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Journal of Progressive Research in Mathematics
Vol 18,1 - 2021
E-ISSN: 2395-0218

Density Matrix Method Begins To Occupy Leading Position In Quantum Physics

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Received: December 17, 2020; Accepted: January 12, 2021; Published: February 13, 2021

Cite this article: Bondarev, B. V. (2021). Density Matrix method begins to occupy leading position in quantum Physics . *Journal of Progressive Research in Mathematics*, *18*(1), 1-23.
Retrieved from http://scitecresearch.com/journals/index.php/jprm/article/view/1996.

Abstract.
This article focuses on how quantum mechanics has been discovered and developed over the past century, and how its development has been hindered by many false theories. Some of these theories have come to light because a new tool has not yet been born that would ensure the existence of new theories. Other false quantum theories appeared due to the authors ignorance of the basics of quantum mechanics and are still taught to students.

This work opens up new paths of quantum physics that start with the Lindblad equation for the statistical operator and the equation for the density matrix. The last equation is equivalent to the equation for the statistical operator.

Keywords: *Fokker –Planck Equation. SchrÖdinger equation. Statistical operator. Density matrix. Liouville –von Neumann equation. Lindblad Equation. Equation for density matrix. Quantum kinetic equation. Dissipative diffusion and attenuation operators. Variational principle.*

1. Introduction

In 1976, a new instrument was born, which somehow remained almost unnoticed by most scientists [1]. This is the Lindblad equation, where the unknown quantity is the statistical operator $\hat{\varrho}$. In this equation, there is only one unknown term $\hat{D}$, which can be called a **dissipative** operator. Before you start solving the Lindblad equation, you need to find this operator.

In 1994, the author of this article derived an equation for the **density matrix**$\varrho_{nn'}$ [2]. The following consequences are automatically derived from this equation: 1) the matrix $\gamma_{nm,m'n'}$, which defines the structure of this equation, is uniquely related to the dissipative operator $\hat{D}$ in the Lindblad equation, 2) when the density matrix has a diagonal form, this equation turns into a **quantum kinetic** equation for the probability $w_n(t)$, 3) the probability p_{mn} of the transition obeys an equation called the **Fermi Golden rule.**

I have sent my article to almost all physicists who should understand the simple language of quantum physics, but they are somehow silent. Only a few professors answered me. Among them there are even two academicians of the Russian Academy of Sciences. But it's been a quarter of a century since my article was published in the journal of "Theoretical and mathematical physics". And it's been almost half a century since Lindblad discovered his equation.

I read a review by a scientist about a report at a conference. He did not specify his name, but he wrote the correct words: "There are no theories that would be accepted by all at once - such good times are long gone. Today, few people will understand a deep theory or model, and even more so, they will immediately accept it. It is usually necessary that entire generations of adherents of the old views die out. Therefore progress must be made in small steps ... “

2. Liouville equation

The Liouville equation describes the evolution in time of the distribution function in phase space. This is the fundamental equation of non-equilibrium statistical mechanics.

Joseph Liouville (1809–1882)

Consider a dynamical system of N particles that have coordinates q_k and conjugate pulses p_k, where k = 1, ..., N . Then the distribution function

$f = f(t, q, p)$,

where $q = q_1, \ldots, q_N; p = p_1, \ldots, p_N$; defines the number of dN particles in the system

$dN = f(t, q, p)\, dq dp$,

for which their q_k coordinates and p_k pulses will be located in a small volume

$dq dp = \sum_{k=1}^{N} dq_k\, dp_k$.

The Liouville equation governing the evolution of the system will have the form$\partial f/\partial t +$

$$\sum_{k=1}^{N} \left(\partial f/\partial q_k\, dq_k/dt + \partial f/\partial p_k\, dp_k/dt \right) = 0 , \tag{2.1}$$

where the functions $q_k = q_k(t)$ and $p_k = p_k(t)$ satisfy the Hamilton equations

$$dq_k/dt = \partial H/\partial p_k \, , dp_k/dt = -\partial H/\partial q_k , \tag{2.2}$$

$H = H(t, q, p)$ is a Hamilton function.

Liouville's theorem States that the distribution function $f = f(t, q, p)$ is constant along any trajectory in phase space. Since this equation demonstrates the conservation of density in phase space, we write the continuity equation:Since this equation demonstrates the conservation of density in phase space, we write the continuity equation:

$$\partial f/\partial t + \sum_{k=1}^{N} \{ \partial (f \dot{q}_k)/\partial q_k + \partial (f \dot{p}_k)/\partial p_k \} = 0 .$$

Open the derivatives of the products $f\dot{q}_k$ and $f\dot{p}_k$. We get

$$\partial f/\partial t + \sum_{k=1}^{N} (\partial f/\partial q_k \dot{q}_k + \partial f/\partial p_k \dot{p}_k) + f \sum_{k=1}^{N} \{\partial \dot{q}_k/\partial q_k + \partial \dot{p}_k/\partial p_k\} = 0 .$$

The last sum after substituting Hamilton's equations into it will be zero:

$$\sum_{k=1}^{N} \{\partial \dot{q}_k/\partial q_k + \partial \dot{p}_k/\partial p_k\} = \sum_{k=1}^{N} \{\partial^2 H/\partial q_k \partial p_k - \partial^2 H/\partial p_k \partial q_k\} = 0 .$$

When the Liouville equation is solved and the distribution function $f = f(t, q, p)$ is found, then the total number of particles in the system can be calculated using the formula

$$N = \int f(t, q, p) \mathrm{d}q\mathrm{d}p \tag{2.3}$$

In the simplest case, when a particle moves in space in a field of force $\boldsymbol{F}$ with coordinates $\boldsymbol{r}$ and momentum $\boldsymbol{p}$, Liouville's theorem can be written as

$$\partial f/\partial t + \dot{\boldsymbol{r}}\nabla f + \dot{\boldsymbol{p}}\nabla_{\boldsymbol{p}} f = 0 , \tag{2.4}$$

where

$$\dot{\boldsymbol{r}} = \boldsymbol{v} , \qquad \dot{\boldsymbol{p}} = \boldsymbol{F}/m . \tag{2.5}$$

A generalization of the Liouville equation to systems with collisions is the Boltzmann equation and the chain of Bogolyubov equations. In plasma physics, this equation is called the Vlasov equation.

3. Probability

There are systems whose behavior cannot be described by the laws of dynamics alone. In such systems, processes occur that cannot be predicted exactly and are called **random.**

In some phenomena, randomness is present as a result of incomplete knowledge of the observer about all the details of the system under study, about its past and about the effects to which it is subjected. Other phenomena may be random because of their physical nature. In any case, statistical methods should be used to describe random events. In particular, this applies to macroscopic systems consisting of a very large number of particles.

Theoretically, it is possible to write in symbolic form the equations of motion of all the particles that make up the macrosystem, taking into account all the forces acting on them. Therefore, for the quantitative description of multi-partial systems, we have to use a different mathematical apparatus based on the concept of probability. When applied to systems in which random processes occur, the laws of dynamics partially or completely lose their force and give way to laws of another property, called **statistical**.

An event that may or may not occur for reasons beyond the control of the observer is called a random event. A random process is a sequence of random events that occur in some physical system. It is not possible to make a complete deterministic description of the behavior of such a system. But even, it would seem, in a completely chaotic behavior is possible to distinguish certain patterns.

The main quantitative characteristic of a random event or random process is **probability**. Probability is a measure of the possibility of a random event occurring. In **statistical physics**, probability is determined using a so-called statistical ensemble, which is a collection of a large number of imaginary or actual identical instances of the system under study.

Let the set of different States of the system under study be finite or countable, i.e. each state of the system can be put in one-to-one correspondence with a natural number i = 1, 2, 3,... Simply put, all system States can be renumbered. Such systems are called **discrete** systems. The set of internal States of atoms and molecules is countable. In physics, such States are called **quantum** States.

