

I. Elements of A. Einstein radiation theory.

In classical electrodynamics, any body moving with acceleration emit electromagnetic energy. The energy emitted per one second can be calculated by this way:

$$W_{classical} = \frac{2e^2}{3c^3} \bar{r} \quad \text{here } \bar{r} \text{ is average acceleration. For harmonic oscillator this energy is proportional to}$$

amplitude of oscillations. In classical physics charged body radiates energy continuously.

In quantum mechanics, systems (for example, an atom, a body, a harmonic oscillator, etc.) emit or absorb energy only when passing from one discrete level to another for example $n \rightarrow n'$. The first consideration of the problem of radiation was proposed by A. Einstein. He introduced the coefficients characterizing the induced transitions (due to external perturbation) $B_{nn'}$ and spontaneous transitions

$A_{nn'}$. The basis idea of Einstein approach is looks like so: if electron of some system locate on excited energy level E_n then there is a certain probability to per second $A_{nn'}$ for spontaneous transition to lower level $E_{n'}$. This transition is accompanied by emission of photon with energy $\hbar \omega$. If number of such excited atoms is N_n then the energy emitted (due to spontaneous transitions) per one second can be calculated as follows:

$$W^s = N_n A_{nn'} \hbar \omega .$$

The spontaneous transition is possible only for transition from upper levels to down. An external electromagnetic field leads to the appearance of additional, so called induced, transitions. This transitions are possible in both directions from top to lower and from down to up. If denote $\rho(\omega)$ as a spectral density of electromagnetic radiation then the emitted and absorbed energies are:

$$W_{emitted}^i = N_n B_{nn'} \hbar \omega \quad W_{absorb.}^i = N_{n'} B_{n'n} \hbar \omega$$

In thermodynamic equilibrium state:

$$N_n A_{nn'} + N_n B_{nn'} \rho = N_{n'} B_{n'n} \rho .$$

The number of electron on levels n and n' determined by Maxwell distribution function

$$N_n = C e^{-E_n/kT} \quad N_{n'} = C e^{-E_{n'}/kT} .$$

After substitution to previous equation and simplification for spectral function of radiation $\rho(\omega)$ we have:

$$\rho(\omega) = \frac{\frac{A_{nn'}}{B_{nn'}}}{\frac{B_{n'n}}{B_{nn'}} e^{\frac{\hbar \omega}{kT}} - 1} \quad \text{but the Planck function for absolutely black body is } \rho(\omega) = \frac{\hbar \omega^3}{\pi^2 c^3} \frac{1}{e^{\frac{\hbar \omega}{kT}} - 1} .$$

comparison of two last equations gives for Einstein coefficients next relationships: $B_{nn'} = B_{n'n}$ and for

probability of spontaneous and induced transitions $B_{nn'} = \frac{\hbar \omega^3}{\pi^2 c^3} A_{nn'}$. The existence of spontaneous

transitions from the physical point of view is very important. This means that in the absence of external perturbation, the atom always simultaneously passes to the ground state (to the state with minimum energy). Then the reciprocal value for coefficient $A_{nn'}$ can be interpreted as the lifetime of electron in a given state and electron cannot be in an excited state for an infinitely long time.

But one more question remains. If the induced transition can be explained by the action of an external electric field (electromagnetic wave), then what external influence leads to the appearance of spontaneous transitions? What is the physical reason of it? Unfortunately, this explanation cannot be found within the framework of the classical approach to the electromagnetic field. In quantum mechanics the electromagnetic wave can be represented as a set of harmonic oscillators (similarly to the vibration of atoms in crystal lattices). In the ground state, the energy of a harmonic oscillator has a non-zero value (zero oscillations) and spontaneous transitions are associated with the influence of this zero oscillations of the electromagnetic field

on the electrons of atoms. Exact calculation show that $A_{m'n'} \sim |r_{m'n'}|^2 = \left| \int \varphi^* \hat{r} \varphi dV \right|^2$. The elements of matrix $B_{m'n'} = B_{n'm'}$ can be calculated by using “golden rule” of quantum mechanics.

II. The basis ideas from relativistic quantum mechanics.

II.a Spin–statistics theorem

There is a spin–statistics theorem in quantum mechanics relates the intrinsic spin of a particle (angular momentum not due to the orbital motion) to the particle statistics it obeys. In units of the reduced Planck constant \hbar , all particles that move in 3 dimensions have either integer spin or half-integer spin. According to this theorem all particles can be divided into two classes.

