

The Schrodinger Equation only Describes Approximately the Properties of Motion of Microscopic Particles in Quantum Mechanics

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Abstract -- We used a nonlinear Schrodinger equation to replace the linear Schrodinger equation and to study further the natures and states of microscopic particles due to plenty of difficulties of quantum mechanics. From this investigation we find that the states and properties of microscopic particles are considerably changed relative to those in quantum mechanics. An outstanding and obvious change is that the microscopic particles have a wave-corpucle duality in such a case. The solution of the nonlinear Schrodinger equation contains an envelop and carrier waves with determinant frequency which can propagation in medium in a certain velocity. These display the wave feature of particle. However the solutions have all a mass centre and possess a determinant size and mass, momentum and energy, which satisfy also the conservation laws of mass, momentum and energy, at the same time, they meet the collision law of classical particles. These embody the corpucle feature of the microscopic particles. Finally we seek the reasons and roots generating these changes, which are due to the nonlinear interactions among the particles or between the particles and background field to be considered in the nonlinear Schrodinger equation. The nonlinear interactions provide a double-well potential to make the microscopic particle to be localized as a soliton, and break also through the fundamental hypothesis for the independence of Hamiltonian operator of the systems with wave function of states of particles in quantum mechanics. Therefore we conclude that the microscopic particle should be described by the nonlinear Schrodinger equation, instead of the linear Schrodinger equation, and the quantum mechanics should develop towards the direction of nonlinear domain.

Index Terms -- Quantum mechanics, Microscopic particle, Schrodinger equation, Motion law, Wave, Corpuscles duality.

I. FUNDAMENTAL HYPOTHESESIS OF QUANTUM MECHANICS

As is known, the states and properties of motion of microscopic particles are depicted by quantum mechanics, which is a foundation of modern science and was established by several great scientists such as Bohr, Born, Schrodinger and Heisenberg, etc., in the early 1900s [1-6]. The theoretical hypotheses of quantum mechanics can be outlined as follows.

(1) The states of microscopic particles are represented by a vector of states $|\psi\rangle$ in Hilbert space, or a wave function $\psi(\vec{r}, t)$ in coordinate representation. It reflects the properties of wave of motion of the microscopic particles and can be normalized (i.e., $\langle\psi|\psi\rangle=1$). If β is a constant number, then both $|\psi\rangle$ and $\beta|\psi\rangle$ describe a same state.

(2) A mechanical quantity of microscopic particle, such as, coordinate x , momentum p and energy E , etc., is represented by an operator in Hilbert space. An observable mechanical quantity corresponds to a Hermitean operator, its eigenvector of state constructs a basic vector in the Hilbert space. This shows that the

values of the physical quantity are just eigenvalues of these operators. The eigenvalues of Hermitean operator are a real number. The eigenvectors corresponding to different eigenvalues are orthogonal with each other. A common eigenstates of commutable Hermitean operators are constituted as an orthogonal and complete set $\{\psi_L\}$. Any vector of state $\psi(\vec{r}, t)$ may be expanded by it into a series as follows

$$\begin{aligned}\psi(r, t) &= \sum_L C_L \psi_L(r, t), \\ |\psi(r, t)\rangle &= \sum_L \langle\psi_L|\psi\rangle |\psi_L\rangle\end{aligned}\quad (1)$$

where $C_L = \langle\psi_L|\psi\rangle$ is the wave function in representation L . If the spectrum of L is continuous, then the summation in Eq. (1) should be replaced by an integral: $\int dL\dots$. Eq. (1) can be regarded as a projection of wave function $\psi(\vec{r}, t)$ of the microscopic particle system, hence it is the foundation of transformation between different representations in quantum mechanics. In the quantum state described by $\psi(\vec{r}, t)$, the probability getting the L' in the measurement of L is $|C_{L'}|^2 = |\psi_{L'}|^2 = |\langle\psi_{L'}|\psi\rangle|^2$ in the case of discrete

spectrum, the probability is $|\langle \psi_L | \psi \rangle|^2 dL$ in the case of continuous spectrum. In a single measurement of any mechanical quantity, only one of the eigenvalues of corresponding operator can be obtained, the system is then said to be in the eigenstate belonging to this eigenvalue.

The two hypotheses are most important assumptions and stipulate how the states of the microscopic particles are represented in quantum mechanics.

(3) A mechanical quantity in an arbitrary state $|\psi\rangle$ can only take an average value by

$$\begin{aligned} \langle \hat{A} \rangle &= \frac{\langle \psi | \hat{A} | \psi \rangle}{\langle \psi | \psi \rangle} \\ \langle \hat{A} \rangle &= \langle \psi | \hat{A} | \psi \rangle \end{aligned} \quad (2)$$

at $\psi(\vec{r}, t)$ is normalized, i.e., possible values of the physical quantity A may be obtained by calculating this average. In order to find out these possible values, a wave function of states must be firstly known. Condition for determination value the quantity A has in this state is $\overline{(\Delta A)^2} = 0$. Thus we can obtain the eigenequation of the operator \hat{A} to be as follows

$$\hat{A} \psi_L = A' \psi_L \quad (3)$$

From this equation we can determine the spectrum of eigenvalues A' of the operator \hat{A} and its corresponding eigenfunction ψ_L , the eigenvalues of \hat{A} are possible values observed from experiment for this physical quantity. All possible values of \hat{A} in any other states are nothing but its eigenvalues in its own eigenstates. This hypothesis reflects the statistical nature in the description of microscopic particle in quantum.

(4) Hilbert space is a linear one and the mechanical quantity corresponds to a linear operator. Then corresponding eigenvector of state, or wave function, satisfies the linear superposition principle, i.e., if two states $|\psi_1\rangle$ and $|\psi_2\rangle$ are ones of a particle, then their linear superposition

$$|\psi\rangle = C_1 |\psi_1\rangle + C_2 |\psi_2\rangle \quad (4)$$

also describes the state of the particle, where C_1 and C_2 are two arbitrary constants. The linear superposition principle of quantum state is determined by the linear characteristics of the operators and this is why the quantum theory is referred to as linear quantum mechanics. However, it is noteworthy to point out that such a superposition is different from that of classical wave, it does not result in changes in probability and intensity of particle.

