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Extension of the Schrodinger equation

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Abstract. Extension of the Schrodinger equation is submitted by removing its limitations appearing due to the limitations of the formalism of Hamilton, based on which this equation was obtained. For this purpose the problems of quantum mechanics arising from the limitations of classical mechanics are discussed. These limitations, in particular, preclude the use of the Schrodinger equation to describe the time symmetry violation. The extension of the Schrodinger equation is realized based on the principle of duality symmetry. According to this principle the dynamics of the systems is determined by the symmetry of the system and by the symmetry of the space. The extension of the Schrodinger equation was obtained from the dual expression of energy, represented in operator form. For this purpose the independent micro - and macro-variables that determine respectively the dynamics of quantum particle system relative to its center of mass and the movement of the center of mass in space are used. The solution of the extended Schrodinger equation for the system near equilibrium is submitted. The main advantage of the extended Schrodinger equation is that it is applicable to describe the interaction and evolution of quantum systems in inhomogeneous field of external forces.

1 Introduction

The constructions of any physical theory are performed based on the basic provisions: models, hypotheses, axioms. As a rule, these basic provisions are taken in a simplified way, to allow us to describe the basic regularities, observed in experiments. For example the structureless material of point (MP) was used as a body model for construction of Newtonian mechanics [1]. This simplification has resulted in a serious contradiction between nature and its physical picture. Indeed, in according with the formalisms of classical mechanics all processes in nature are reversible. In reality we are witnessing of the irreversible picture. This contradiction was classified as a one of the chief problem of the physics [2, 3].

The explanation of the mechanism of irreversibility in the frames of the laws of the classical mechanics was found by the expansion of classical mechanics [4-6]. Expansion was achieved by replacing the material point, which used in Newtonian motion equation, on the particle, which has a structure. As a result, Newtonian mechanics became a special case of the new enhanced mechanics. The replacement MP on structural particle (SP) allowed us to remove the above mentioned contradiction between the reversible theoretical picture and the irreversible picture of the real nature [6].

The Schrodinger equation is the basis of quantum mechanics [7-10]. And like in the case of classical mechanics, it is faced with some difficulties, in particular in the description of the symmetry

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breaking and irreversible processes [11, 12]. We shall not discuss them. It is enough to say that classical mechanics is the limiting case of quantum mechanics. Therefore, the proof of existence of irreversibility in the frame of the laws of classical mechanics is a proof of the existence of the irreversible dynamics in the quantum mechanics. And we can suggest that the approach to the removal of the restrictions in quantum mechanics will be similar to the approach that has been used for the expansion of classical mechanics.

In this paper we consider the following questions: what restrictions of the Schrodinger equation follow from the restrictions of classical mechanics; how to remove these restrictions from the Schrodinger equation; how to obtain the extended Schrodinger equation.