Consider a statistical ensemble consisting of N identical discrete systems, each of which has a random process. Let $N_i(t)$ be among the systems of this ensemble in the state with number i at some time t. It is obvious that the sum of all these numbers is equal to the number of N systems in the ensemble:

$$\sum_i N_i(t) = N(t)\ . \tag{3.1}$$

The probability that one of the ensemble systems is in the i-th state at time t is called the value

$$w_i(t) = \lim_{N \to \infty} N_i/N, \tag{3.2}$$

that is, the limit to which the ratio of the number $N_i(t)$ to the number $N(t)$ of systems in the ensemble tends, when the latter increases indefinitely. From definition (2.2), it follows that the probability can take any value from zero to one:

$$0 \leq w_i \leq 1\ .$$

We sum up both parts of equality (2.2) for all possible values of the number i. Taking into account (2.1), we obtain the so-called **probability normalization condition** П росуммируемобечасти

$$\sum_i w_i = 1. \tag{3.3}$$

The state of a real discrete system, except for the number I, is characterized by one or more quantities that have a certain physical meaning. For Example, each system consists of a certain number of particles and has some energy. Let's denote one of these values by the letter x, and its value corresponding to the i-th state is x_i. The set of values that the value E can take is **discrete**. Therefore, this value is called a discrete random variable. The sum of all values of the value E is called the **spectrum** of its values.

Let's assume that for each of N systems of the ensemble, the values of the value x are measured at time t. The average value $\bar{x}$ of this value is determined by the formula

$$\bar{x} = \sum_i x_i\, w_i. \tag{3.4}$$

The task of statistical physics is to find the distribution function $w_i = w_i(t)$ and use it to calculate the average values of physical quantities that characterize the system under study.

4. Thermodynamics. Canonical Gibbs distribution

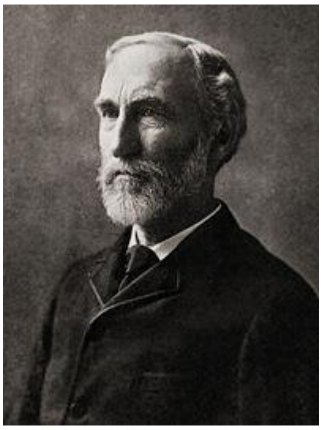
A substance is a collection of a colossal number of molecules. Such parameters of matter as volume, internal energy, and entropy require knowledge of probability for their determination. In other words, the state of a substance is determined by the distribution functions of molecules. For example, the internal energy and entropy will be equal

$$U = U\{w_i(t)\} \qquad \text{and} \qquad S = S\{w_i(t)\}.$$

Consider a large chunk of matter that is in an equilibrium state. Then the probability will not depend on time and must have a structure common to all equilibrium systems. The type of this function was set by Gibbs:

$$w_i = \nu \exp\left(-\beta E_i\right)\ . \tag{4.1}$$

This expression is called the **canonical Gibbs distribution**. It is of fundamental importance in the theory of equilibrium States of macroscopic systems.



Josiah Gibbs (1839–1903)

The equilibrium distribution function (4.1) depends on the energy of the system E_i in state I and contains two parameters ν and β. The Formula (4.1) allows us to calculate the probability w_i that the equilibrium system will be in the i-th state at some point in time.

The parameter β in formula (4.1) takes only positive values: $\beta > 0$. It can be shown that the parameter β is inversely proportional to the absolute temperature T:

$$\beta = 1/(k_\mathrm{B}\, T), \tag{4.2}$$

where k_B is the Boltzmann continuous.
Note: Currently a more General formula is used

$$\beta = 1/(\,\hbar\,\omega + \,k_\mathrm{B}\, T)\,,$$

where $\hbar\ \omega$ is the energy of radiation that is part of the thermostat.

To find the parameter ν, we will refer to the probability normalization condition (3.3). Then we will have

$$\sum_i w_i = \nu \sum_i \exp\,(\,-\beta E_i) = 1.$$

From here we get

$$\nu = 1/\sum_i \exp\ (\,-\beta E_i)\ . \tag{4.3}$$

5. Boltzmann Equation

The Boltzmann equation, known as the kinetic Boltzmann equation, is named after Ludwig Boltzmann, who first considered it. It describes a statistical distribution

$$f=f(t, \boldsymbol{r}, \boldsymbol{p})$$

particles in a gas or liquid and is one of the most important equations of physical kinetics. This is the field of statistical physics that describes systems in a state of thermodynamic equilibrium or far from equilibrium, for example, in the presence of temperature gradients and an electric field.

Ludwig Boltzmann (1844 −1906)

The physical meaning of the distribution function $f = f(t, \boldsymbol{r}, \boldsymbol{p})$ is that the number of dN particles that are in the volume d$\boldsymbol{r}$= dxdydz and have pulses ending in d$\boldsymbol{p}$= dp_xdp_ydp_z will be equal to

dN= $f(t, \boldsymbol{r}, \boldsymbol{p})$ d$\boldsymbol{r}$d$\boldsymbol{p}$ **.**

The Boltzmann equation has the form

$$\partial f/\partial t + \nabla f\ \partial \boldsymbol{r}/\partial t + \nabla_v f\, \partial \boldsymbol{v}/\partial t = \partial f/\partial t\,|_{\text{collisions}}\ , \tag{5.1}$$

where the right side of this equation describes the collisions of particles with each other and has yet to be determined. If you put it in this equation

$$\partial \boldsymbol{r}/\partial t = \boldsymbol{v}\ , \partial \boldsymbol{v}/\partial t = \boldsymbol{F}/m\ , \tag{5.2}$$

then we will have

$$\partial f/\partial t + \boldsymbol{v}\,\nabla f + \boldsymbol{F}/m\,\nabla_v f = \partial f/\partial t\,|_{\text{collisions}}\ . \tag{5.3}$$

The simplest description of a collision member is

$$\partial f/\partial t\,|_{\text{collisions}}\ = -(f - f_{\text{o}})/\tau, \tag{5.4}$$

where f_{o} is a function that is a solution of the Liouville equation

$$\partial f/\partial t + \boldsymbol{v}\,\nabla f + \boldsymbol{F}/m\,\nabla_v f = 0\ . \tag{5.5}$$

Now the equation takes the form

$$\partial f/\partial t + \boldsymbol{v}\,\nabla f + \boldsymbol{F}/m\,\nabla_v f = -(f - f_{\text{o}})/\tau\ . \tag{5.6}$$

Another more complex description of collisions of two particles is carried out using an integral, in which there is a product of two functions $f_1 f_2$.

6. Maxwell - Boltzmann Statistics

We apply the Gibbs distribution to describe a particle of an ideal gas when it is in a state of thermal equilibrium. The energy of the particle is equal to

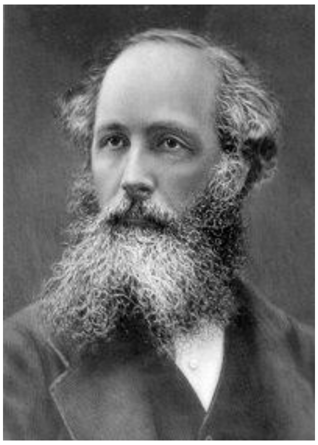
$$E(\boldsymbol{r}, \boldsymbol{v}) = mv^2/2 + U(\boldsymbol{r}) \; . \tag{6.1}$$

Then the Gibbs distribution gives

$$w(\boldsymbol{r}, \boldsymbol{v}) = \nu \exp \{ -\beta \, (mv^2/2 + U(\boldsymbol{r}) \} \; . \tag{6.2}$$

It is not difficult to verify that this function satisfies the Liouville equation (2.4) or the Boltzmann equation (5.5), if we remember that

$\boldsymbol{F} = -\nabla U.$



James Maxwell(1831−1879)

7. Vlasov Equation

Vlasov found that in the Boltzmann equation, the collision integral, which is determined by the paired interactions of molecules, only fits when the interaction forces of the particles act close enough to them. The proximity or distance of forces is characterized by the radius of their influence. Coulomb forces act between charged particles. The calculation of the radius of action of these forces showed that it is greater than the radius of influence of forces acting between uncharged molecules. Therefore, Coulomb forces are called long-range. Vlasov suggested that the influence of electromagnetic interaction between charged particles should not be carried out directly, but only by means of an electromagnetic field.