(5) Correspondence principle. If the classical mechanical quantities A and B satisfy the Poisson brackets: $\{A, B\} = \sum_n [(\partial A / \partial q_n) \times (\partial B / \partial p_n) - (\partial A / \partial p_n) \times (\partial B / \partial q_n)]$, where q_n and p_n are generalized coordinate and momentum in classical system, respectively, then the corresponding operators \hat{A} and \hat{B} in quantum mechanics satisfy the following commutation relations

$$[A, B] = (AB - BA) = -ih\{A, B\} \quad (5)$$

where $i = \sqrt{-1}$ and h is the Planck's constant. If A and B are substituted by q_n and p_n , respectively, then $[\hat{p}_n, \hat{q}_m] = -ih\delta_{nm}$, $[\hat{p}_n, \hat{p}_m] = 0$. This reflects the fact that the values taken for physical quantity are quantized. Based on this fundamental principle, the Heisenberg uncertainty relation can be obtained by

$$\overline{(\Delta A)^2} \overline{(\Delta B)^2} \geq \frac{|C|^2}{4} \quad (6)$$

where $iC = [\hat{A}, \hat{B}]$ and $\Delta A = \langle \hat{A} \rangle - \langle \hat{A} \rangle$. For the coordinate and momentum operators, the Heisenberg uncertainty relation takes the usual form: $\Delta x \Delta p > h/2$.

(6) The time dependence of a quantum state $|\psi\rangle$ of a microscopic particle is determined by the following Schrodinger equation

$$\begin{aligned} -\frac{\hbar}{i} \frac{\partial}{\partial t} |\psi\rangle &= H |\psi\rangle \\ \text{or } i\hbar \frac{\partial \psi}{\partial t} &= -\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r}, t) \psi \end{aligned} \quad (7)$$

where $\hbar^2 \nabla^2 / 2m$ is the kinetic energy operator, $V(\vec{r}, t)$ is the externally applied potential operator, m is the mass of particles, $\psi(\vec{r}, t)$ is a wave function describing the states of particles, \vec{r} is the coordinate or position of the particle, and t is the time. This is a fundamental dynamic equation for the microscopic particle in time-space. However the Hamiltonian operator of the systems H is given by

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hbar^2}{2m} \nabla^2 + \hat{V} \quad (8)$$

where \hat{T} is an operator of kinetic energy and \hat{V} an operator of potential energy. In other words, the properties of the systems at any time are determined by the Hamiltonian of the systems, the states and features of the particle at any position and time is determined by Schrodinger equation (7), which is a linear equation for the wave function $\psi(\vec{r}, t)$, thus we call ever it as linear Schrodinger equation. This is another of reasons to be referred to it as linear quantum mechanics.

If the state vector of the system at time t_0 is $|\psi(t_0)\rangle$ then the mechanical quantity and wave vector at time t are associated with those at time t_0 by a unitary motive operator $\hat{U}(t, t_0)$, namely $|\psi(t)\rangle = \hat{U}(t, t_0) |\psi(t_0)\rangle$, where $\hat{U}(t, t_0) = 1$, $\hat{U}^\dagger \hat{U} = \hat{U} \hat{U}^\dagger = I$. If $\hat{U}(t, 0) = \hat{U}(t)$, thus the equation of motion becomes

$$-\frac{\hbar}{i} \frac{\partial}{\partial t} \hat{U}(t) = \hat{H} \hat{U}(t) \quad (9)$$

when H does not depend explicitly on an time t and $\hat{U}(t) = \exp(-it\hat{H}/\hbar)$. If H is an explicit function of time t , then

$$\hat{U}(t) = 1 + \frac{1}{ih} \int_0^t dt_1 \hat{H}(t_1) + \frac{1}{(ih)^2} \int_0^t dt_1 \hat{H}(t_1) \int_0^{t_1} dt_2 \hat{H}(t_2) + \dots \quad (10)$$

This equation shows a causality relation of the microscopic law of motion. Obviously, there is an important assumption here: the Hamiltonian operator of the system is independent on the wave function of state of the particle. This is a fundamental assumption in quantum mechanics.

(7) Principle of full-identity. No new physical state occurs when two same particles exchange mutually their positions in the systems, in other words, it satisfies

$$p_{kj}|\psi\rangle = \lambda|\psi\rangle, \text{ where } \hat{p}_{kj} \text{ is a exchange operator, .}$$

The wave function for an system consisting of identical particles must be either symmetric Ψ_s , ($\lambda = +1$) or antisymmetric Ψ_a , ($\lambda = -1$), and this property remains invariant with time and is determined only by the nature of the particle. The wave function of a boson particle is symmetric and that of fermion is antisymmetric.

(8) Assumption of measurement of physical quantities in quantum systems. There was no assumption made about measurement of physical quantities at the beginning of quantum mechanics. It was introduced later to make the quantum mechanics complete. However, this is a nontrivial and controversial topic which has been a focus of scientific debate. This problem will not be discussed here. Interested reader can refer to some literatures.

In one word, these hypothesizes stipulate the representation forms of states and mechanical quantities and Hamiltonian of microscopic particles and the relationships satisfied by them. Concretely speaking, the states of microscopic particle is represented by a wave function, which satisfies the linear Schrodinger equation (7) and linear superposition principle in Eq. (4) and normalization condition, the square of its absolute value represents the probability of the particle at certain point in space-time, and is used to indicate the corpuscle feature of microscopic particle. The mechanical quantities of microscopic particle are represented by the operators, which satisfy the commutation relation in Eq. (5) and uncertainty relation in Eq. (6), their values are denoted by some possible average values or eigenvalues of corresponding operators in any states or eigenstates, The Hamiltonian operator of the systems is independent on the wave function of state of the particles and denoted only by kinetic and potential energy operators in Eq. (8), which determine the states of the particles by virtue of Eq. (7). These are just the quintessence and creams of quantum mechanics.