The first are Bose (bosons) particles, which have an integer spin value, such as 0,1,2, etc. In each quantum state, there can be an infinitely large number Bose particles. All Bose particles in a given state have the same wave function. The probability of finding a particle in a state with energy E (due to thermal excitation) can be calculated using the Bose-Einstein distribution function:

$$f(E, T) = \frac{1}{e^{E/kT} - 1} .$$

An example of such particles are photons, phonons.

The second are Fermi (fermions) particles, which have an half-integer spin value, such as 1/2,3/2,5/2, etc. Only one Fermi particles can be located in given quantum state. This rule is called the Pauli exclusion principle. The probability of finding a particle in a state with energy E (due to thermal excitation) can be calculated using the Fermi-Dirac distribution function:

$$f(E, T) = \frac{1}{e^{(E-\mu)/kT} + 1} .$$

Here μ – chemical potential. For metals at room temperature the chemical potential can be replaced by the Fermi energy. The proton,neutron,electron are Fermi particles.

II.b Klein -Gordon equations

The Schrödinger equation in the non-relativistic case can be formally obtained from the expression for the classical total energy:

$$E = \frac{p^2}{2m} + U .$$

The conversion from classical physics to quantum mechanics can be carried out by replacing classical physical quantities with the corresponding operators. But what kind of operators? In classical physics, the law of conservation of energy is the result of the symmetry of space with respect to infinitesimal displacements in time, and the law of conservation of momentum is the result of the symmetry of space with respect to infinitesimal space displacements. The corresponding operators of space transformations (taken from the theory of so-called Lie and Poincaré groups) are looks like as follows:

$$\text{for } E \rightarrow \hat{E} = i\hbar \frac{d}{dt} \text{ and for space displacement in x-direction } \hat{p}_x \rightarrow -i\hbar \frac{d}{dx} \text{ and generally } \hat{p} = -i\hbar \hat{\nabla} .$$

After substitution into the previous equation, we have:

$$i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \Delta \psi + U \psi .$$

In special relativity (the potential energy is omitted) the total energy of particle is (see first lecture):

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

Klein-Gordon equation can be obtained by the same way. After substitution energy and momentum with corresponding operators we will get:

$$\frac{1}{c^2} \frac{d^2}{dt^2} \psi - \Delta \psi + \frac{m_0^2 c^2}{\hbar^2} \psi = 0$$

By using of so called d'Alembert operator $\square = \frac{1}{c^2} \frac{d^2}{dt^2} - \Delta$ finally we have the Klein-Gordon equation for free particles:

$$\square \psi + \frac{m_0^2 c^2}{\hbar^2} \psi = 0 .$$

This equation can be used to describe properties of so-called Bose particles .

The solution of this equation (for free particle) is: $\psi(t, x) = \frac{1}{V} e^{\frac{i}{\hbar}(p \cdot x - Et)}$ where $E = \pm \sqrt{p^2 c^2 + m_0^2 c^4}$. The negative value of energy should be discarded because there is no mechanism for transition from positive to negative energies states. But if we take into the account external electromagnetic field (this formally can be done by changes $E \rightarrow E + q \varphi$ and $\vec{p} \rightarrow \vec{p} - \frac{q}{c} \vec{A}$, here q-charge of particle, φ – electrostatic potential and A-magnetic potential) the solution of this new Klein-Gordon equation can be expressed as a superposition of solutions for free particle (due to the fact that this wavefunctions form a complete set of functions). But this representation is possible only if we take into the account the positive and negative values of energy. Later this result served as the basis to justify the possibility of the existence of antimatter and these two worlds (matter and antimatter) can interact through the electromagnetic field. The Klein-Gordon equation is suitable to describe the properties of non-spin particles.

II.c Dirac equation

The Dirac equation is another representation of the relativistic Schrödinger equation. The Hamilton operator in relativistic approximation is looks like this: $\hat{H} = \sqrt{\sum_{i=1,2,3} (\hat{p}_i c)^2 + m_0^2 c^4}$ here 1,2,3 \equiv x,y,z . Dirac

boldly suggested that for Fermi particles (particles with half-integer spin), the square root can be represented as a simple linear combination of the individual terms of the square root:

$$\sqrt{\sum_{\alpha=1,2,3} (\hat{p}_\alpha c)^2 + m_0^2 c^4} = \beta m_0 c^2 + \sum_{i=1,2,3} \alpha_i \hat{p}_i c , \text{ here } \alpha_i \text{ and } \beta$$

are a suitable coefficients but this equality cannot be true for plain numbers. Dirac showed it is possible if you are dealing with matrices (the minimum possible order of the matrices for this should be equal 4). In particular, it works if the coefficients are given by :

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad \alpha_1 = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} \quad \alpha_2 = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} \quad \alpha_3 = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} \text{ and}$$

matrices α_i are satisfy to the next conditions (to be consistent with Klein-Gordon equation): $\alpha_i^2 = \beta^2 = I$,

for $i \neq j$ $\alpha_i \alpha_j + \alpha_j \alpha_i = 0$ and $\alpha_i \beta + \beta \alpha_i = 0$. Here $\sigma_x, \sigma_y, \sigma_z$ are so-called 2×2 Pauli Spin matrices:

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

The formal derivation of "classical" time-dependent Schrödinger equation.