For plasma, which consists of electrons and ions, Vlasov equations are used

$$\partial f^{(e)}/\partial t + \boldsymbol{v}\nabla f^{(e)} - e\,(\boldsymbol{E} + [\,\boldsymbol{vB}]/c)\,\nabla_{\boldsymbol{p}} f^{(e)} = 0 \, , \tag{7.1}$$
$$\partial f^{(i)}/\partial t + \boldsymbol{v}\nabla f^{(i)} + e\,(\boldsymbol{E} + [\,\boldsymbol{vB}]/c)\,\nabla_{\boldsymbol{p}} f^{(i)} = 0 \, , \tag{7.2}$$

where $f^{(e)}$ and $f^{(i)}$ are the distribution functions of electrons and ions, e is the elementary electric charge, $\boldsymbol{E}$ is the electric field strength, and $\boldsymbol{B}$ is the magnetic field induction. These equations should be supplemented with Maxwell's equations of charge and current:

$$\text{rot}\, \boldsymbol{E} = -1/\text{c}\, \partial \boldsymbol{B}/\partial t \, , \qquad \text{div}\, \boldsymbol{E} = 4\,\pi\rho \, , \tag{7.3}$$

$$\text{rot}\, \boldsymbol{B} = 4\,\pi \boldsymbol{j}/\text{c} + 1/\text{c}\, \partial \boldsymbol{E}/\partial t \, , \qquad \text{div}\, \boldsymbol{B} = 0 \, , \tag{7.4}$$

$$\rho = e \int (f^{(i)} - f^{(e)})\, \text{d}^3 p \, , \qquad \boldsymbol{j} = e \int (f^{(i)} - f^{(e)})\, \boldsymbol{v} \text{d}^3 p \; . \tag{7.5}$$

If the magnetic field can be ignored in these equations, the resulting equations will be called Vlasov– Poisson equations:

$$\partial f^{(\alpha)}/\partial t + \boldsymbol{v}\nabla f^{(\alpha)} + q_\alpha \boldsymbol{E}\, \nabla_{\boldsymbol{p}} f^{(\alpha)} = 0 \, , \nabla \boldsymbol{E} = 4\,\pi\rho \, , \tag{7.6}$$

where $\alpha = e$ or i, $q_e = -e, q_i = e$.

8. Bogolyubov's Equations

Consider a system of N particles with a pair interaction located in an external field. Let q_i and p_i be the generalized coordinates and pulses of the i -th particle, $\Phi_i(q_i)$ be the interaction potential with the external field, and $\Phi_{ij}(q_i, q_j)$ be the potential energy of the interaction of particles. Distribution function of the complete system

$$f_N = f_N(t, q_1, \dots, q_N, p_1, \dots, p_N)$$

satisfies the Liouville equation

$$\partial f_N/\partial t + \sum_{i=1}^{N} \dot{q}_i \, \partial f_N/\partial q_i - \sum_{i=1}^{N} \left(\partial \Phi_i/\partial q_i + \sum_{j=1, j\neq i}^{N} \partial \Phi_{ij}/\partial q_i\right) \partial f_N/\partial p_i = 0 \quad (8.1)$$

Define the function f, which specifies only s pairs of numbers q_i and p_i, by the ratio

$$f_s = f_s(t, q_1, \dots, q_s, p_1, \dots, p_s) = \int f_N(t, q_1, \dots, q_N, p_1, \dots, p_N)\, \mathrm{d}q_{s+1} \mathrm{d}p_{s+1} \dots \mathrm{d}q_N \mathrm{d}p_N \,.$$

This function will satisfy the equation

$$\partial f_s/\partial t + \sum_{i=1}^{s} \dot{q}_i \, \partial f_s/\partial q_i - \sum_{i=1}^{s} \left(\partial \Phi_i/\partial q_i + \sum_{j=1, j\neq i}^{s} \partial \Phi_{ij}/\partial q_i\right) \partial f_s/\partial p_i =$$

$$= (N - s) \sum_{i=1}^{s} \partial/\partial p_i \int \partial \Phi_{is+1}/\partial q_i \, f_{s+1} \mathrm{d}q_{s+1} \mathrm{d}p_{s+1} \,. \quad (8.2)$$

Let's put in equation (7.2) the number s = 1, 2, ..., we will have

$$\partial f_1/\partial t + \dot{q}_1 \, \partial f_1/\partial q_1 - \partial \Phi_1/\partial q_1 \, \partial f_1/\partial p_1 =$$

$$= (N - 1)\, \partial/\partial p_1 \int \partial \Phi_{12}/\partial q_1 \, f_2 \mathrm{d}q_2 \mathrm{d}p_2 \,, \quad (8.3)$$

$$\partial f_2/\partial t + \sum_{i=1}^{2} \dot{q}_i \, \partial f_2/\partial q_i - \sum_{i=1}^{2} \left(\partial \Phi_i/\partial q_i + \sum_{j=1, j\neq i}^{2} \partial \Phi_{ij}/\partial q_i\right) \partial f_2/\partial p_i =$$

$$= (N - 2) \sum_{i=1}^{2} \partial/\partial p_i \int \partial \Phi_{i\,3}/\partial q_i \, f_3 \mathrm{d}q_3 \mathrm{d}p_3 \,, \dots \quad (8.4)$$

All these equations are called the Bogolyubov chain of equations. To be more precise, they are called BBGKY-equations, where the abbreviation bbgki contains the names of scientists: N. Bogolyubov, M. Bourne, J. Green, J. Kirkwood and J. Yvon, who contributed to these equations.

9. Fokker –Planck Equation

Until now, probability has not been explicitly mentioned in all these equations. Now we will write down an equation that describes the time evolution of the probability of events occurring in the system under study.

Let the state of a certain system be determined by the set of numbers $x_1, x_2, \dots, x_N$, which change randomly over time. The probability density is used to describe such a system

$$w = w(t, x_1, x_2, \dots, x_N)\,.$$

If we know this function, the probability that the system parameters are in a small part of $\mathrm{d}x_1\ \mathrm{d}x_2\ \ldots\ \mathrm{d}x_N$ is equal to

$\mathrm{d}w = w(t,\ x_1, x_2, \ldots, x_N)\ \mathrm{d}x_1\ \mathrm{d}x_2\ \ldots\ \mathrm{d}x_N$.

The normalization condition will look like this

$$\int w(t,\ x_1, x_2, \ldots, x_N)\ \mathrm{d}x_1 \mathrm{d}x_2\ \ldots\ \mathrm{d}x_N = 1 \qquad (9.1)$$

The General form of the equation for the probability density is

$$\partial w/\partial t = -\sum_{i=1}^{N} \partial(D_i^{(1)}\ \mathrm{w})/\partial x_i + \sum_{i=1}^{N}\sum_{j=1}^{N} \partial^2(D_{ij}^{(2)}\ \mathrm{w})/\partial x_i\, \partial x_j\ , \qquad (9.2)$$

where $D_i^{(1)}$ and $D_{ij}^{(2)}$ are unknown functions of variables t and $x_1, x_2, \ldots, x_N$. This equation was written by scientists **Adrian Fokker** and **Max Planck**. In our literature, it is known as the Kolmogorov equation.

For the first time, the equation was used to statistically describe the Brownian motion of a particle in a liquid, when the motion can be described using the probability density:

$w = w(\,t, \boldsymbol{r}, \boldsymbol{p}\,)$.

In this case, the probability

$$\mathrm{d}w = w(t, \boldsymbol{r}, \boldsymbol{p}\,)\ \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{p} \qquad (9.3)$$

says that the particle at time t has vectors $\boldsymbol{r}$ and $\boldsymbol{p}$ that end in the volume d$\boldsymbol{r}$d$\boldsymbol{p}$. Now the Fokker −Planck equation can have the form

$$\partial w/\partial t = -\ \nabla(\,\boldsymbol{A}_1 w\,) + \nabla(\,\boldsymbol{B}_1 \nabla \mathrm{w}\,) - \nabla_{\boldsymbol{p}}(\,\boldsymbol{A}_2\ w\,) + \nabla_{\boldsymbol{p}}\big(\boldsymbol{B}_2 \nabla_{\boldsymbol{p}} \mathrm{w}\,\big)\,, \qquad (9.4)$$

where the vectors $\boldsymbol{A}_{\boldsymbol{\alpha}}$ and $\boldsymbol{B}_{\alpha}$ ($\alpha = 1, 2$) depend on t, $\boldsymbol{r}$, $\boldsymbol{p}$.