2 The basic ideas of the quantum mechanics

Quantum mechanics was created as a result of solving problems to explain of the experimentally observed effects: quantization of energy, wave-particle duality. These properties characterize the behavior of quantum particles. It was found that the quantum particles combine the properties of conventional particles and waves. These properties, unusual for the classical mechanics, determine dynamics of the quantum particles. The quantization is associated with the observed discrete states of atomic systems [9-11]. The wave-particle duality manifested itself in that the separate particle during its registration, for example, by means of photographic plates, falls into a separate point on the plate, as it takes place for ordinary classical particles. At the same time, this point is not determined by the equations of motion or electrodynamics equations. The experiments showed that the spatial distribution of these particles was described by the wave equation [7]. According to experimental data, the energy and momentum with the defined frequency and wavelength can be associated with each micro-particle [2-5]: $E = h\nu = \hbar\omega$, $p = h\nu/c$. Here $\hbar = h/2\pi$ is a Planck's constant [7]; c is a velocity of light; $\omega = 2\pi\nu$ is an angular frequency; λ is a de Broglie wavelength. This allowed us to put the wave function into conformity with to the quantum particle. As it was found, the wave function of a free particle was a plane mono-chromatic de Broglie wave [9-11]: $\psi(r,t) = A\exp(i(kr - \omega t)/h)$, where $k = p/h$. As it can be seen from the experiments, the consistent scattering of particles, for example, on the crystal lattice, is equivalent to the scattering of the simultaneous flow of independents particles. In accordance with this result, the wave function of the aggregate of particles must satisfy the principle of superposition. Analysis of the experimental results of research of the dynamic properties of particles led Schrodinger to the idea that their dynamics was described by the wave equation but not by the Newton equation of motion [7-10]. The solution of the wave equation is the wave function, which is defined by the points in the configuration space. So, due to the quantum-wave dualism, particles can be associated with a wave field, which determines their spatial distribution. The amplitude of this field depends on the coordinates and time. Therefore this function is expressed through the so-called wave function $\psi(r,t) \equiv \psi(x,y,z,t)$. The value, $|\psi(x,y,z,t)|^2 dV$, means the probability of finding a particle at a time t in the volume element dV. It can be written as: $dW = |\psi(x,y,z,t)|^2 dV$. Based on the Hamilton formalism, Schrodinger found the equation for the wave function of the particles that described the experimental data [7]. The key idea, which helped him to assign the classical mechanics with the quantum mechanics was that the action in classical mechanics, up to a constant factor, was equal to Planck's constant, and coincided with the phase of the wave. There are several ways to obtain the Schrodinger equation. But the most logical way, which helps us to understand the relationship of this equation with the classical mechanics, belongs to Schrodinger [7]. Let us briefly describe the path that led Schrodinger to his equation.

3 How the Schrodinger equation was built

Schrodinger drew attention to the importance of conformity of the Hamilton-Jacobi equations [1] and the equations of geometrical optics. It consists in the fact that the action $S = \int_{t_0}^{t}(T - U)dt$ is equivalent to the phase of the wave (see Hamilton-Jacobi equation [1]). Here T is a kinetic energy, U-is a potential energy, t-is a time. Based on this, he decided to use the fact that for the wave function, the phase of which up to a constant factor coincides with the action, the following equation holds [9]: $u^2\nabla^2\psi(r,t) - \partial^2\psi(r,t)/\partial t^2 = 0$. If we substitute into this equation the value: $u = E/\sqrt{2m(E-U)}$, where m is a mass of the particle, and if we take into account that $\partial^2\psi(r,t)/\partial t^2 = -\omega^2\psi(r,t)$, $E\psi(r,t) = ih\partial\psi(r,t)/\partial t$, we get to the following equation [8-10]:

$$i\hbar\partial\psi(r,t)/\partial t = \{-\hbar^2\nabla^2/2m + U(r,t)\}\psi \tag{1}$$

It is the Schrodinger equation for one particle. For him the superposition principle holds. The Schrodinger equation is a first order in time. That is, the wave function for particles is uniquely determined by its initial value. The Schrodinger equation for a system can be obtained from the energy expression for the total energy of the particles. If we replace the energy and the momentum by the relevant operators, the Schrodinger equation for a system will have the form [9]:

$$\{i\hbar\partial/\partial t + \sum_{i=1}^{N}[\hbar^2\nabla^2/2m_i - U(r_i,t)] - W_{int}(r_1,r_2...r_N)\}\psi(r_1,r_2...r_N,t) = 0 \tag{2}$$

Here $W_{int}(r_1,r_2...r_N)$ - is the energy of interaction of particles, depending on the distance between them; $i = 1,2...N$; $U(r_i)$ is a potential energy of the i -th particle in the field of external forces.

We emphasize that the eq. (2) is applicable to systems of interacting particles. If the interactions are absent, for the stationary case the solution of eq. (2) can be represented as the product of the wave functions for each particle: $\psi = \psi_1(r_1), \psi_2(r_2)...\psi_N(r_N)$. This is equivalent to the sum of independent solutions for each particle.

In the general case the variables of the eq. (2) are not decoupled. The nature of the engagement variables in the eq. (2) is similar to the nature of the engagement of the variables for MP system which moves in a non-uniform force field. The variables in the laboratory coordinate are not orthogonal because they belong to the different symmetry groups [4, 6].

