{ikr}}{r}\ .$$

We see that our problem reduces to the calculation of amplitude $f(\theta,\varphi)$ of scattered particles. It allows to find the flux of particles which are scattered in certain fixed direction. Since incoming particles are described by the plane wave e^{ikz}, the flux of incoming particles is proportional to its velocity

$$j_l=\frac{\hbar k}{M}=v\ .$$

Since the flux of scattered particles is given by

$$j_h(\theta,\varphi)=\frac{\left|f(\theta,\varphi)\right|^2 v}{r^2}\ ,$$

the differential cross section is expressed as

$$d\sigma(\theta,\varphi)=\left|f(\theta,\varphi)\right|^2 d\Omega\ .$$

As we see the amplitude of scattered wave gives us the differential cross section.

30.2 Green functions method. Next we use the Green functions method and prove that the solution has indeed the above given form. We started from

$$(\Delta+k^2)\psi=\frac{2MU}{\hbar^2}\psi\ .$$

Next we introduce the Green function $G(\vec{r},\vec{r}\,')$, which satisfies

$$(\Delta+k^2)\,G(\vec{r},\vec{r}\,')=\delta(\vec{r}-\vec{r}\,')\,.$$

Using the Green function (see the Appendix at the end) the general solution is given as

$$\psi(\vec{r})=\psi_0(\vec{r})+\int G(\vec{r},\vec{r}\,')\frac{2M}{\hbar^2}U(\vec{r}\,')\psi(\vec{r}\,')\,dV'\ ,$$

where $\psi_0(\vec{r})$ is the solution of corresponding homogeneous equation

$$(\Delta+k^2)\psi_0=0\ .$$

Of course that solution may be given as the plane wave e^{ikz}.

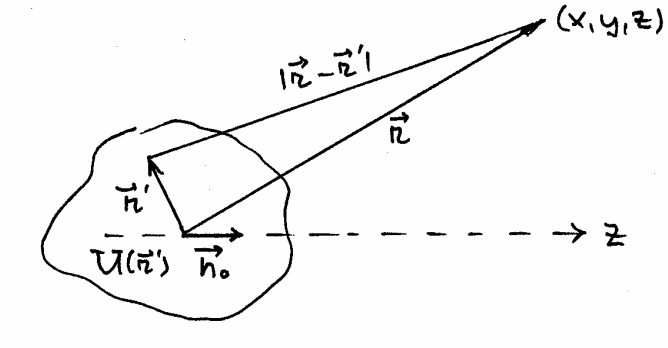
For our problem the corresponding Green function is (see Aappendix)

$$G(\vec{r},\vec{r}') = -\frac{1}{4\pi}\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} .$$

As a result, we have obtained an integral equation for $\psi(\vec{r})$

$$\varphi(\vec{r}) = e^{ikz} - \frac{M}{2\pi\hbar^2}\int \frac{e^{ik|\vec{r}-\vec{r}'|}U(\vec{r}')\varphi(\vec{r}')dV'}{|\vec{r}-\vec{r}'|} .$$

Next we analyse the integral and demonstrate that for large values of r we indeed get the solution in above given form. Assume that potential energy is nonzero at distances where $r' \le R$. (In all practical cases one always finds the distance R, where potential energy is so small, that we may neglect it). Distances



$$r >> R ,$$

we consider as large ones (then $r >> r'$) and therefore we may write

$$|\vec{r}-\vec{r}'| = \sqrt{(\vec{r}-\vec{r}')^2} = \sqrt{r^2 - 2\vec{r}\cdot\vec{r}'} = r - \frac{\vec{r}\cdot\vec{r}'}{r} .$$

As a result the solution takes the form

$$\psi(\vec{r}) = e^{ikz} - \frac{e^{ikr}}{r}\frac{M}{2\pi\hbar^2}\int e^{-i\vec{k}\cdot\vec{r}'}U(\vec{r}')\psi(\vec{r}')dV' ,$$

where $\vec{k} = k\vec{r}/r$. Scattering amplitude is therefore the following

$$f(\theta,\varphi) = -\frac{M}{2\pi\hbar^2}\int e^{-i\vec{k}\cdot\vec{r}'}U(\vec{r}')\psi(\vec{r}')dV' .$$

As a final result we found the needed general form of solutions, but the way to real solutions is yet quite far. Here we reduced the Schrödinger equation to integral equation, which is more complicated in comparison with differential equation, but it helps to prove the general form of solutions. As follows we analyse some simple cases, where it is possible to use some approximation methods and where the integral form turns out to be useful.