II. THE SUCCESS AND DIFFICULTIES OF QUANTUM MECHANICS AND ITS ROOTS

On the basis of several fundamental hypothesises mentioned above, Heisenberg, Schrodinger, Bohn, Dirac, etc., have founded up the theory of quantum mechanics which describes the law and properties of motion of the microscopic particles. This theory states that once the externally applied potential fields and the conditions at the initial states for the particle are given, the states and features of the particles at any time later and any position can be easily determined by linear Schrodinger equations (7) and (8) in the case of nonrelativistic motion. The quantum states and their

occupations of electronic systems, atom, molecule, and the band structure of solid state matter, and any given atomic configuration are completely determined by the above equations. Macroscopic behaviours of the systems, such as, mechanical, electrical and optical properties may be also determined by these equations. This theory can also describe the properties of microscopic particle systems in the presence of external electromagnetic-field, optical and acoustic waves, and thermal radiation. Therefore, to a certain degree, the linear Schrodinger equation describes the law of motion of microscopic particles of which all physical systems are composed. It is the foundation and pillar of modern science.

The quantum mechanics had great successes in descriptions of motion of microscopic particles, such as, electron, phonon, photon, exciton, atom, molecule, atomic nucleus and elementary particles, and in predictions of properties of matter based on the motion of these quasi-particles. For example, energy spectra of atoms (such as hydrogen atom, helium atom) and molecules (such as hydrogen molecule) and compounds, the electric, magnetic and optical properties of atoms and condensed matters can be calculated based on the quantum mechanics and the calculated results are in good agreement with experimental measurements. Being the foundation of modern science, the establishment of the theory of quantum mechanics has revolutionized not only physics, but also many other science branches, such as, chemistry, astronomy, biology, etc., and at the same time, created many new branches of science, for example, quantum statistics, quantum field theory, quantum electronics, quantum chemistry, quantum biology, quantum optics, etc. One of the great successes of quantum mechanics is the explanation of the fine energy-spectra of hydrogen atom, helium atom and hydrogen molecule. The energy spectra predicted by quantum mechanics for these simple atoms and molecules are completely in agreement with experimental data. Furthermore, modern experiments have demonstrated that the results of Lamb shift and superfine structure of hydrogen atom and anomalous magnetic moment of electron predicted by the theory of quantum electrodynamics are coincident with experimental data. It is therefore believed that the quantum electrodynamics is one of successful theories in modern physics.

Despite the great successes of quantum mechanics, it nevertheless encountered some problems and difficulties. In order to overcome these difficulties, Einstein had disputed with Bohr, and others for the whole of his life and the difficulties remained still up to now. The difficulties of quantum mechanics are well known and have been reviewed by many scientists. When one of founders of the quantum mechanics, Dirac, visited to Australia in 1975, he gave a speech on development of quantum mechanics in New South Wales University. During his talk, Dirac mentioned that at the time, great difficulties existed in the quantum mechanical theory. One of the difficulties referred to by Dirac was about an accurate theory for interaction between cat one point, we shall find that the energy of a point charge is infinite. This problem had puzzled

physicists for more than 40 years. Even after the establishment of renormalization theory, no actual progress had been made. Therefore, Dirac concluded his talk by marking the following statements: "It is because of these difficulties, I believe that the foundation for the quantum mechanics has not been correctly laid down. I cannot accept that the present foundation of the quantum mechanics is completely correct".

However, have what difficulties in the quantum mechanics on earth evoked these contentions and raised doubts about the theory among physicists in the world? It was generally accepted that the fundamentals of the quantum mechanics consist of Heisenberg matrix mechanics, Schrodinger wave mechanics, Bohr's explanation of probability for the wave function and Heisenberg uncertainty principle, etc.. These were also the focal points of debate and controversy. In other word, the debate was about how to interpret the quantum mechanics. Some of the questions being debated concern the interpretation of the wave-corpucle duality, probability explanation of wave function, Heisenberg uncertainty principle, Bohr complementary (corresponding) principle, the quantum mechanics which describes on earth whether the law of motion for a single particle or for an assembly consisting of a great number of particles, the problems of microscopic causality and chance, the difficulties in controlling interaction between measuring instrument and objects being measured, etc. Meanwhile, the quantum mechanics can not describe the physical systems with many body and many particles. When it is used to depict such systems, plenty approximations must be done to find out some approximate solutions, thus a lot of true and important phenomena and effects are artificially eliminated or thrown away. This is very sorry for developments of physics. Therefore most of these problems relate to an important problem that the quantum mechanics is or is not the theory of real physics. Since modern quantum mechanics was born in 1920s, these problems were all situated in heated disputes among various points of views and different schools. It was an exceptional phenomenon in history of physics, that so wide the scope was and so high the related physicist's positions in different schools were. The main trend was Copenhagen School regarded Bohr as its head. As early as 1920s, heated disputes on statistical explanation and incompleteness of wave function arose ever between Bohr and other physicists, such as Einstein, de Brooglie, Schrodinger, Lorentz, etc. Thus, a long-drawn-out dispute occurred. Such a great polemic is unprecedented. This polemic may be divided into three stages.

When the quantum mechanics had just been founded from 1924 to 1927 as the first stage, Einstein proceeded from his own philosophical conviction and his scientific aim pursued (a description of exact causality towards physical world) to nurse a strong grievance against the probability interpretation of the quantum mechanics. He said in this letter: "although the quantum mechanics is imposing, there is an internal sound which tells me that the quantum mechanics is not so real yet, in any case, I believe that God is not to throw dice".

The second stage was from 1927 to 1930. After Bohr had set forward his complementary principle and had formed his orthodox interpretation, Einstein nursed an extreme grievance. Because the complementary principle was set forward based on the Heisenberg uncertainty relation, thus, the spearhead of Einstein's criticism was directed at the uncertainty relation.

The third stage was from 1930 until Einstein died. An expression was sharply concentrated on the reply to Bohr, in which "EPR" paradox had been set forward by Einstein together with Podolsky and Rosen. Because this paradox was referred to the basic problem of the LQM, i.e., whether it satisfied the deterministic localized theory and the microscopic causality or not. Because some of recent experiments are advantageous to the LQM, instead of the Bell inequality, so it is necessary to understand the contents and meaning of the EPN paradox.