4 Why it is necessary to expanded the Schrodinger equation

We will proceed from the fact that to describe a system of interacting particles in quantum mechanics, like in classical mechanics, the eq. (2) shall be converted in accordance with the principle of duality symmetries (PDS) [4, 5]. The PDS means that the dynamic of the system is determined by the internal symmetry of the system and symmetry of space. That is, the energy of a system must be submitted as a sum of the motion energy and internal energy of the system. Then the nature of the violation of the time symmetry is connected with the transformation of the motion energy of the system into the internal energy [5]. The reasons for using the PDS are following. According to the laws of classical mechanics, matter is divisible to infinity. Therefore all the elements, including elementary particles, are structured. Note that there are no experiments, which would be contrary to this fact. Therefore, we assume that in quantum mechanics all particles have structure. Indeed, according to quantum mechanics, firstly, the energy of the ground state of the particles is different from zero, and secondly, the energy of the ground state of a quantum oscillator is not equal to zero. At the same time, the energy of the ground state is determined by the uncertainty principle. These facts

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agree with each other if we assume that all particles are structured and therefore have the internal energy. The minimum of this energy is determined by the Planck's constant. In turn, the forces determined by internal energy and the energy of motion, respectively. Therefore if the energy is not present in the dual form, it becomes possible to describe the violation of time symmetry when they move in inhomogeneous fields of external forces because the violation of time symmetry is caused by the transformation of the motion energy of the system in its internal energy. An example that confirms this view is the problem of the quantum oscillator [10].

There are also arguments, which are in favor of expansion of the Schrodinger equation. Due to the wave properties of the dynamics of the particles, the so-called Heisenberg's uncertainty principle takes place: $\Delta p \Delta r \geq \hbar$. This gives rise to the following questions. How is the violation of time symmetry connected with the uncertainty principle? How is it related to the infinite divisibility of matter? How the principle of uncertainty is associated with the fact that the accuracy of determining the dynamics of the particles cannot exceed the accuracy of determining the energy of motion at each point of the phase space, which is limited to changes of the internal energy of the system? Let us explain that the answers to these and many other questions must be sought on the basis of *PDS* [5,6].

There are at least two approaches to the interpretation of the uncertainty principle. Bohr argued that the uncertainty principle should be taken as a real manifestation of nature, without trying to look for an explanation. Einstein saw it as a restriction of the theory itself. From the standpoint of structuring matter at all hierarchical levels [8], we can propose an explanation of the uncertainty principle, that corresponds to the point of view of Einstein.

Let us take a system of interacting particles. For example, the scattering of the of the high energy electron flux on nucleons. Then assume that new particles appear as a result. This means that there must be a change in the internal energy of the reaction products while maintaining the total energy of the interacting systems. Since in this case the energy of motion of the system is reduced due to its conversion into internal energy, the violation of the symmetry of the time takes place. It means that $\delta A = A^d \neq 0$, where A^d is a right hand part in the variation of the least of action for any systems moving in inhomogeneous space [4, 5]. Then the nature of the uncertainty principle can be explained by the fact that the motion energy transforms into the internal energy resulting in strong particles interaction or motion systems in inhomogeneous space and we will have: $A^d \geq h$ or the A^d never equal to zero [4].

Transformation of the motion energy of the system into the internal energy, in classical mechanics determines the dissipative processes, which constitute the essence of the second law of thermodynamics for sufficiently large systems. It is natural to assume that for the quantum mechanics it will be similar. In extension of the Schrodinger equation, taking *PDS* into account, we replace the independent variables by the micro-and macro-variables. These variables create two independent groups of variables. Micro-variables determine the motion of the particle relative to the center of mass of the system. Macro-variables determine the motion of the center of mass of the system in the space [4,5].