30.3 Born approximation. Next we assume that the scattering potential is small. Then we can use aproximation methods and take as the zeroth approximation for wave function the wave function of incoming particles, which we write as

$$\psi_0(\vec{r}) = e^{ikz} = e^{i\vec{k}_0\cdot\vec{r}} \ ,$$

where $\vec{k}_0 = k\,\vec{n}_0$ is the wave vector along the z-axis.

Now the scattering amplitude is expressed as integral

$$f(\theta,\varphi) = -\frac{M}{2\pi\hbar^2}\int e^{i\vec{K}\cdot\vec{r}'}U(\vec{r}')\,dV' \ ,$$

where

$$\vec{K} = \vec{k}_o - \vec{k} \ .$$

(Vector $\vec{K}$ is sometimes called collision vector.) If the explicit expression for potential energy is given it is possible to calculate the first approximation of scattering amplitude and also the scattering cross section.

Next we analyse the frequently appearing case, when the potential is central symmetric

$$U = U(r) \ .$$

Since it does not depend from angles, it is possible to integrate over the angles. Let us denote the angle between vectors $\vec{K}$ and $\vec{r}'$ as ϑ and since $\vec{K}\cdot\vec{r}' = K\,r'\cos\vartheta$, we have

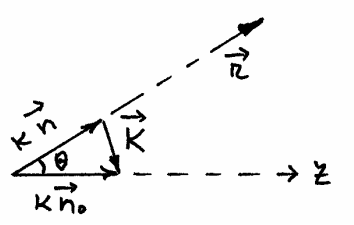
$$f(\theta) = -\frac{M}{2\pi\hbar^2}\int_0^{\infty}U(r')\,r'^2dr'\int_0^{\pi}e^{iKr'\cos\vartheta}\sin\vartheta\,d\vartheta\int_0^{2\pi}d\varphi \ .$$

Simple integration over angles gives

$$f(\theta) = -\frac{2M}{\hbar^2 K}\int_0^{\infty}U(r')\sin(Kr')\,r'dr'$$

Angle θ (see figure) is the angle between z-axis and the direction of scattered particles, therefore the scattering amplitude depends only from that angle, since

$$K = k\left|\vec{n}_0 - \vec{n}\right| = 2k\sin\frac{\theta}{2} \ .$$



Example. Yukawa potential energy. Next we calculate the scattering amplitude using Yukawa potential energy for the scattering centre. Yukawa derived that potential energy for nuclear forces and he takes it as the Coulomb potential energy (inversely proportional to distance) and cut it with decreasing exponent. Yukawa potential energy has a general form

$$U(r) = -A\frac{e^{-ar}}{r} \ .$$

Exponent quarantees that the radius of forces is small, the quantity $r_0 = 1/a$ is called the action radius of forces.

Substituting potential energy, we must calculate the following integral

$$f(\theta) = -\frac{2M}{\hbar^2 K}\int_0^\infty U(r')\sin(K r')\, r' dr' = \frac{2M A}{\hbar^2 K}\int_0^\infty e^{-a r'}\sin(K r')\, dr' \ .$$

Here we use the following integral, given in tables

$$\int_0^\infty e^{-a x}\sin(b x)\, dx = \frac{b}{a^2 + b^2} \ ,$$

and which gives the following scattering amplitude for the Yukawa potential

$$f(\theta) = \frac{2M A}{\hbar^2}\frac{1}{a^2 + K^2} = \frac{2M A}{\hbar^2}\frac{r_0^2}{1 + (r_0 K)^2}$$

(we assumed that the forces are small).