Many scientists who followed closely the thought of localization and incomplete view of the LQM which were set forward by Einstein etc thought of that there could exist hidden variables theory hidden behind the LQM, which might interpret the behaviour of probability for the MIP. This thought of "the hidden variables" had early been suggested when the LQM was just born. However, Von Neumann Law had negated it in 1932. For a long time since then, no one talked longer to this problem. After the 2nd World War, after Einstein had expressed a grievance to the LQM and suggested that any actual state would completely be described.

Bohm put forward a systematic "hidden variable theory" in 1952. He considered that the statistical characteristics of the LQM come from the fluctuation of subquantum systems. If the hidden function determining the MIP could be found, then a deterministic description could be made for a single particle. How does the existence of such hidden variables be proved? He suggested experimental alternatives for measuring the spin correlation function of single proton and the polarizing correlation in annihilating radiation of photons. Bohm's theory was improved later because in Bohm's theory the single state $\psi(\vec{r}, t)$ is essentially a smooth variational state which describes only state of the fluid with random fluctuation, but the wave function in the LQM can not take into this random fluctuation. Thus, new hidden variables would not be introduced in such a case. Then Bohm's theory can be only referred to as a random hidden-variables theory.

However, if the motion of particle in the system was taken as a stable Markov process, then a steady solution of Schrodinger equation can be given from steady distribution of Markov chain, if the Fock-Planck equation was taken as dynamic equation of the MIP, then the new "hidden variables theories" of the LQM can also be set up. In 1996, Bell set up Bell's inequality on the basis of Bohm deterministic "localized variables theory" and attempted to verify by experiment this theory and the LQM which was right and which was wrong. As mentioned above, at that time, majority of the experiments supported the LQM. Thus the localized "hidden variables theory" which could not completely

repeat all the statistical predictions of the LQM was negated at present.

In one word, the long-dated dispute between Bohr and Einstein schools was focused on three problems: The first is that Einstein upheld to believe that the microscopic world being the same as the macroscopic one in which the particles is a matter of objective existence independent of sensational and the theoretical description to it should be deterministic in principle. The second is that Einstein always considered that the theory of the LQM was not an ultimate and complete one. From the point of view of Einstein, the objective truth of the LQM is similar to the classical optics. They all seem to be a kind of theory with statistical law, i.e., when the probability $|\psi(\vec{r}, t)|^2$ of a particle at moment t and in location r is given, an average value of observable quantities with which the experimental results may be compared can be calculated out by statistics. But the process of individual particle state is locking in full understanding yet. Hence, $\psi(\vec{r}, t)$ has not ended the understanding of microscopic object, namely the statistical interpretation can not be ultimate and complete. The third is how to interpret physically the LQM. He had a grievance against that the theory of the LQM made an attempt at completely describing single particle. This had fully been expressed in his speech in 5th Selway International Meeting of Physics. He put forward again that the states of a single particle could not be described by the wave function Ψ in any case in his book of "Physics and reality" published in 1936, it is referred to many particles. In the light of term in statistical mechanics, the system should be referred to as an assembly. He considered further that the uncertainty relation resulted from incompleteness of the description for an particle by $\psi(\vec{r}, t)$, because a description of completeness should be definite for all observable quantities. Additionally, he did not accept the statistical interpretation for wave function in the LQM, because he did not believe that the electron possessed free will. Thus, Einstein's grievance against the LQM did not direct towards the mathematic forms of the LQM, but its fundamental hypotheses and the physical interpretation. He also considered that this is due to the incomplete understanding of the properties of the MIP. Moreover, since the contradiction of relativity theory to the theoretical fundamental of the LQM had ever once resulted in a dispute. Thus Einstein formed a thought to unite the relativity theory and LQM and want to interpret the atomic structure by field theory. In a word, the divergences about several fundamental problems of the LQM between Einstein and Bohr schools are deep-going, concrete and deeply considerable. Above introductions of the disputes between them are helpful to deeply understand natures and question of the LQM and to promote further bearing of non-linear quantum mechanics.

However, what are the roots of these difficulties of quantum mechanics on earth? As is known, the Schrodinger equation in Eq. (7), which is used to describe the properties and rules of motion of microscopic particles, is a wave equation, if only the externally applied potential is known, we can find the

solutions of the equation [7-9]. However, for all externally applied potentials, the solutions of the equation are always a linear or dispersive wave, for example, at $V(\vec{r}, t) = 0$, its solution is a plane wave

$$\psi(\vec{r}, t) = A' \exp[i(\vec{k} \cdot \vec{r} - \omega t)] \quad (11)$$

where k is the wave-vector of the wave, ω is its frequency, and A' is its amplitude. This solution denotes the state of a freely moving microscopic particle with an eigenenergy of

$$E = \frac{p^2}{2m} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2), (-\infty < p_x, p_y, p_z < \infty) \quad (12)$$

This is a continuous spectrum. It states that the probability for the particle to appear at any point in the space is the same, thus the microscopic particle propagates and distributes freely in a wave in total space, this means it cannot be localized and have nothing about corpuscle feature.

If the free particle is artificially confined in a small finite space, such as, a rectangular box of dimension a , b and c , then the solutions of Eq. (7) are standing waves

$$\psi(x, y, z, t) = A \sin\left(\frac{n_1 \pi x}{a}\right) \sin\left(\frac{n_2 \pi y}{b}\right) \sin\left(\frac{n_3 \pi z}{c}\right) e^{-iEt/\hbar} \quad (13)$$

In such a case, there is still dispersion effect for the microscopic particle, namely, it appears still with a determinant probability at each point in the box with a quantized eigenenergy

$$E = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right) \quad (14)$$

The corresponding momentum is also quantized. This means that the wave feature of microscopic particle has been not changed in this condition.