5 The expansion of the Schrodinger equation for the system

Now let us show how to obtain the extended Schrodinger equation in connection with *PDS* for the system of two particles in the stationary case when the interaction between particles depends on the distance between them. In this case from eq. (2) we will have [9, 10]:

$$\{E + [\hbar^2 \nabla_R / 2M - U(r, R)] + [\hbar^2 \nabla_r^2 / 2\mu - W_{int}(r)]\}\psi(r, R) = 0 \tag{3}$$

Here $M = m_1 + m_2$ is a the total mass of the system, $\mu = m_1 m_2/(m_1 + m_2)$, $R = (m_1 r_1 + m_2 r_2)/(m_1 + m_2)$ are the coordinates of the center of mass (CM) of system, $r = r_1 - r_2$, E_{int} is an internal energy of the system, E_{cm} is energy of motion of the system CM, and $E_{int} + E_{cm} = E$. Eq. (3) is obtained by transition to the micro- and macro-variables. They characterize the movement of the CM of oscillator and the motion of each particle with respect to the CM. If $U(r, R) = W(r) + V(R)$, the variables are separated, and the wave function can be written as: $\psi(r, R) = \psi(r)\psi(R)$. In this case, eq. (3) is divided into two independent equations:

$$\{E_{int} + \hbar^2\nabla_r^2/2\mu - W(r) - W_{int}(r)\}\psi(r) = 0(a); \{E_{cm} + \hbar^2\nabla_R/2M - V(R)\}\psi(R) = 0\ (b) \tag{4}$$

Eq. (4 a) defines the relative movement of the particles in the CM system. Its solution is consistent with the one of a quantum oscillator in the case when the Hamiltonian has the form [8]: $\hat{H} = 1/2(\hat{p}^2/\mu + \mu\omega^2\hat{r})$, where $\hat{p}, \hat{r}$ are the operators of momentum and coordinate, ω is a the natural frequency of the oscillator.

Eq. (4 b) determines the motion in the space of the CM of oscillator. In the absence of an external field of forces, its solution has the form: $\psi(R) = exp(i/\hbar PR)$, where $P = \sqrt{2}ME_{cm}$. Micro- and macro-variables form two groups of independent variables. For the interacting systems, or when the system is moving in non-uniform field forces, these variables are connected with each other. As a result, as in classical mechanics, invariant is a sum of the energy of motion of the system and its internal energy.

The nature of the symmetry breaking is completely determined by the nonlinear terms, containing simultaneously the micro-and the macro-variables and describing the mutual transformation of the motion energy of the system and of the internal energy while maintaining their sum [4-6]. This means that in the general case the principle of superposition of the solutions for particles is not realized.

Thus, to describe the processes of the system dynamics and its evolution, in general, when the violation of time symmetries takes place, we need to use the total energy recorded in the micro- and macro-variables. For this purpose, the energy system of particles must be written as a sum of the energy of motion and the internal energy in the form of the operator. For quantum mechanics, this means that the Hamiltonian operator must be constructed as a sum of operators which describe the internal dynamics of the system and operators which determine the motion of the system in a heterogeneous space. Replacing the energy and momentum of the system by operators, we obtain from eq. (2) for stationary case:

$$\{E + \hbar^2\nabla_R^2/2M - U(\tilde{r}_1, \tilde{r}_2...\tilde{r}_N, R) + \sum_{i=1}^{N}[\hbar^2\nabla_{\tilde{r}_i}^2/2m - W_{int}(\tilde{r}_i)]\}\psi(\tilde{r}_1, \tilde{r}_2...\tilde{r}_N, R) = 0 \tag{5}$$

Here R is a CM coordinate system, $\tilde{r}_i$ are the coordinates of the i-th particle relative to CM of the system. We call this equation the extended Schrodinger equation. Contrary to the classical equation, it allows to take into account the transformation of the energy of motion of a quantum system in its internal energy. This transformation takes place when the system is moving in an inhomogeneous field of external forces. Without such transformation it is impossible to describe the formation of new attractors or quantum systems.

