

# THE NONLINEAR QUANTUM MECHANICAL THEORY AND ITS APPLICATIONS

**Pang Xiao Feng**

Institute of Life Science and Technology, University of Electronic Science and Technology of China, Chengdu  
610054, China

International Centre for Materials Physics, Chinese Academy of Science, Shenyang 110015, China  
E-mail: pangxf2006@yahoo.com.cn

## ABSTRACT

The properties of quantum mechanics and its difficulties and problems are discussed, the reasons resulting in these difficulties and direction of development of quantum mechanics are carefully studied. In practice, quantum mechanics neglects the real motions of the microscopic particles and background field as well as the real interactions between them. Therefore it can describe approximately the states of microscopic particles. For solving these difficulties of quantum mechanics, we proposed and established a nonlinear quantum mechanics based on the properties of macroscopic quantum effect and theories of superconductivity and superfluidity. In the new theory the elementary principles are proposed, its properties are also investigated. Subsequently, the motion laws and some main properties of microscopic particles in nonlinear quantum systems, including the wave-particle duality of the solution of the nonlinear Schrödinger equation, the stability of microscopic particles described by nonlinear quantum mechanics and the classical rule of microscopic particle motion, are studied using these elementary principles and theories. We obtained a lot of new and interesting results from this investigation, for example, the microscopic particles have really a wave-corpuscle duality in nonlinear quantum mechanics. The microscopic particles are localized due to the nonlinear interaction, have a determinant size, mass, energy and momentum. Thus the microscopic particles have not only a corpuscle but also a wave features, which are completely different from those in quantum mechanics. Hence we conclude that nonlinear quantum mechanics is a new physical theory, a correct representation of describing microscopic particles and a necessary result of the development of quantum mechanics, but traditional quantum mechanics is only its an approximation and especial case at the nonlinear interaction to be equal to zero, it can solve the difficulties and problems disputed for about a century by scientists in quantum mechanics field. In the meanwhile, we use the new theory of nonlinear quantum mechanics to study properties of the excitons and phonons in an organic crystal (acetanilide). The results obtained show that the excitons and phonons become as a soliton having a wave-corpuscle duality in this system. Thus the correctness and availability of nonlinear quantum mechanics are demonstrated using these experiments. We can predict that it has extensive applications in physics, chemistry, biology and polymers, etc.. Finally we state how the difficulties and problems in quantum mechanics are solved by the new theory of nonlinear quantum mechanics. Thus we can affirm from these investigations that the nonlinear quantum mechanics established by us is correct, quantum mechanics is only an approximate theory.

**Keywords:** *Quantum mechanics, nonlinear interaction, microscopic particle, nonlinear Schrödinger equation, nonlinear theory, wave-particle duality, nonlinear systems.*

## 1. INTRODUCTION, WAVE FEATURE OF MICROSCOPIC PARTICLES AND DIFFICULTIES OF QUANTUM MECHANICS

It is well known that several great scientists, such as Bohr, Born, Schrödinger and Heisenberg, etc. established quantum mechanics in the early 1900s[1-6], which is the foundation and pillar of modern science and provides a unique way of describing the properties and rules of motion of microscopic particles (MIP) in microscopic systems. In quantum mechanics the state of microscopic particles is described by the Schrödinger equation:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r}, t) \psi \quad (1)$$

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 theory states that once the externally applied potential field and initial states of the microscopic particles are given, the states of the particles at any time later and any position can be determined by the

Schrödinger equation (1) in the case of nonrelativistic motion. In this theory the Hamiltonian operator of the system corresponding Eq.(1) is

$$\hat{H}(t) = \hat{T}^2 / 2m + V(\vec{r}, t) + \quad (2)$$

where  $\hat{T} = \hat{T}^2 / 2m$  is the kinetic energy operator,  $V$  the external potential energy operator.