If the potential field is further varied, for example, the microscopic particle is subject to a conservative time-independent field, $U(\vec{r}, t) = U(\vec{r}) \neq 0$, then the microscopic particle satisfies the time-independent linear Schrodinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi' + V(\vec{r}) \psi' = E \psi' \quad (15)$$

where

$$\psi = \psi'(\vec{r}) e^{-iEt/\hbar} \quad (16)$$

When $V = \vec{F} \cdot \vec{r}$, here \vec{F} is a constant field, such as, a one dimensional uniform electric field $V(x) = -eEx$, the solution of Eq. (15) is $\psi' = A \sqrt{\xi} H_{1/2}^{(1)}[(2/3) \cdot \xi^{3/2}]$, $\xi = x/l + \lambda$, where $H^{(1)}(x)$ is the first kind Hankel function, A is a normalized constant, l is the characteristic length and λ is a dimensionless quantity. The solution is still a dispersed wave. When $\xi \rightarrow \infty$, it approaches $\psi'(\xi) = A' \xi^{-1/4} e^{-2\xi^{3/2}/3}$ to be a damped wave.

If $V(x) = Fx^2$, the eigenwave function and eigenenergy are $\psi'(x) = N_n e^{-\alpha^2 x^2/2} H_n(\alpha x)$, and $E_n = (n + 1/2) \hbar \omega$, ($n = 0, 1, 2, \dots$), respectively, here $H_n(\alpha x)$ is the Hermite polynomial. The solution obviously has a decaying feature, and so on. These properties of solutions show clearly that the linear Schrodinger

equation is only a wave equation, its solutions have only a wave with dispersion feature, not the corpuscle feature. We can only use the $|\psi(\vec{r},t)|^2$ to represent the probability of particle occurred at position \vec{r} and time t . The above results show that the wave feature of the microscopic particle cannot be changed with variations of the time and external potential V . However, these features are incompatible and contradictory with regard to the traditional concept of particles [7-9], thus a great difficulty and trouble of quantum mechanics, such as, the uncertainty relationship between the position and momentum, the mechanical quantities have some average values in any state. These difficulties and contradictions are the intrinsic and inherent in quantum mechanics, and cause a duration controversy in physics [8-12]. More surprising, the way and method solving these problems have not sought up to now. Therefore it is very necessary to clarify the essences of these problems and to find the roots generating these problems [8-12].

As is known, Hamiltonian operator in Eq. (8) of the system corresponding Eq. (7) consists only of kinetic and potential operator of particles; the latter is only determined by an externally applied field, and not related to the state or wave function of the particle. We can keep changing the form of the external potential field $V(\vec{r})$, but soon we will find out that the dispersion and decaying nature of the microscopic particle persists no matter what form the potential field takes. This means that the external potential field $V(\vec{r})$ can only change the shape of the microscopic particle, i.e., its amplitude and velocity, but not its fundamental property such as dispersion as mentioned above. Therefore, the natures and features of microscopic particle are only determined by the kinetic energy term, $(\hbar^2/2m)\nabla^2 = \hat{p}^2/2m$, with dispersive effect, which cannot always be balanced and suppressed by an external potential field $V(\vec{r},t)$ in Eq. (7). Thus the particle has only the dispersive or wave feature. Because microscopic particles are always in motion, the dispersion effect of the kinetic energy term always exists. Then, microscopic particles have permanently a wave or dispersive feature, not the corpuscle feature. This is just the root the microscopic particles have only a wave feature in quantum mechanics.

III. SCHRODINGER EQUATION ONLY DESCRIBES APPROXIMATELY THE PROPERTIES OF MOTION OF MICROSCOPIC PARTICLES

The above results show that the quantum mechanics is so simple that it delineates and represents not essential and complete motions and interactions of all particles, which constitute the microscopic systems. Under the indication of this theory, when the quantum mechanics is used to study the properties of motion of microscopic particles in the complicated systems of many bodies and many particles, such as atoms of many electrons, molecule, solid and polymer, we have to freeze the motions of nuclei, or other particles (or electrons) or lattice field, and represent further their effects on the studied particle by using a mean field, or

periodic potential or other approximate potentials, which replace the real interactions between them, without respect to how complexity of the interactions among the particles or between the particles and background fields. This means that real motions and many interactions among them are all completely and thoroughly rubbed and neglected, thus the natures and features of microscopic particle are only determined by the kinetic energy term, $(\hbar^2/2m)\nabla^2 = \hat{p}^2/2m$, with dispersive effect, thus the particle has only the dispersive or wave feature. Then, microscopic particles have permanently a wave or dispersive feature, not the corpuscle feature. This is just the root the microscopic particles have only a wave feature in quantum mechanics. Obviously, this is not reasonable and appropriate to practical case. The above problems and difficulties are just the inherent shortcomings of linear quantum mechanics and cannot be overcome in itself framework. Therefore, it is not difficult to conclude from the above studies that the linear quantum mechanics is only an approximate theory and need develop forwards.

On the contrary, if the real motions of each particle or background field and the interactions among the particles or between the particle and background field are now considered, where the background field may be the lattice field in solid and condensed matter, in which the microscopic particles are possibly the electron or exciton or polaron, thus we can give the dynamical equations of the particles and background field, which can be represented by

$$i\hbar \frac{\partial}{\partial t} \phi = -\frac{\hbar^2}{2m} \nabla^2 \phi + V(x,t) + \chi \phi \frac{\partial F}{\partial x} \quad (17)$$

$$\frac{\partial^2 F}{\partial t^2} - v_0^2 \frac{\partial^2 F}{\partial x^2} = -\chi \frac{\partial}{\partial x} |\phi|^2 \quad (18)$$

where ϕ denotes the state of a microscopic particle, F denotes the dynamics of a background field or another particle with velocity v_0 , χ is a coupling interaction coefficient between them. This coupling changes themselves states. Eq. (17) and (18) mean that when the background field vibrates harmonically around its equilibrium position, instead of is frozen, the states of the particles will be changed through the interaction between them, such as electron-phonon coupling, but its counteraction force also the background field to make the forced vibration. This is just the physical meanings of Eq. (17)-(18). From Eq. (18) we can find out

$$\frac{\partial F}{\partial x} = -\frac{\chi}{v^2 - v_0^2} |\phi|^2 \quad (19)$$

Inserting Eq. (19) into Eq. (17) yields

$$i\hbar \frac{\partial}{\partial t} \phi = -\frac{\hbar^2}{2m} \nabla^2 \phi + V(x,t) - b |\phi|^2 \phi \quad (20)$$

where $b = \frac{\chi^2}{v^2 - v_0^2}$. This equation is just the nonlinear

Schrodinger equation of the microscopic particle, which is different from linear Schrodinger equation (7). This result shows clearly the nonlinear interaction comes

from the interactions among the particles or between the particles and background field. In practice, all realistic physics systems are composed of many particles and many bodies, the system composed of one particle does almost exist not in nature. Then in these systems, including the hydrogen atom, the nonlinear interactions exist always and generally in any conditions, if only the real motions of each particle or background field and the interactions among them are considered [10-15]. This means that we should all use the nonlinear Schrodinger equation in Eq. (20), instead of the linear Schrodinger equation in Eq. (7) in quantum mechanics, to study the states and properties of microscopic particles in any realistic-physics systems.