In the absence of engagement micro-variables with macro-variables, the total energy is a sum of the energy of motion of the whole system and the internal energy, respectively, i.e., $E = E_{int} + E_{cm}$. In this case the eq. (5) is divided into two equations:

$$\{E_{cm} + \hbar^2\nabla_R^2/2M - V(R)\}\psi(R) = 0 \tag{6}$$

$$\{E_{int} + \sum_{i=1}^{N}[\hbar^2\nabla_{\tilde{r}_i}^2/2m - W_{int}(\tilde{r}_i) - W(\tilde{r}_1, \tilde{r}_2...\tilde{r}_N)\}\psi(\tilde{r}_1, \tilde{r}_2...\tilde{r}_N) = 0 \tag{7}$$

where $\psi(\tilde{r}_1, \tilde{r}_2...\tilde{r}_N, R) = \phi(R)\varphi(\tilde{r}_1, \tilde{r}_2...\tilde{r}_N)$, $U(\tilde{r}_1, \tilde{r}_2...\tilde{r}_N) = W(\tilde{r}_1, \tilde{r}_2...\tilde{r}_N) + V(R)$.

6 Solutions of the Schrodinger equation for systems near equilibrium

Let us consider the case when the system moving in the field of external forces near equilibrium. In this case the potential energy of the system in external field can be written as: $U_N = (\alpha \sum_{i=1}^{N} r_i^2)/2$, where α is a positive coefficient (the value of the second derivative $\partial^2 U/\partial^2 r$ when $r = r_0$). Here all particles are identical. The quadratic functions of the potential energy of the system in an external field can be written in terms of the quadratic function, in which the arguments are the coordinates of the particles with respect to the CM and the CM coordinate system [4-6]. It follows from the equation: $N \sum_{i=1}^{N} r_i^2 = (\sum_{i=1}^{N} r_i)^2 + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} r_{ij}^2$, where $r_i - r_j = r_{ij}$. After completing in this equality the replacement $R_N = (\sum_{i=1}^{N} r_i)/N$, we will have for potential energy: $U_N = \alpha[R_N^2 + 1/N \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} r_{ij}^2]/2$. Here the first term in the right hand side is the potential energy of the motion of the system in the field of external forces. The second term is determined by the differences between the coordinates of the micro-particles.

Let us transform the energy by replacing: $r_i = R_N + \tilde{r}_i$, where $\tilde{r}_i$ are coordinate of the micro-particles relative to CM. Because $\sum_{i=1}^{N} \tilde{r}_i = 0$ we obtain $U_N = \alpha[R_N^2 + \sum_{i=1}^{N} \tilde{r}_i{}^2]/2$. Here the second term is equal to the energy of motion of particles relative to CM. Hence, the potential energy of the system in the external field near the equilibrium point is divided into the potential energy of motion of its CM and the amount of potential energy of motion of all particles relative the CM: $U_N = U_N^{tr} + U_N^{ins}$, where $U_N^{tr} = \alpha R_N^2/2$, $U_N^{ins} = \alpha \sum_{i=1}^{N} \tilde{r}_i{}^2/2$. I.e., the internal energy of the system can be written in the coordinates and velocities of the particles with respect to the CM. In this case the eqs. (6, 7) can be written as:

$$\{E_{cm} + \hbar^2 \nabla_R^2/2M - \alpha R_N^2/2\}\phi(R) = 0 \tag{8}$$

$$\{E_{int} + \sum_{i=1}^{N}[\hbar^2 \nabla_{\tilde{r}_i}^2/2m - W_{int}(\tilde{r}_i) - \alpha \tilde{r}_i^2/2]\}\varphi(\tilde{r}_1, \tilde{r}_2 ... \tilde{r}_N) = 0 \tag{9}$$

where $\psi(\tilde{r}_1, \tilde{r}_2 ... \tilde{r}_N, R) = \phi(R)\varphi(\tilde{r}_1, \tilde{r}_2 ... \tilde{r}_N)$.