Let's assume that

$\boldsymbol{A_1} = \boldsymbol{p}/m, \quad \boldsymbol{A_2} = \boldsymbol{F}\,, \quad \boldsymbol{B}_{\alpha} = 0\,.$

Now the Fokker − Planck equation becomes the Boltzmann equation

$\partial w/\partial t = -\boldsymbol{p}/m\,\nabla w - \boldsymbol{F}\,\nabla_{\boldsymbol{p}} w\,.$

10. Questions that classical physics could not answer

Here are some of these questions.

1. Atomic structure. It is impossible to explain from the point of view of classical physics why atoms there are consistently.

2. Linear spectra of light emission and absorption by atoms. Classical theory cannot explain why light is emitted and absorbed by different atoms at discrete frequencies. In addition these spectra are expressed by simple algebraic relations.

3. The radiation of a black body. No explanation of the dependence of the radiation intensity of a heated body on frequency and temperature.

11. Thermal radiation Photons

Now it's time to talk about quantum mechanics, the Foundation of which was first laid by Max Planck. He studied the spectrum of thermal radiation, for the explanation and quantitative description of which he had to assume that light and electromagnetic radiation are a collection of particles. These particles are called **quanta** of light, or **photons**.

Max Planck (1858 –1947)

Like any other particle of matter, a photon has energy and momentum. The energy ε of a single photon is proportional to the frequency ω of the electromagnetic radiation of which it is a particle:

$$\varepsilon = \hbar\omega, \tag{11.1}$$

where the fundamental constant $\hbar$ is called the **Planck constant**. The photon's pulse modulus is related to its energy by the ratio

$$p= \varepsilon/c, \tag{11.2}$$

where c is the speed of light. In vector form, this relation has the form

$$\boldsymbol{p}= \hbar\boldsymbol{k} , \tag{11.3}$$

$\boldsymbol{k}$ is the wave vector. Recall that a monochromatic electromagnetic wave is described by the function cos ($\boldsymbol{k}\,\boldsymbol{r} + \omega t + \alpha$). This is how the idea of light as a wave, or as a particle, appears.

Calculations based on the photon hypothesis led Planck to the following dependence of the energy density of equilibrium thermal radiation on frequency and temperature:

$$w(\omega, T) = \hbar\,\omega^3/\{\,\pi^2 c^3[\exp(\,\beta\,\hbar\,\omega) - 1\,]\,\}\,. \tag{11.4}$$

Here appeared the constant $\hbar$ that Planck found. This constant suggests that the equation where it appears belongs to quantum physics.

12. Frequency spectrum of light emitted by hydrogen atom

When observing the light emitted by individual atoms, it was experimentally established that the spectrum of this light has a linear character. And each atom has a spectrum inherent only to this atom. The easiest is the spectrum of the hydrogen atom. The first person to derive a formula for this spectrum was Niels Bohr. He proposed the so-called orbit quantization rule, which must be satisfied by the stationary orbits of electrons in an atom. According to this rule when an electron moves in a stationary orbit its moment of momentum L is equal to an integer number of Planck constants $\hbar$:

$$L = n\hbar , \tag{12.1}$$

where the integer n = 1, 2, 3, ... is called a **quantum number**.

Bohr's theory has produced remarkable results when describing a hydrogen atom consisting of a proton with a charge of + e and an electron with a charge of $-e$. Therefore the electron from the core will be affected by the force of attraction
of the Coulomb

$$F = e^2/(4\,\pi\varepsilon_0 r^2), \tag{12.2}$$

where r is the distance between the nucleus and the electron.

Niels Bohr (1885– 1962)

Since the mass of the nucleus is much larger than the mass of the electron, the nucleus can be considered stationary, and the electron - moving around it. Consider the movement of an electron around the nucleus on a circle of radius r. Write down Newton's second law:

$$m\,v^2/r = e^2/(4\,\pi\varepsilon_0 r^2), \tag{12.3}$$

where m and v are the mass of the electron and its velocity.
The quantization rule (12.1) can now be written as follows:

$$m\,v\,r = n\hbar\,. \tag{12.4}$$

Equations (12.3) and (12.4) form a system with two unknowns v and r. Now we find the velocity v and the distance r from the electron to the nucleus:

$$v = e^2/(4\,\pi\varepsilon_0 n\hbar), \quad r = 4\,\pi\varepsilon_0 n^2\,\hbar^2/(m\,e^2)\,. \tag{12.5}$$

As can be seen from this formula, the velocity v and radius of the electron's orbit depend on the number n. Therefore, the number n is considered as the number of the orbit. The radius r_B of the first orbit, for which n =1, is called the **Bohr radius**.

The internal energy E of hydrogen is the total mechanical energy of an electron moving around a stationary nucleus. Coulomb interaction an electron with a nucleus corresponds to the potential energy

$U = -e^2/(4\,\pi\varepsilon_0 r)$.

Therefore, the total mechanical energy of the electron according to the formula (6.1) will be equal to

$$E = mv^2/2 - e^2/(4\pi\varepsilon_o r). \qquad (12.6)$$

Substituting the formulas (12.5) here leads to the value of the total energy of the hydrogen atom

$$E_n = -R\hbar/n^{\mathbf{2}}\mathbf{,} \qquad (12.7)$$

where R is the Rydberg constant.

Bohr then suggested that an atom emits a photon when an electron moves from one orbit to another. In this case the energy lost by the electron is converted into the energy of the photon:

$$E_{n_2} - E_{n_1} = \hbar\omega_{n_1 n_2}, \qquad (12.8)$$

where $n_2 > n_1$. Let's substitute the energy of an electron into this formula and we will have

$$\omega_{n_1 n_2} = R(\,1/n_1^2 - 1/n_2^2)\,. \qquad (12.9)$$

This formula accurately describes the spectrum of frequencies emitted by the hydrogen atom. At this point, a new theory begins, which became known as quantum mechanics.

13. Schrödinger Equation

Erwin Schrödinger (1887 – 1961)

The Schrödinger equation is considered to be the basis of **quantum mechanics**. In this equation the unknown quantity is the so called**wave function**

$$\psi=\psi(\,t,q\,)\,, \qquad (13.1)$$

where t is time, and q is a quantum variable that determines the state of the system. The meaning of the wave function is that the product

$$\psi^*(\,t,\,q\,)\,\psi(\,t,\,q\,) = w(\,t,\,q\,) \qquad (13.2)$$

it is possible to detect the system in state q at time t. The probability must meet the normalization condition:

$$\int \psi^*(\,t,\,q\,)\,\psi(\,t,\,q\,)\mathrm{d}q = 1\,. \qquad (13.3)$$

The Schrödinger equation itself can be written as follows

$$i\hbar\, \partial\psi/\partial t=\widehat{H}\psi, \tag{13.4}$$

where $\widehat{H}=\widehat{H}(t, q)$ is the energy operator of the system. This operator explains what to do with the wave function $\psi(t, q)$ so that it gives us the average energy $E(t)$ of the system at time t:

$$E(t) =\int \psi^*(t,q)\widehat{H}(t, q)\, \psi(t, q)\mathrm{d}q\ . \tag{13.5}$$

From the Schrödinger equation, you can deduce everything that Bohr came up with, and much more.

14. Eigenfunctions and eigenvalues of energy

The total energy operator $\widehat{H}$ is equal to the sum of the kinetic and potential energy operators. For an electron in a hydrogen atom it is equal to

$$\widehat{H}\ = -\,\hbar^2/(2\,m)\,\nabla^2-\mathrm{e}^2/r. \tag{14.1}$$

The function ψ can be represented as

$$\psi(t,\mathbf{r}) = \varphi(\mathbf{r})\ \exp\,(-\ \mathrm{i}\ \omega\ t)\ , \tag{14.2}$$

where ω is a constant having the dimension of frequency. Setting this function in the Schrodinger equation gives

$$\widehat{H}\varphi= E\varphi, \tag{14.3}$$

where E is the electron energy. Equation (14.3) is called the stationary Schrodinger equation. This equation is called the equation for eigenfunctions φ of the Hamiltonian $\widehat{H}$, and the energy E is called the eigenvalue of this operator.