At present, it is deserve to study whether the nonlinear interaction $b|\phi|^2\phi$ related to the state of the particle can cancel and suppress the dispersion effect of the kinetic term in Eq. (20) and result at last in the localization of the particle. For this purpose we investigate the changes of nature of the particles by using Eq. (20) at $V(x, t) = 0$.

In the one-dimensional case, equation (20) at $V(x, t) = 0$ is represented by

$$i\phi_t + \phi_{x'x'} + b|\phi|^2\phi = 0 \tag{21}$$

where $x' = x/\sqrt{\hbar^2/2m}$, $t' = t/\hbar$. We now assume the solution of Eq. (21) to be of the form

$$\phi(x', t') = \varphi(x', t')e^{i\theta(x', t')} \tag{22}$$

Inserting Eq. (22) into Eq. (21) we can obtain

$$\varphi_{x'x'} - \varphi\theta_{t'} - \varphi\theta_{x'}^2 - b\varphi^2\varphi = 0, (b > 0) \tag{23}$$

$$\varphi\theta_{x'x'} + 2\varphi_x\theta_{x'} + \varphi_{t'} = 0 \tag{24}$$

If let $\theta = \theta(x' - v_e t')$, $\varphi = \varphi(x' - v_e t')$, then Eq. (23)-(24) become

$$\varphi_{x'x'} - v_e\varphi\theta_{t'} - \varphi\theta_{x'}^2 - b\varphi^3 = 0 \tag{25}$$

$$\varphi\theta_{x'x'} + 2\varphi_x\theta_{x'} - v_e\varphi_{t'} = 0 \tag{26}$$

If fixing the time t' and further integrating Eq. (26) with respect to x' we can get

$$\varphi^2(2\theta_{x'} - v_e) = A(t') \tag{27}$$

Now let integral constant $A(t') = 0$, then we can get $\theta_{x'} = v_e/2$. Again substituting it into Eq. (25), and further integrating this equation we then yield

$$\int_{\phi_0}^{\phi} \frac{d\phi}{\sqrt{Q(\phi)}} = x' - v_e t' \tag{28}$$

where $Q(\phi) = -b\phi^4/2 + (v_e^2 - 2v_e v_e)\phi^2 + c'$.

When $c' = 0$, $v_e^2 - 2v_e v_e > 0$, then $\phi = \pm\phi_0$, $\phi_0 = [(v_e^2 - 2v_e v_e)/2b]$ is the roots of $Q(\phi) = 0$ except for $\phi = 0$. Thus from Eq. (18) we obtain the solution of Eq. (23)-(24) is $\varphi(x', t') = \phi_0 \operatorname{sech} h[\sqrt{\frac{b}{2}}\phi_0(x' - v_e t')]$. Then the solution of nonlinear Schrodinger equation in Eq. (21) eventually is of the form

$$\phi(x, t) = A_0 \operatorname{sech} h \left\{ \frac{A_0 \sqrt{bm}}{\hbar} [(x - x_0) - vt] \right\} e^{i[m(x-x_0) - Et]/\hbar} \tag{29}$$

where $A_0 = \sqrt{\frac{mv^2/2 - E}{2b}}$, v is the velocity of motion

of the particle, $E = \hbar\omega$. The solution of Eq. (29) can be also found by the inverse scattering method [13, 14, 16]. This solution is completely different from Eq. (2), and contains a envelop and carrier waves, the former is

$$\varphi(x, t) = A_0 \operatorname{sech} \left\{ A_0 \left[\sqrt{mb}(x - x_0) - vt \right] / \hbar \right\}$$

and a bell-type non-topological soliton with an amplitude A_0 , the latter is the $\exp\{i[mv(x - x_0) - Et]/\hbar\}$. This solution is shown in Fig. 1. Therefore, the microscopic particle described by nonlinear Schrodinger equation (21) is a soliton [13-17]. The envelop $\varphi(x, t)$ is a slow varying function and the mass centre of the particle, the position of the mass centre is just at x_0 , A_0 is its amplitude, and its width is given by $W = 2\pi\hbar/(\sqrt{mb}A_0)$. Thus, the size of the particles is $A_0W = 2\pi\hbar/\sqrt{mb}$ and a constant.

This shows that the particle has exactly a mass centre and determinant size, thus is localized at x_0 . According to the soliton theory [13-17], the bell-type soliton in Eq. (29) can move freely over macroscopic distances in a uniform velocity v in space-time retaining its form, energy, momentum and other quasi-particle properties. Just so, the vector \vec{r} or x has definitively physical significance, and denotes exactly the positions of the microscopic particles at time t . Then, the wave-function $\phi(\vec{r}, t)$ or $\varphi(x, t)$ can represent exactly the states of the particle at the position \vec{r} or x and time t . These features are consistent with the concept of particles. Thus the feature of corpuscle of microscopic particles is displayed clearly and outright.

At the same time, we show also the collision property of two soliton solutions of Eq. (21) by numerical simulation technique in Fig. 1(c). From this figure we see clearly that the two particles can go through each other while retaining their form after the collision, which is the same with that of the classical particles. Therefore, the microscopic particle depicted by the nonlinear Schrodinger equation (21) has an obvious corpuscle feature.