If the condition $W_{int}(\tilde{r}_i) = \beta \sum_{i=1}^{N} \tilde{r}_i^2/2$ is satisfied, then we have: $\varphi(\tilde{r}_1, \tilde{r}_2 ... \tilde{r}_N) = \Pi_{i=1}^{N} \varphi_i(\tilde{r}_i)$. In this case the eq. (9) splits into independent equations for oscillators:

$$\{E_i + [\hbar^2 \nabla_{\tilde{r}_i}^2/2m - (\alpha + \beta)\tilde{r}_i^2/2]\}\varphi(\tilde{r}_i) = 0 \tag{10}$$

when condition $E_{int} = \sum_{i=1}^{N} E_i$ takes place. Here E_i is kinetic energy of motion of each particle of the system relative to its CM. This is the equation for the independent quantum oscillators. For the wave function $\varphi(\tilde{r}_i)$ the energy levels are given by [5]: $\varepsilon_{n_i} = \hbar\omega_i(n_i + 1/2)$, where $\omega_i = (\sqrt{(\alpha + \beta)})/m$. The index i is shown here only in order to emphasize the affiliation of the energy levels of the particle.

Thus, near equilibrium in the external and internal fields, the eqs. (6, 7) separate into independent oscillator equations for each particle, as well as for the system as a whole. The integrability of the equations follows from the fact that near the equilibrium the system is described by the Hamiltonian formalism. The characteristic frequency of these oscillators is defined as the forces of interaction of micro-particles as well as of the external forces. The external field of forces plays the role of the additive for independent vibrations of the atoms near their equilibrium. But the oscillation of the system in an external field of force is independent from the internal forces. The same is the case for the system of MP classical mechanics near the equilibrium of the internal and external forces fields [6]. In the general case of an inhomogeneous field of external forces, the variables in the eqs. (6, 7) are engaged. This leads to violation of time symmetry.

7 Conclusion

Thus, the restrictions of the classical mechanics which led to the reversibility of the hamiltonian systems, lead to restrictions of the Schrodinger equation. To remove these restrictions, it is necessary to write the Schrodinger equation in accordance with the *PDS* by using energy operators written in the micro- and macro-variables. In this case, the Hamiltonian splits into two parts. Micro-variables determine the dynamics of particle system with respect to the CM, and macro-variables determine the motion of a system in space as a whole. This equation can describe nonlinear processes symmetry breaking for the system moving in inhomogeneous fields of forces. Symmetry breaking determined by the nonlinear terms in the expansion of the forces, which depend simultaneously on micro- and macro-variables. These nonlinear terms, as in the case of classical mechanics, associated with the D-entropy of quantum systems [5, 6]. The D-entropy determines the part of the motion energy of the system which is transformed into the internal energy.

If the system is close to equilibrium, the Schrodinger equation is splitted into independent equations of the oscillations of the entire system as a whole, and each of the particles relative to the center of mass. The dynamic of the each particle is determined by the field of external forces and the forces of their interaction. The dynamics of the system is determined by the external forces only.

The main advantage of the extended Schrodinger equation is that it is applicable to describe the interaction and evolution of quantum systems.

References

[1] K.Lanczos, *Variation principles of mechanics* (Mir, Moscow, 1962) 408
[2] V.L.Ginzburg, UFN, **177**, 346 (2007)
[3] I.Prigogine, *From Being to Becoming* (Nauka, Moscow, 1980) 342
[4] V.M.Somsikov, PoS (Baldin ISHEPP XXII) 047 (2014)
[5] V.M.Somsikov, Modern Physics Letters B **4**, 1-11 (2016)
[6] V.M.Somsikov, *To the basics of evolution of the physics* (Sci., Almaty, 2016) 306
[7] A.Schrodinger, Phys.Rev. **28**, 1049-1070 (1926)
[8] L.D.Landau, E.M.Lifshitz, *Quantum mechanics* (Sci., Moscow, 1989) 767
[9] V.G.Levich, Y.Vdovin, V.A. Myamlin, *Course of Theoretical Physics II* (Sci., Moscow, 1962) 820
[10] V.G.Zelevinskii, *Lectures on quantum mechanics* (Siberian university, Novosibirsk, 2002) 504
[11] B.B.Kadomtsev, UFN **165**, 967-973 (1995)
[12] J.Greenstein, A.Zajonc, *Quantum challenge. Modern research foundations of quantum mechanics* (Intelligence, Dolgoprudny, 2012) 432
[13] M.J.Klein, UFN **92**, 679-700 (1967)
[14] V.M.Somsikov, Intern. Journal of Sci. **4**, 30-36 (2015)