Scattering cross section is the following

$$\sigma(\theta) = \left| f(\theta) \right|^2 = \frac{4M^2 A^2 r_0^4}{\hbar^4 (1 + (r_0 K)^2)^2} \ .$$

In conclusion we shall analyse two special cases: 1) $r_0 K << 1$ ja 2) $r_0 K >> 1$.

1) Special case $r_0 K << 1$. That special case is connected with small forces and slowly moving particles. *K* is expressed via the velocity of incoming particles as

$$K = 2k\sin\frac{\theta}{2} = \frac{2p}{\hbar}\sin\frac{\theta}{2} = \frac{2Mv}{\hbar}\sin\frac{\theta}{2} \ .$$

The final result is

$$\sigma = \frac{4M^2 A^2 r_0^4}{\hbar^4} \ .$$

It means that the scattering of slow particles on forces with small action radius is isothropic and do not depend on direction at all.

2) In another special case $r_0 K >> 1$ we get the result

$$\sigma(\theta) = \frac{4M^2 A^2}{\hbar^4 K^4} \ .$$

It means that for fast particles the result does not depend action radius $r_0 = 1/a$.

The last result allows to apply it also in the case of Coulomb forces ($r_0 \to \infty$). Treating, as an example, the scattering of α-particles on atomic nucleous, we take

$$U(r) = -\frac{Z\,b\,e^2}{r} \ ,$$

(here $A = Z\,b\,e^2$) and get the well known Rutherford formula

$$\sigma(\theta) = \frac{Z^2 b^2 e^4 M^2}{4\,p^4 \sin^4 \dfrac{\theta}{2}} \ .$$

Appendix.

1. Green function's method. Suppose, we have an equation

$$\hat{F}\psi = \varphi \ ,$$

where $\hat{F}$ is some differential operator and φ some given function. The problem is to find function ψ.

To solve our equation we need the inverse operator $\hat{F}^{-1}$ for operator $\hat{F}$. Inverse operator is defined as operator which satisfies

$$\hat{F}^{-1}\hat{F} = \hat{F}\,\hat{F}^{-1} = 1 \ .$$

Applying the inverse operator we get the solution

$$\psi = \hat{F}^{-1}\varphi \ .$$

If operator $\hat{F}$ is a differential operator, the inverse operator is an integral operator. We write the solution $\psi = \hat{F}^{-1}\varphi$ as (to simplify the analysis, we restrict ourselves to one-dimensional case)

$$\psi(x) = \int G(x,x')\varphi(x')\,dx' \ .$$

If we apply operator $\hat{F}$ and use $\hat{F}\psi = \varphi$, we have

$$\hat{F}\psi(x) = \int \hat{F}\,G(x,x')\,\varphi(x')\,dx' = \varphi(x) \ .$$

The last equality holds, if

$$\hat{F}\,G(x,x') = \delta(x-x') \ .$$

Function $G(x,x')$, which is the solution of the above given equation, is called the Green function of equation $\hat{F}\psi = \varphi$. In order to solve our differential equation we must find the corresponding Green function.

Since the equation, we started with, is inhomogeneous, the general solution is some special solution of $\hat{F}\psi = \varphi$ plus the general solution of corresponding homogeneous equation $\hat{F}\psi_0 = 0$. Therefore the general solution is

$$\psi(x) = \psi_0(x) + \int G(x,x')\varphi(x')\,dx' \ .$$

In solving scattering problems the method of Green functions is also used, but in that case $\varphi(x)$ also depends on the function we tried to find, something like $\varphi(x) = A(x)\psi(x)$. That equation is more complicated and used in cases if one can apply some approximate methods.