However, the envelope of the solution in Eq. (19) is a solitary wave. It has a certain wavevector and frequency as shown in Fig. 1(b), and can propagate in space-time, which is accompanied with the carrier wave. The feature of propagation depends only on the concrete nature of the particle. Fig. 1(b) shows the width of the frequency spectrum of the envelope $\varphi(x, t)$, the frequency spectrum has a localized structure around the carrier frequency ω_0 . Therefore, the microscopic particle has exactly a wave-particulate duality [10-15].

Fig. 1(a) and Eq. (29) are just a perfect and beautiful representation and embodiment of the wave-particulate duality of the microscopic particles. This result also consists of de Broglie's relation formula of wave-particulate duality as well as Davisson and Germer's

experimental result of electron diffraction on double seam in 1927 [6-8].

However, we also demonstrate that the solution of Eq. (29) is not the solution Eq. (11) of linear Schrodinger equation in Eq. (7), even though the nonlinear interaction approaches to zero. To see this clearly, we now re-write the solution Eq. (29) as the following form

$$\phi(x,t) = 2\sqrt{\frac{2}{b}}k \operatorname{sech}\left\{2k\left[(x'-x'_0)-v_e t'\right]\right\} e^{i v_e [(x'-x'_0)-v_e t']/2} \quad (30)$$

where $2^{3/2}k/b^{1/2} = A_0$, $A_0 = \sqrt{\frac{v_e^2 - 2v_c v_e}{2b}}$, v_e is the

group velocity of the particle, v_c is the phase speed of the carrier wave. For a certain system, v_e and v_c are determinant and do not change with time. According to the soliton theory [13-17], the above solution with weak nonlinear interaction ($b \ll 1$) and small skirt $\phi(x',t')$ may be approximated by ($x' > v_e t'$)

$$\phi = 4\sqrt{2/b}k e^{-2k(x'-v_e t')} e^{i v_e (x'-x'_0 - v_e t')/2} \quad (31)$$

Thanks to the small term $b|\phi|^2 \phi$, then Eq. (21) can be approximated by

$$i\phi_t + \phi_{x'x'} \approx 0 \quad (32)$$

Substituting Eq. (31) into Eq. (32), we can examine that it satisfies Eq. (32), and can get $v_e \approx 4k$, which is the group speed of the particle. (Near the top of the peak, we must take both the nonlinear and dispersion terms into account because their contributions are of the same order. The result is the group speed.). Here, we have only checked the formula for the region where $\phi(x,t)$ is small; that is, when a particle is approximated by Eq. (31), it satisfies the approximate wave Eq. (32) with $v_e \approx 4k$.

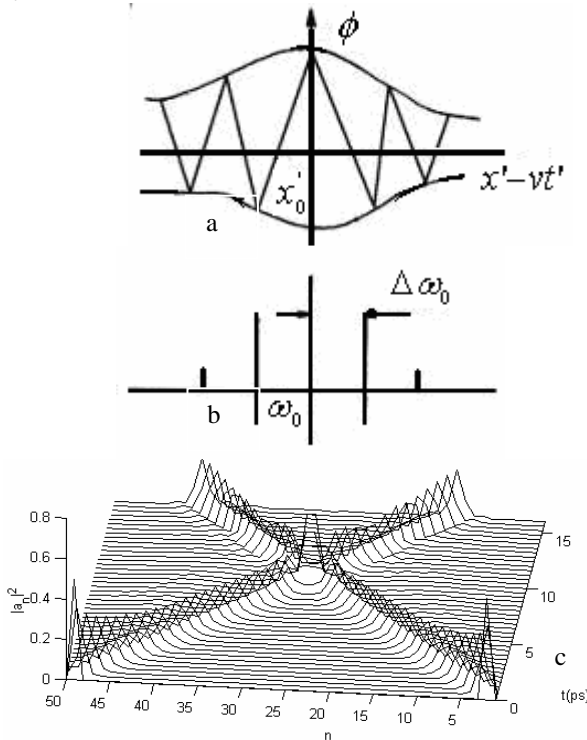


Fig.1. The solution in Eq. (29) at $V = A = 0$ in Eq. (11) and its features.

However, if Eq. (32) is treated as a linear Schrodinger equation, its solution is of the form:

$$\phi'(x,t) = A e^{i(kx - \omega t)} \quad (33)$$

We now have $\omega = k^2$, which gives the phase velocity ω/k as $v_c = k$ and the group speed $\partial\omega/\partial k = v_{gr} = 2k$. Apparently, this is different from $v_e = 4k$. This is because the solution Eq. (31) is essentially different from Eq. (33). Therefore, the solution Eq. (32) is not the solution of nonlinear Schrodinger equation (20) with $V(x,t) = 0$ in the case of weak nonlinear interactions. Solution Eq. (31) is a “divergent solution” ($\phi(x,t) \rightarrow \infty$ at $x \rightarrow -\infty$), which is not an “ordinary plane wave”. The concept of group speed does not apply to a divergent wave. Thus, we can say that the soliton is made from a divergent solution, which is abandoned in the linear waves. The divergence develops by the nonlinear term to yield waves of finite amplitude. When the nonlinear term is very weak, the soliton will diverge; and suppression of divergence will result in no soliton. These circumstances are clearly seen from the soliton solution in Eq. (30) in the case of nonlinear coefficient $b \neq 1$. If the nonlinear term approaches zero ($b \rightarrow 0$), the solitary wave diverges ($\phi(x,t) \rightarrow \infty$). If

we want to suppress the divergence, then we have to set $k = 0$. In such a case, we get Eq. (33) from Eq. (30). This illustrates that the nonlinear Schrodinger equation can reduce to the linear Schrodinger equation if and only if the nonlinear interaction and the group speed of the particle are zero. Therefore, we can conclude that the microscopic particles described by the nonlinear Schrodinger equation in the weak nonlinear interaction limit is also not the same as that in linear Schrodinger equation in quantum mechanics. Only if the nonlinear interaction is zero, the nonlinear Schrodinger equation can reduce to the linear Schrodinger equation. However, real physical systems or materials are made up of a great number of microscopic particles, and nonlinear interactions always exist in the systems. The nonlinear interactions arise from the interactions among the microscopic particles or between the microscopic particles and the environment. The nonlinear Schrodinger equation should be the correct and more appropriate theory for real systems. It should be used often and extensively, even in weak nonlinear interaction cases. However, the linear Schrodinger equation in quantum mechanics is an approximation to the nonlinear Schrodinger equation and can be used to study motions of microscopic particles in systems in which there exist only very weak and negligible nonlinear interactions.