Finally for Dirac equation we have:

$$i \hbar \frac{d \psi}{dt} = (\beta m_0 c^2 + \sum_{i=1,2,3} \alpha_i \hat{p}_i c) \psi = \hat{H} \psi .$$

The wave function must be a so-called four-component Dirac Spinor function (due to the fact that matrices α_i have order 4): $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$. After substitution matrices and using Pauli units ($\hbar=c=1$) we have:

$$i \frac{\partial}{\partial t} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = i \frac{\partial}{\partial x} \begin{pmatrix} -\psi_4 \\ -\psi_3 \\ -\psi_2 \\ -\psi_1 \end{pmatrix} + i \frac{\partial}{\partial y} \begin{pmatrix} -\psi_4 \\ +\psi_3 \\ -\psi_2 \\ +\psi_1 \end{pmatrix} + i \frac{\partial}{\partial z} \begin{pmatrix} -\psi_3 \\ +\psi_4 \\ -\psi_1 \\ +\psi_2 \end{pmatrix} + m_0 \begin{pmatrix} +\psi_1 \\ +\psi_2 \\ -\psi_3 \\ -\psi_4 \end{pmatrix} .$$

Frequently Dirac equation can be presented in more compact form by using γ -matrices representation:

$$(i \gamma^0 \frac{\partial}{\partial t} + i \vec{\gamma} \vec{\nabla} - m) \psi = 0 \quad \text{here}$$

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad \gamma^1 = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix} \quad \gamma^2 = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix} \quad \gamma^3 = \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix} \quad \text{and can be expanded into matrix form:}$$

$$\begin{pmatrix} i \frac{\partial}{\partial t} - m & 0 & i \frac{\partial}{\partial z} & i \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \\ 0 & i \frac{\partial}{\partial t} - m & i \frac{\partial}{\partial x} - \frac{\partial}{\partial y} & -i \frac{\partial}{\partial z} \\ -i \frac{\partial}{\partial z} & -i \frac{\partial}{\partial x} - \frac{\partial}{\partial y} & -i \frac{\partial}{\partial t} - m & 0 \\ -i \frac{\partial}{\partial x} + \frac{\partial}{\partial y} & i \frac{\partial}{\partial z} & 0 & -i \frac{\partial}{\partial t} - m \end{pmatrix} \begin{pmatrix} \psi^1 \\ \psi^2 \\ \psi^3 \\ \psi^4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} .$$

The probability density can be identified as: $\psi^2 = |\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2$ and must be normalized on unit.

II.d Some remarks about magnetic properties of electron and spin.

It is make sense to give the physical justification for the relationship between the Pauli Spin matrices and the spin magnetic moment.

The classical magnetic moment for the orbital motion of an electron around nuclei is $\vec{\mu} = \frac{q}{2m} \vec{L}$ and corresponding quantum mechanical operator $\hat{\mu} = \frac{q}{2m} \hat{L}$, here \hat{L} - angular moment operator. The energy of interaction of the magnetic moment with an external magnetic field looks like this $-\vec{\mu} \vec{B}$.

The Dirac equation for a free electron can be improved by includes the interaction with an external electromagnetic field (see corresponding substitutions in II.b) this gives the so-called Schrödinger-Pauli equation. But in this new equation, an additional potential energy appears, which looks like this $-\frac{q}{2m} \vec{\sigma} \vec{B}$.

It is important to emphasize that the particle moves translationally in an external electromagnetic field. This means that this additional energy is associated with the interaction of an external electromagnetic field with additional internal degrees of freedom of particle related to the its own internal magnetic field - the Spin.

Then the Spin magnetic moment is look like so: $\vec{\mu}_s = \frac{q}{2m} \vec{\sigma}$ or in term of spin vector $\vec{\mu}_s = \frac{q}{m} \vec{S}$. It is clear that the electron Spin does not disappear outside the electromagnetic field. Spin is an additional physical property of fermions and Dirac equation describes the behavior of spin-1/2 fermions in relativistic quantum field theory.