2. Green function for $(\Delta + k^2)\psi = \varphi$. Now the Green function satisfies

$$(\Delta + k^2)\,G(\vec{r},\vec{r}') = \delta(\vec{r} - \vec{r}') \ .$$

To find it, we present $G(\vec{r},\vec{r}')$ as a Fourier' integral

$$G(\vec{r},\vec{r}') = \frac{1}{(2\pi)^{3/2}} \int g(\vec{q})\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}')}\, d^3q \ ,$$

for the Dirac delta function $\delta(\vec{r} - \vec{r}')$ we use integral

$$\delta(\vec{r} - \vec{r}') = \frac{1}{(2\pi)^3} \int e^{i\vec{q}\cdot(\vec{r}-\vec{r}')} d^3q \ .$$

Since

$$(\Delta + k^2)\,G(\vec{r},\vec{r}') = \frac{1}{(2\pi)^{3/2}} \int (k^2 - q^2)\, g(\vec{q})\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}')}\, d^3q$$

and it must give as a result δ-function, we get

$$g(\vec{q}) = \frac{1}{(2\pi)^{3/2}} \frac{1}{k^2 - q^2} \ .$$

Therefore the Green function is presented as integral

$$G(\vec{r},\vec{r}') = \frac{1}{(2\pi)^3} \int \frac{e^{i\vec{q}\cdot(\vec{r}-\vec{r}')}\, d^3q}{k^2 - q^2} \ .$$

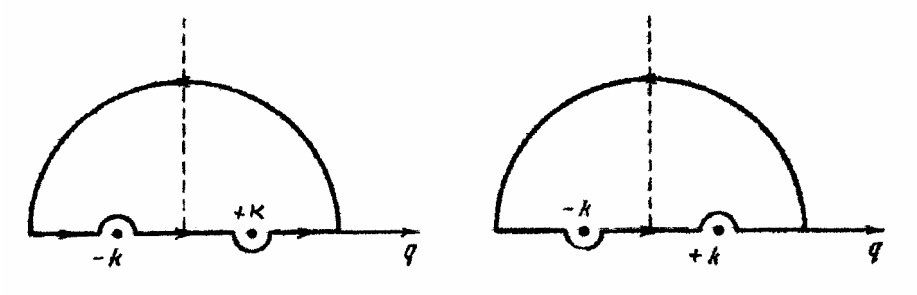
Nex we calculate that integral using in q-space spherical coordinates. Then the integral, we have to calculate, is the following

$$G(\vec{r},\vec{r}') = \frac{1}{(2\pi)^3} \int_0^\infty \frac{q^2 dq}{k^2 - q^2} \int_0^\pi e^{iq|\vec{r}-\vec{r}'|\cos\theta} \sin\theta\, d\theta \int_0^{2\pi} d\varphi \ .$$

Integrating over angles it remains the integral over q (but now from -∞ to +∞)

$$G(\vec{r},\vec{r}\,') = \frac{1}{4\pi^2 i\left|\vec{r}-\vec{r}\,'\right|}\int_{-\infty}^{+\infty}\frac{e^{iq\left|\vec{r}-\vec{r}\,'\right|}\,q\,dq}{k^2-q^2}\ .$$

Since the given integral is integral from some function of complex variables which has two singular points $q=\pm k$, the result is not unique, but depends on that, of how we choose the contour of integration.



There are different choices, but the mostly used ones are the following two: one of the singularities remains inside the cntour, the other is outside (as in above given figures). For such integrals the method of residues is used and the result is $2\pi i$ multiplied to residue in singular point. In the first case ($q=+k$) we get the result

$$G_+(\vec{r},\vec{r}\,') = -\frac{e^{ik\left|\vec{r}-\vec{r}\,'\right|}}{4\pi\left|\vec{r}-\vec{r}\,'\right|}$$

and in the second case ($q=-k$) we get the result

$$G_-(\vec{r},\vec{r}\,') = -\frac{e^{-ik\left|\vec{r}-\vec{r}\,'\right|}}{4\pi\left|\vec{r}-\vec{r}\,'\right|}\ .$$

In the first case we have the spherical waves which go away from the scattering centre (outcoming waves), in the second case we have incoming spherical waves. Calculating scattering amplitudes we must use Green function $G_+(\vec{r},\vec{r}\,')$, since scattering waves are outcoming waves.