However, how could a microscopic particle be localized in such a case? In order to shed light on conditions for localization of microscopic particle in the nonlinear Schrodinger equation, we return to discuss the property of nonlinear Schrodinger equation (20). The time-independent solution of Eq. (20) is assumed to have the form of [5-10]

$$\phi(x,t) = \phi(x,t) e^{-iEt/\hbar} \quad (34)$$

Then Eq. (20) becomes as

$$-\frac{\hbar^2}{2m}\nabla^2\varphi'+[V(\vec{r})-E]\varphi'-b|\varphi'|^2\varphi'=0 \quad (35)$$

For the purpose of showing clearly the properties of this system, we here assume that $V(\vec{r})$ and b are independent of \vec{r} . Then in one-dimensional case, equation (35) may be written as

$$\frac{\hbar^2}{2m}\frac{\partial^2\varphi'}{\partial x^2}=-\frac{d}{d\varphi'}V_{eff}(\varphi') \quad (36)$$

$$V_{eff}(\varphi')=\frac{1}{4}b|\varphi'|^4-\frac{1}{2}(V-E)|\varphi'|^2 \quad (37)$$

When $V > E$ and $V < E$, the relationship between $V_{eff}(\varphi')$ and φ' is shown in Fig. 2. From this figure we see that there are two minimum values of the potential, corresponding to two ground states of the microscopic particle in the system, i.e., $\varphi'_0 = \pm\sqrt{(V-E)/b}$. This is a double-well potential, and the energies of the two ground states are $-(V-E)^2/4b \leq 0$. This shows that the microscopic particle can be localized due to the fact that the microscopic particle has negative binding energy. This localization is achieved through repeated reflection of the microscopic particle in the double-well potential field. The two ground states limit the energy diffusion, thus the energy of the particle is gathered, soliton is formed, and the particle is eventually localized. Obviously, this is a result of the nonlinear interaction because the particle is in normal, expanded state if $b=0$. In the latter, there is only one ground state of the particle which is $\varphi' = 0$. Therefore, only if $b \neq 0$, the system can have two ground states, and the microscopic particle can be localized. Its binding energy, which makes the particle to be localized, is provided by the attractive nonlinear interaction, $-b(\varphi'\varphi'^*)^2$, in the systems. Only if the coupling interaction between them equal to zero or exists not, then Eq. (20) can degenerate to the linear Schrodinger equation in Eq. (7). This indicates again that the linear Schrodinger equation in quantum mechanics can only describe the states and properties of a single particle in vacuum without the nonlinear interaction. However, such physical systems are not existent in nature. Therefore we conclude from this investigation that the linear Schrodinger equation is an approximate and linear theory and cannot correctly describe the states and properties of the microscopic particle in the realistic physics systems. In previous investigations plenty of scientific workers use it to study the states and properties of microscopic particles in the systems of many particles and many bodies and obtain a lot of approximate results, in which some complicated and really nonlinear interaction among these particles, which could determine the essences and natures of particles, are ever replaced by a simple and uniform average-potential unassociated with the states of particles in virtue of different approximate methods. Thus the effects and results arising from these complicated effects and nonlinear interactions are ignored completely. Then the state and properties of particles determined by the average potential are not real and correct. It is very necessary to re-study these problems by the nonlinear Schrodinger equation and

corresponding quantum theory. These results show clearly that quantum mechanics need very develop towards the direction of nonlinear domain [22-25].

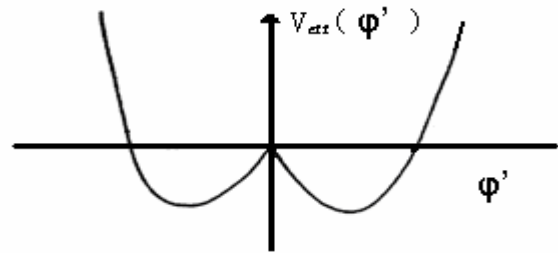


Fig.2. The effective potential of nonlinear Schrodinger equation.

IV. CONCLUSION

Since there are plenty of difficulties in quantum mechanics, in which the states and properties of microscopic particles are described by a linear Schrodinger equation, thus we here used a nonlinear Schrodinger equation to replace it and to study further the nature and states of microscopic particles. From this investigation we find that the states and properties of microscopic particles are considerably changed relative to those in quantum mechanics. An outstanding and obvious change is that the microscopic particles have a evident wave-corpucle duality which are obtained from the natures and properties of the solutions of nonlinear Schrodinger equation in the cases of different external potentials, the significances of wave function and conservation laws met by it. The solution of the nonlinear Schrodinger equation contains an envelop and carrier waves with determinant frequency which can propagation in medium in a certain velocity. These display the wave feature of particle. However the solutions have also a mass centre and possesses a determinant size and mass, momentum and energy, which satisfy also the conservation laws of mass, momentum and energy, at the same time, they meet the collision law of classical particles. These embody the corpucle feature of the microscopic particles. Finally we seek the reasons and roots generating these changes, which are due to the nonlinear interactions among the particles or the particles and background fields in the systems described by the nonlinear Schrodinger equation. In the meanwhile, we verified that the linear Schrodinger equation can only describe the states and properties of a single microscopic particle in vacuum without non linear interaction, the quantum mechanics is an approximate and linear theory and cannot represent in truth the properties and states of motion of the microscopic particles. For a realistic physics systems composed of many particles and many bodies we should use the nonlinear Schrodinger equation in Eq. (10) to describe the states and properties of the microscopic particles. The nonlinear interactions introduced in the nonlinear Schrodinger equation break through the fundamental hypothesis for the independence of Hamiltonian operator of the systems with wave function of states of particles in quantum

mechanics. Thus these microscopic particles are localized and have a real wave-corpucle duality. Therefore our investigations point out the direction of development of quantum mechanics and raise our knowledge and understanding to the essences and natures of microscopic particles.

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