Substitute the Hamiltonian (14.1) in equation (14.3). Receive

$$\{ -\hbar^2/(2\,m)\,\nabla^2-\mathrm{e}^2/r\ \}\ \varphi= E\varphi\ . \tag{14.4}$$

Surprisingly, this equation has a solution not for any negative values of energy E, but only for some quantum values. So the wave function depends on three indexes

$$\varphi_{nlm}\ = \varphi_{nlm}\,(\mathbf{r})\ . \tag{14.5}$$

The number n takes the values 1, 2, 3, ... and is called the **main quantum number**. For a given value n, the number l, called the **orbital number**, takes one of the n values 0, 1, 2,..., $n-1$. Finally, the **magnetic quantum number**m takes the values $-l$, $-l$+ 1, ..., -1, 0, 1, 2, ..., $l-1$, l. In total, for a given value of l, the number m takes 2 l + 1 values. The main quantum number n determines the possible values of the electron energy in the hydrogen atom:

$$E_n\ = -\,R\hbar/n^2, \tag{14.6}$$

All eigenvalues of the total energy operator $\widehat{H}$ for which these equations have a solution form the so-called **energy spectrum**, or the spectrum of possible values of the particle's energy. Among the possible values of the particle's energy, there is always the smallest. The wave function corresponding to the lowest energy value describes the so-called **ground state** of the particle.

After that, the eigenvalues of the energy of other atoms were calculated using approximate methods from the Schrodinger equation. The approximate formula will look like

$$E_n\ \cong -\,Z\,R\hbar/n^2, \tag{12.7}$$

where Z is the number of electrons in an atom. The light spectrum is determined by the formula (12.9). This spectrum is consistent with the observed spectrum. This is how the Schrodinger equation appeared, which is still considered the main equation of quantum mechanics.

15. Coordinate and wave representation of quantum particle

Physicist Louis de Broglie proposed to consider a quantum particle not only as a point particle, but also as a wave, which is characterized by a vector

$$\boldsymbol{k} = \boldsymbol{p}/\hbar\ . \tag{15.1}$$

Louis de Broglie (1892-1987)

In the coordinate representation the coordinate operators $\hat{\boldsymbol{r}}$ and momentum $\hat{\boldsymbol{p}}$ will be equal

$$\hat{\boldsymbol{r}} = \boldsymbol{r},\ \ \hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla\ . \tag{15.2}$$

But in the wave representation these same operators will be equal

$$\hat{\boldsymbol{r}} = -\,\mathrm{i}\nabla_{\boldsymbol{k}},\qquad \hat{\boldsymbol{p}} = \hbar\boldsymbol{k}\,. \tag{15.3}$$

Let's find out how these representations are related. To do this, assuming that the operators act on the same function $U = U(\boldsymbol{k}, \boldsymbol{r})$, equate the right parts of the results of the operators actions:

$-$

$\mathrm{i}\nabla_{\boldsymbol{k}}U = \boldsymbol{r}U\ , -\mathrm{i}\nabla U = \boldsymbol{k}\ U\,.$

These equations have the same solution:

$U \sim \exp(\mathrm{i}\boldsymbol{kr})$.

The function U is called **unitary**.

The transition from the coordinate representation of a particle to the wave representation and the reverse transition are performed using the **unitary matrix**$U_{\boldsymbol{kr}}$, which is defined by the relation

$$\sum_{\boldsymbol{k}} U_{\boldsymbol{kr}}\, U^{*}_{\boldsymbol{kr}'} = \delta_{\boldsymbol{rr}'}\,, \tag{15.4}$$

where $\delta_{\boldsymbol{rr}'}$ is the Kronecker symbol. The simplest unitary matrix is

$$U_{\boldsymbol{kr}} = A \exp (\mathrm{i}\boldsymbol{k}\,\boldsymbol{r}) . \tag{15.5}$$

There are other rare types of unitary matrix.

16. Statistical operator and density matrix

In addition to the wave function ψ, which describes the state of a quantum system, **J. von Neumann** came up with another more General way of describing it – the statistical operator

$$\hat{\varrho} = \hat{\varrho}(q, t) . \tag{16.1}$$

The statistical operator is related to the density matrix $\varrho_{nn'}(t)$ (t) by the formula

$$\varrho_{nn'}(t) = \int \varphi_n^*(q, t)\, \hat{\varrho}(q, t)\, \varphi_{n'}(q, t)\, \mathrm{d}q . \tag{16.2}$$

where the functions $\varphi_n(q,\ t)$ can be found from the Schrödinger equation. Formula (16.2) sets the density matrix $\varrho_{nn'}(t)$ in the *n*-representation. The diagonal element $\varrho_{nn'}$ of the density matrix is the probability $w_n = w_n(t)$ that the system is in state *n*:

$$\varrho_{nn}(t) = w_n(t) . \tag{16.3}$$

If the statistical operator is equal to

$$\hat{\varrho}(q) = \delta(q - q_{\mathrm{o}}) , \tag{16.4}$$

where $\delta(q - q_{\mathrm{o}})$ is the Dirac Delta function, and q_{o} is a constant. Then the state of the system is called **pure**. Formula (16.2) gives

$$\varrho_{nn'}(t) = \varphi_n^*(q_{\mathrm{o}}, t)\varphi_{n'}(q_{\mathrm{o}}, t) . \tag{16.5}$$

Otherwise, the system state is called **mixed**.
For the statistical operator, the equation was derived from the Schrödinger equation

$$\mathrm{i}\hbar\, \partial\hat{\varrho}/\partial t = [\ \hat{H}\hat{\varrho}] , \tag{16.6}$$

which is called the **Liouville – von Neumann equation**.

17. Liouville – von Neumann equation and density matrix in coordinate and wave representations

For the density matrix, equation (16.6) will look like this

$$\mathrm{i}\hbar\, \partial\varrho_{nn'}/\partial t = \textstyle\sum_m \left(H_{nm}\, \varrho_{mn'} - \varrho_{nm}\, H_{mn'} \right) , \tag{17.1}$$

where $H_{nn'}$ are matrix elements of the Hamiltonian $\hat{H}$ of the system. By analogy with the formula (16.2), we write

$$H_{nn'}(t) = \int \varphi_n^*(q, t)\, \hat{H}(q, t)\, \varphi_{n'}(q, t)\, \mathrm{d}q . \tag{17.2}$$

If it turns out that the matrix elements $H_{nn'}$ are diagonal, i.e. they have the form

$$H_{nn'}(t) = \varepsilon_n(t)\, \delta_{nn'}\,, \qquad (17.3)$$

where ε_n are the eigenvalues of the system's energy, and $\delta_{nn'}$ are the Kronecker symbols. Then equation (17.1) takes the form

$$\mathrm{i}\hbar\, \partial\varrho_{nn'}/\partial t = \{\, \varepsilon_n(t) - \varepsilon_{n'}(t)\, \}\varrho_{nn'}\,. \qquad (17.4)$$

For $n = n'$ we get

$$\partial\varrho_{nn}/\partial t = 0 \qquad \text{or} \partial w_n/\partial t = 0\,. \qquad (17.5)$$

Were obtained from the Liouville – von Neumann equation of the density matrix in coordinate and wave representations. So in coordinate representation the density matrix for a free particle has the form

$$\varrho(t, \boldsymbol{r}, \boldsymbol{r}') = (\alpha/\pi)^{3/2} \exp\{\, -\alpha\, [(\boldsymbol{r} + \boldsymbol{r}')/2 - \boldsymbol{r}_{\mathrm{o}} - \boldsymbol{v}_{\mathrm{o}} t\,]^2\, \} \cdot$$

$$\cdot \exp\{ - \mathrm{i} m \boldsymbol{v}_{\mathrm{o}}(\, \boldsymbol{r} - \boldsymbol{r}')/\hbar\, \}\,. \qquad (17.6)$$

This function describes the free particle that started its movement at the point $\boldsymbol{r}_{\mathrm{o}}$ and continues to move at the speed $\boldsymbol{v}_{\mathrm{o}}$.

In wave representation, the free particle is described by a density matrix of the form

$$\varrho(\boldsymbol{k}, \boldsymbol{k}') = \exp\{\, -\mathrm{i}\, \hbar/m(\boldsymbol{k} - \boldsymbol{k}')\, \}\ \delta\{(\boldsymbol{k} + \boldsymbol{k}')/\boldsymbol{2}\ - \boldsymbol{k}_{\mathrm{o}}\boldsymbol{\}}\,, \qquad (17.7)$$

where $\delta(\boldsymbol{k})$is the Delta-function.

18. Lindblad Equation

A quantum system that is in contact with other systems around it is called an **open** system. The equation describing the state of such a system was discovered by Lindblad:

$$\mathrm{i}\hbar\, \partial\hat{\varrho}/\partial t = [\, \hat{H}\hat{\varrho}] + \mathrm{i}\hbar\hat{D}, \qquad (18.1)$$

where $\hat{\varrho}$ is the statistical operator, $\hat{H}$ is the Hamiltonian of the system, and $\hat{D}$ is the **dissipative operator**, which is equal to

$$\hat{D} = \sum_{jk} C_{jk}\, \{\, 2\, \hat{a}_j\, \hat{\varrho}\hat{a}_k^{+} - \hat{a}_k^{+}\hat{a}_j\, \hat{\varrho} - \hat{\varrho}\hat{a}_k^{+}\hat{a}_j\, \}\,, \qquad (18.2)$$

C_{jk} is some matrix, and $\hat{a}_j$ is an unknown operator that still needs to be found.

The Lindblad equation opens up new possibilities in the future of quantum physics.

19. Equation for density matrix

In [2], the motion of a non-equilibrium quantum system S that is in contact with an equilibrium heat reservoir R was considered. the equation for the density matrix $\varrho_{nn'}$ of the system S was derived

$$\mathrm{i}\hbar\, \partial\varrho_{nn'}/\partial t = \sum_m\, (H_{nm}\, \varrho_{mn'} - \varrho_{nm}\, H_{mn'}) + \mathrm{i}\hbar D_{nn'}\,, \qquad (19.1)$$

where H_{nm} are the matrix elements of the Hamiltonian $\hat{H}$, $D_{nn'}$ is a dissipative matrix that is equal to

$$D_{nn'} = \sum_{m\,m'} \gamma_{nm,m'n'}\, \varrho_{mm'} - 1/2 \sum_{m} \left(\gamma_{nm}\, \varrho_{mn'} + \varrho_{nm} \gamma_{mn'}\right) \;, \tag{19.2}$$

$\gamma_{nm,m'n'}$ – some matrix,

$$\gamma_{nn'} = \sum_{m} \gamma_{mn',nm} \,. \tag{19. 3}$$

Here the number n denotes the quantum state of the system S in some n-representation.

20. Quantum kinetic equation

Let it turn out that the density matrix has a diagonal form:

$$\varrho_{12} = w_1 \delta_{12} \;, \tag{20.1}$$

where $w_1 = w_{n_1}$ is the probability that system S is in the state n_1, δ_{12} is the Kronecker symbol. Then equation (19.1)

turns into a quantum kinetic equation

$$\partial w_1 / \partial t = \sum_{n_2} \{p_{12} w_2 - p_{21} w_1\} \;, \tag{20. 2}$$

where

$$p_{12} = p_{nm} = \gamma_{nm,mn} = (2\,\pi/\hbar) \sum_{NM} |v_{nN,mM}|^2\, W_M\, \delta(\,\varepsilon_n - \varepsilon_m + E_N - E_M\,) \tag{20. 3}$$

there is a probability of transition of the system S in a unit of time from the state m to the state n,

$W_N = v\exp(-\,\beta E_N)$

– the probability that the equilibrium system R is in the state N with energy E_N, v is the normalizing factor, $\beta = 1/(k_{\mathrm{B}} T)$ is the inverse temperature of the thermostat; $v_{nN,mM}$ is matrix elements of the Hamiltonian of the interaction of the system S with the thermostat R. the Formula (20.3) is the **Golden rule of Fermi**.

21. Connection of dissipative operator and dissipative matrix

Formulas (18.2) and (19.2) establish the relationship between the dissipative operator and the dissipative matrix

$$\gamma_{nm,m'n'} = 2\sum_{jk} C_{jk}\, a_{nm,j}\, a^{+}_{m'n',k} , \tag{21.1}$$

where $a_{nm,j}$ are matrix elements of the operator $\hat{a}_j$.

22. Dissipative diffusion and attenuation operators

In [3], two operators were introduced

$$\hat{\boldsymbol{a}} = \hat{\boldsymbol{p}} + \mathrm{i}\hbar\beta\, \hat{\boldsymbol{F}}/4 \;, \quad \hat{\boldsymbol{b}} = \hat{\boldsymbol{r}} + \mathrm{i}\hbar\beta\, \hat{\boldsymbol{p}}/(4\,m) \;, \tag{22.1}$$

where $\hat{\boldsymbol{r}}$, $\hat{\boldsymbol{p}}$ and $\boldsymbol{F}$ are the coordinate, momentum, and force operators, and m is the mass of the particle. These operators are called **dissipative diffusion and attenuation operators**. Let's put them in the Lindblad equation

$$i\hbar\, \partial\hat{\varrho}/\partial t = [\,\hat{H}\hat{\varrho}] +$$

$$+\, iD/\hbar\{\, 2\hat{a}\hat{\varrho}\hat{a}^{+} - [\,\hat{a}^{+}\hat{a}\,,\ \hat{\varrho}]_{+}\,\} +$$

$$+\, i\gamma/\hbar\{\, 2\hat{b}\hat{\varrho}\hat{b}^{+} - [\,\hat{b}^{+}\hat{b}\,,\ \hat{\varrho}]_{+}\,\}\,, \qquad (22.2)$$

where

$$\hat{H} = \hat{\boldsymbol{p}}^{2}/(2\,m) + \hat{U} \qquad (22.3)$$

$-$ the Hamiltonian of a particle, $\hat{U}$ is its potential energy, D is the diffusion coefficient, and $\alpha = \beta\,\gamma$ is the coefficient of friction. We assume that the force and potential energy satisfy the relation

$$\boldsymbol{F} = -\nabla U\,. \qquad (22.4)$$

Substituting the operators (22.1) in equation (22.2), we get

$$i\hbar\, \partial\hat{\varrho}/\partial t = [\,\hat{H}\hat{\varrho}]$$

$$-iD/\hbar\{\, [\hat{\boldsymbol{p}}[\,\hat{\boldsymbol{p}}\hat{\varrho}]\,] + i\hbar\,\beta/2[\,\hat{\boldsymbol{p}}[\,\hat{\boldsymbol{F}}\hat{\varrho}]_{+}\,] + (\hbar\,\beta/4)^{2}[\,\hat{\boldsymbol{F}}[\,\hat{\boldsymbol{F}}\hat{\varrho}]\,]\,\} -$$

$$-\, i\,\gamma/\hbar\{\, [\hat{\boldsymbol{r}}[\,\hat{\boldsymbol{r}}\hat{\varrho}]\,] + i\hbar\,\beta/(2\ \mathrm{m})\,[\,\hat{\boldsymbol{r}}[\,\hat{\boldsymbol{p}}\hat{\varrho}]_{+}\,] + \{\hbar\,\beta/(4\,m)\,\}^{2}[\,\hat{\boldsymbol{p}}[\,\hat{\boldsymbol{p}}\hat{\varrho}]\,]\,\}\,. \qquad (22.5)$$

In this equation, we discard the summands containing β^{2}. To do this, add operators

$$\hat{\boldsymbol{a}}_{1} = -i\hbar\beta\,\hat{\boldsymbol{F}}/4\,, \qquad \hat{\boldsymbol{b}}_{1} = -i\hbar\beta\,\hat{\boldsymbol{p}}/(4\,m).$$

Then equation (22.5) takes the form

$$i\hbar\, \partial\hat{\varrho}/\partial t = [\,\hat{H}\hat{\varrho}] \qquad (22.6)$$

$$-iD/\hbar\{\, [\hat{\boldsymbol{p}}[\,\hat{\boldsymbol{p}}\hat{\varrho}]\,] + i\hbar\,\beta/2[\,\hat{\boldsymbol{p}}[\,\hat{\boldsymbol{F}}\hat{\varrho}]_{+}\,]\} -$$

$$-\, i\,\gamma/\hbar\{\, [\hat{\boldsymbol{r}}[\,\hat{\boldsymbol{r}}\hat{\varrho}]\,] + i\hbar\,\beta/(2\ \mathrm{m})\,[\,\hat{\boldsymbol{r}}[\,\hat{\boldsymbol{p}}\hat{\varrho}]_{+}\,]\}\,.$$

23. Equation for density matrix in coordinate representation

The coordinate representation is characterized by operators

$$\hat{\boldsymbol{r}} = \boldsymbol{r}, \quad \hat{\boldsymbol{p}} = -i\hbar\nabla\,.$$

In this representation, equation (22.5) takes the form

$$i\hbar\, \partial\varrho/\partial t = -\,\hbar^{2}/(2\,m)\,(\,\nabla^{2} -\ \nabla'^{2})\varrho + (\,U - \mathrm{U}'\,)\,\varrho\, +$$

$$+\, i\hbar\, D\{\, (\nabla + \nabla')^{2}\varrho - \beta/2\,(\,\nabla + \nabla'\,)\,(\,\boldsymbol{F} + \boldsymbol{F}'\,)\varrho\,\} -$$

$$-\, i\,\gamma/\hbar\{\, (\boldsymbol{r} - \boldsymbol{r}')^{2}\varrho +\ \hbar^{\boldsymbol{2}}\,\beta/(2\ \mathrm{m})\,(\,\boldsymbol{r} - \boldsymbol{r}'\,)\,(\,\nabla - \nabla'\,)\,\varrho\}\,, \qquad (23.1)$$

where $\varrho = \varrho(\,t, \boldsymbol{r}, \boldsymbol{r}'\,)$.

24. Quantum equation for density matrix and Wigner equation

To understand the meaning of dissipative operators, we write equation (23.1) for the Wigner function

$$w(t,\boldsymbol{r},\boldsymbol{p}) = 1/(2\,\pi\,\hbar)^3 \int \varrho(t,\boldsymbol{r}+\boldsymbol{r}'/2,\boldsymbol{r}-\boldsymbol{r}'/2)\exp(-\mathrm{i}\,\boldsymbol{p}\,\boldsymbol{r}'/\hbar)\,\mathrm{d}\boldsymbol{r}', \tag{24.1}$$

which is the **quantum** analog of the classical distribution function. Using the function (24.1), we find that for F = const we have the equation

$$\partial w/\partial t = -\boldsymbol{p}/m\,\nabla w - \boldsymbol{F}\nabla_{\boldsymbol{p}} w + \tag{24.2}$$
$$D(\nabla - \beta\boldsymbol{F})w + \gamma\nabla_{\boldsymbol{p}}(\nabla_{\boldsymbol{p}} + \beta/m\,\boldsymbol{p})w,$$

This equation is the **Fokker −Planck** equation for a Brownian particle. This establishes the relationship between the **quantum** equation (22.6) and the **classical** statistical equation (24.2).

25. Equation for system of identical particles

In [4], an equation was derived for the density matrix $\varrho_{nn'}(t)$, which describes the behavior of a system of identical particles. Based on the statistical operator of this system, a hierarchical sequence of operators $\hat{\varrho}^{(1)}$, $\hat{\varrho}^{(2)}$, … and so on can be constructed [5, 6]. The operator $\hat{\varrho}^{(1)}$ has a trace equal to the number N particles in the system:

$$\mathrm{Tr}\,\hat{\varrho}^{(1)} = N. \tag{25.1}$$

The main property of the operator $\hat{\varrho}^{(2)}$ can only be written if it is expressed in terms of the corresponding density matrix

$$\varrho(\alpha_1,\alpha_2;\ \alpha_1',\alpha_2') \equiv \varrho_{\alpha_1,\alpha_2;\,\alpha_1',\alpha_2'} \equiv \varrho_{12,1'2'}.$$

Here the value α is a quantum variable that characterizes the state of a single particle in some representation. For example, in the coordinate representation, the value of α is equal to the sum of four numbers: $\alpha = \{x, y, z, \xi\}$, where ξ is the spin of the particle. For particles that are either **bosons** or **fermions**, this property looks like this

$$\varrho_{12,1'2'} = \pm\varrho_{21,1'2'} = \pm\varrho_{12,2'1'} = \varrho_{21,2'1'}. \tag{25.2}$$

Here the sign + corresponds to bosons, and the sign −to fermions. If we are interested in only one density matrix $\varrho_{11'}$, then the second density matrix will be:

$$\varrho_{12,1'2'} \cong \varrho_{11'}\varrho_{22'} \pm \varrho_{12'}\varrho_{21'}. \tag{25.3}$$

This matrix will exactly satisfy the relation (25.2).

The simplest and most common type of Hamiltonian of a system of many particles consists of two terms: the operator $\hat{H}^{(1)}$ of one particle and the operator $\hat{H}^{(2)}$ of two particles that interact with each other. Now we can write an expression for the average energy of a system of identical particles

$$E = \sum_{\alpha\alpha'} H_{\alpha\alpha'}\,\varrho_{\alpha'\alpha} + 1/2\sum_{\{\alpha\}} H_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}\,\varrho_{\alpha_1'\alpha_2',\alpha_1\alpha_2}, \tag{25.4}$$

where $\{\alpha\} = \alpha_{1,}\ \alpha_2, \alpha_{1,}'\ \alpha_2'$, $H_{\alpha\alpha'}$ and $H_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}$ are matrix elements of the operators $\hat{H}^{(1)}$ and $\hat{H}^{(2)}$. The matrix elements $H_{\alpha\alpha'}$ are equal to

$$H_{\alpha\alpha'}(t) = \int \varphi_{\alpha}^{*}(q,t)\, \widehat{H}^{(1)}(q,t)\, \varphi_{\alpha'}(q,t)\, \mathrm{d}q\ . \qquad (25.5)$$

Matrix element

$$H_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} \equiv H_{12,1'2'}$$

of the Hamiltonian $\widehat{H}^{(2)}$, the interactions of two particles must satisfy the equalities:

$$H_{12,1'2'} = \pm H_{21,1'2'} = \pm H_{12,2'1'} = H_{21,2'1'}\,. \qquad (25.6)$$

By analogy with the formula (25.5), the formula will be valid

$$H_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} = \int \Phi_{\alpha_1\alpha_2}^{*}(q_1,q_2)\, \widehat{H}^{(2)} \Phi_{\alpha_1'\alpha_2'}(q_1,q_2)\mathrm{d}q_1\, \mathrm{d}q_2\ . \qquad (25.7)$$

In order for these matrix elements to obey the conditions (25.6), the function $\Phi_{\alpha_1\alpha_2}(q_1,q_2)$ must be a Slater function:

$$\Phi_{\alpha_1\alpha_2}(q_1,q_2) = 1/\sqrt{2}\{\ \varphi_{\alpha_1}(q_1,t)\varphi_{\alpha_2}(q_2,t) \pm \varphi_{\alpha_1}(q_2,t)\varphi_{\alpha_2}(q_1,t)\}\ .$$

Substituting the approximate expression (25.3) into the formula (25.4), taking into account the property (25.6) of matrix elements of the Hamiltonian $\widehat{H}^{(2)}$, we have

$$E = \sum_{\alpha\alpha'} H_{\alpha\alpha'}\, \varrho_{\alpha'\alpha} + \sum_{\{\alpha\}} H_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}\, \varrho_{\alpha_1'\alpha_1}\varrho_{\alpha_2'\alpha_2}\ . \qquad (25.8)$$

It is not difficult to prove that

$$\sum_{n_2n_3n_4} [H_{12,34}\varrho_{43\ 21'}] \cong 2 \sum_{n_2n_3n_4} [H_{12,34}, \varrho_{42}\varrho_{31'}]\ . \qquad (25.9)$$

Now you can write the desired equation for the density matrix

$$\mathrm{i}\hbar\, \partial\varrho_{11'}/\partial t = \sum_{n_2} [H_{12}\varrho_{21'}] + \sum_{n_2n_3n_4} [H_{12,34}\ , \varrho_{42}\varrho_{31'}] +$$

$$+\mathrm{i}\hbar/2 \sum_{n_2n_3} (\,2\,\gamma_{12,31'}\varrho_{23} - \gamma_{23,12}\varrho_{31'} - \gamma_{31',23}\varrho_{12}\,) +$$

$$+\mathrm{i}\,\hbar \sum_{n_2n_3n_4} \{(\varrho_{14}\varrho_{23} \pm \varrho_{24}\varrho_{13})\,\gamma_{34,21'} - \gamma_{34,12}\,(\varrho_{24}\varrho_{1'3} \pm \varrho_{1'4}\varrho_{23}) +$$

$$+\gamma_{12,43}(\varrho_{32}\varrho_{41'} \pm \varrho_{42}\varrho_{31'}) - (\,\varrho_{31}\varrho_{42} \pm \varrho_{41}\varrho_{32})\,\gamma_{21',43}\}\ . \qquad (25.10)$$

In some representation the density matrix has a diagonal form:

$$\varrho_{12} = w_1\delta_{12}\ .$$

Substituting this matrix into equation (25.10) turns it into a quantum kinetic equation for n_2=n_1

$$\partial w_1/\partial t = \sum_{n_2} \{p_{12}w_2(\,1 \pm w_1) - p_{21}w_1(\,1 \pm w_2)\}\ , \qquad (25.11)$$

where $p_{12} = \gamma_{12,21}$ is the probability of the particle passing from the state n_2 to the staten_1 in a unit of time.

26. Variation principle

When a quantum system is in an equilibrium state, the law that characterizes this state can be found using the variational principle. To do this, you need to know the energy of the system and its entropy. We only know one approximate expression for entropy, which is valid only in the case of a diagonal density matrix:

$$S = -k_{\mathrm{B}} \sum_{\boldsymbol{k}} \{ (1- w_{\boldsymbol{k}})\ln (1- w_{\boldsymbol{k}}) + w_{\boldsymbol{k}} \ln w_{\boldsymbol{k}} \} . \qquad (26.1)$$

Therefore, the energy of the system must also be diagonal. But the energy of the system, as usual, is recorded in the coordinate representation. You need to find a unitary matrix, which is used to transfer energy from the coordinate views in diagonal:

$$E = \sum_{\boldsymbol{k}} \varepsilon_k w_{\boldsymbol{k}} + 1/2 \sum_{\boldsymbol{k}\boldsymbol{k}'} \varepsilon_{\boldsymbol{k}\boldsymbol{k}'} w_{\boldsymbol{k}} w_{\boldsymbol{k}'} , \qquad (26.2)$$

where $\varepsilon_{\boldsymbol{k}}$ is the kinetic energy of one particle, $\varepsilon_{\boldsymbol{k}\boldsymbol{k}'}$ is the interaction energy of two particles.

Next, the variational principle allows you to write the equation for the probability of the state $w_{\boldsymbol{k}}$. The variational principle begins with the thermodynamic potential

$$\Omega = E - S\,T - \mu N , \qquad (26.3)$$

where T is the absolute temperature and μ is the chemical potential. The number of N particles is related to the probability $w_{\boldsymbol{k}}$ by the equality

$$N = \sum_{\boldsymbol{k}} w_{\boldsymbol{k}} . \qquad (26.4)$$

In our case, the thermodynamic potential is a function of $w_{\boldsymbol{k}}$:

$$\Omega = \Omega(w_{\boldsymbol{k}}) .$$

By differentiating this function by probability and equating the derivative to zero,
we get the equations for the desired function:

$$\ln\ [(1 - w_{\boldsymbol{k}})/w_{\boldsymbol{k}}] = \beta\, (\varepsilon_{\boldsymbol{k}} + \sum_{k'} \varepsilon_{kk'} w_{k'} - \mu) . \qquad (26.5)$$

27. Superconductivity

Unfortunately, it is not possible to solve equation (26.5), unless we accept an approximate formula for the energy $\varepsilon_{\boldsymbol{k}\boldsymbol{k}'}$ of the interaction of two electrons:

$$\varepsilon_{\boldsymbol{k}\boldsymbol{k}'} = I\, \delta_{\boldsymbol{k}+\boldsymbol{k}'} - J \delta_{\boldsymbol{k}-\boldsymbol{k}'} , \qquad (27.1)$$

where I and J are positive constants. Substitute the formula (27.1) in the formula (26.2). After
simple transformations we get

$$E = \sum_k \{ \varepsilon_k w_k + 1/2\, (I w_k w_{-k} - J w_k^2) \} , \qquad (27.2)$$

and putting the formula (27.1) in equation (26.5) gives

$$\ln\ [(1 - w_{\boldsymbol{k}})/w_{\boldsymbol{k}}] = \beta\, (\varepsilon_{\boldsymbol{k}} + I w_{-k} - J\, w_{\boldsymbol{k}} - \mu) . \qquad (27.3)$$

Solving this equation on a computer allows us to explain all the phenomena that have been discovered in superconductivity [5].

28. Conclusion

New theories from quantum physics based on the statistical operator and density matrix are presented in [6]. Here are some of these theories: superconductivity and superfluidity theories, laser theory and the theory of calculating the energy levels of an arbitrary atom, the theory of the oscillator density matrix, and the derivation of the Heisenberg relation. A new theory of ball lightning is presented in [7].

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New theories in quantum physics

I take the liberty of listing new theories in quantum physics that I have published in various scientific journals over the course of my long life. All these theories are based on the well-known mathematical principles of quantum mechanics. The core of these theories were the statistical operator and the density matrix.

1. Correlation theory of bimolecular reactions in solids. Bondarev B. V. Correlation theory of solid-phase reaction kinetics, Kinetics and catalysis, 1982, v. 23, № 2, p. 334-339.

2. Dissipative diffusion and attenuation operators were introduced. How I came up with it these two operators, I don't remember. I think it was God who chose me as his Minister. But even then Lindblad wrote down his equation. He assigned the operator $\widehat{D}$ to the Liouville – von Neumann equation in its most General form without conclusion. So I substituted my diffusion and attenuation operators into this General expression for the operator $\widehat{D}$and deduced that the quantum Lindblad equation goes into the Fokker – Planck equation for probability, which describes the motion of a Brownian particle. This was how quantum theory was linked to classical statistical physics.
Bondarev B.V. Quantum Markovian master equation for a system of identical particles interacting with a heat reservoir, Physica A, 1991, v. 176, № 2, p. 366-386.

3. An equation for the density matrix was derived from the Liouville – von Neumann equation. Bondarev B. V. Derivation of the quantum kinetic equation from the Liouville – von Neumann equation, TMF, 1994, v. 100, № 1, p. 33-43.

4. A new theory of superconductivity. Bondarev B. V. On some features of the electron distribution function for Bloch States. Bulletin of the MAI, 1996, v. 3, №2, p. 56-65.

5. A new theory of superfluidity. Bondarev B. V. Application of the variational density matrix method for describing the thermodynamic properties of a quantum Bose gas, Vestnik MAI, 1998, v. 5, № 2, p. 53-60.

6. A new theory of the quantum oscillator. Dissipative matrix. Bondarev B.V. Lindblad Equation for Harmonic Oscillator. Uncertainty Relation Depending on Temperature, Applied Mathematics, 2017, v. 8, p. 1529-1538.

7. A new theory for calculating the energy levels of electrons in an arbitrary atom. Bondarev B.V. Density Matrix Method in Theory of Atom. Advanced Materials. Springer. 2018, v. 207, p. 145-159.

8. A new theory of the laser. Bondarev B.V. New theory of laser. Method of density matrix. Advanced Materials. Springer. 2019, v. 224, p. 163.

9. A new theory for the density matrix of a quantum oscillator, when a dissipative attenuation operator is inserted into the Lindblad equation. Calculations show that the average value of the coordinate exactly satisfies the differential equation of damped oscillations. Bondarev B. V. Method of density matrices in the theory of quantum oscillator. Dissipative matrix. Scientific discussion, 2018, v. 1, № 19, p. 52-55.

10. A new theory of the equation for the density matrix of a system of identical particles.
Bondarev B.V. Equation for the density matrix of the system of identical particles. Advanced Materials. Springer. 2020, p. 141.

11. A new theory LED. Bondarev B. V. method of density matrices in quantum LED theory. Scientific discussion, 2019, v. 1, № 31, p. 43-50.

12. A new theory of ball lightning.Bondarev B.V. Ball lightning. Density matrix method. Scientific discussion, 2019, v. 1, № 38, p. 37-44.

13. A new spaser theory.Bondarev B.V. Spaser's quantum theory. Method of density matrix. Scientific discussion, 2020, v. 1, № 41. p. 21-27.

14. A new theory of graphene. Bondarev B.V. Method of density matrix. Quantum theory of graphene. Superconductivity. Scientific discussion, 2020, v. 1, № 42. p. 6-12

15. A new theory of nuclear forces. Bondarev B.V. Equation for the statistical operator and the state of nucleons in the atomic nucleus. Scientific discussion, 2020, v. 1, № 46. p. 34-41.

These theories begin a new stage in the development of quantum physics. which will be taken over by new young physicists. I wish you good luck.