The quantum mechanics has achieved a great success in descriptions of motions of microscopic particles, such as, the electron, phonon, exciton, polaron, atom, molecule, atomic nucleus and elementary particles, and in predictions of properties of matter based on the motions of these quasi-particles. For example, energy spectra of atoms (such as hydrogen atom, helium atom), molecules (such as hydrogen molecules) and compounds, electrical, optical and magnetic properties of atoms and condensed matters can be calculated based on linear quantum mechanics and the calculated results are in basic agreement with experimental measurements. Thus considering that the quantum mechanics is thought of as the foundation of modern science, then 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 instance, quantum statistics, quantum field theory, quantum electronics, quantum chemistry, quantum optics and quantum biology, etc. Therefore, we can say the quantum mechanics has achieved a great progress in modern science. One of the great successes of linear quantum mechanics is the explanation of the fine energy spectra of hydrogen atom, helium atom and hydrogen molecule. The energy spectra predicted by the quantum mechanics are in agreement with experimental data. Furthermore, new experiments have demonstrated that the results of the Lamb shift and superfine structure of hydrogen atom and the anomalous magnetic moment of the electron predicted by the theory of quantum electrodynamics are in agreement with experimental data. It is therefore believed that the quantum electrodynamics is one of the successful theories in modern physics.

Studying the above postulates in detail, we can find [7-13] that the quantum mechanics has the following characteristics.

(1) Linearity. The wave function of the particles,  $\psi(\vec{r}, t)$ , satisfies the linear Schrödinger equation (1) and linear superposition principle, that is, if two states,  $|\psi_1\rangle$  and  $|\psi_2\rangle$  are both eigenfunctions of a given linear operator, then their linear combination holds:

$$|\psi\rangle = C_1 |\psi_1\rangle + C_2 |\psi_2\rangle$$

where  $C_1$  and  $C_2$  are constants relating to the state of these particle. The operators are some linear operators in the Hilbert space. This means that the quantum mechanics is a linear theory, thus it is quite reasonable to refer to the theory as the linear quantum mechanics.

The independence of Hamiltonian operator on the wave function. From Eq. (2) we see clearly that the Hamiltonian operator of the systems is independent on the wave function of state of the particles, in which the interaction potential contained relates also not to the state of the particles. Thus the potential can change only the states of the particles, such as the amplitude, but not its natures. Therefore, the natures of the particles can only be determined by

the kinetic energy term,  $\hat{T} = \hat{T}^2 / 2m$  in Eqs. (1) and (2).

(3) The wave feature. The Schrödinger equation (1) is in essence a wave equation and has only wave solutions, which do not include any corpuscle feature. In fact, let the wave function be  $\psi = f \exp[-iEt/\hbar]$  and substitute it into Eq. (1), we can obtain

$$\frac{\partial^2 f}{\partial x^2} + k_0^2 n^2 f = 0$$

where  $n^2 = (E - U)/(E - C) = k^2 / k_0^2$ ,  $C$  is a constant,  $k_0^2 = 2m(E - C)/\hbar^2$ . This equation is nothing but that of a light wave propagating in a homogeneous medium. Thus, the linear Schrödinger equation (1) is unique one able to describe the wave feature of the microscopic particle. In other words, when a particle moves continuously in the space-time, it follows the law of linear variation and disperses over the space-time in the form of a wave of microscopic particles. Therefore, the dynamic equation (1) of the particles is a wave equation in essence, thus the microscopic particles are only a wave. This is a basic or essential nature of the microscopic particles in quantum mechanics.

This nature of the particles can be also verified by using the solutions of Eq. (1)[7-18]. In fact, at  $V(\vec{r}, t)=0$ , its solution is a plane wave:

$$\psi(\vec{r}, t) = A' \exp[i(\vec{k} \cdot \vec{r} - \omega t)] \quad (3)$$

where  $k$ ,  $\omega$ ,  $A'$  and are the wavevector, frequency, and amplitude of a wave, respectively. This solution denotes the state of a freely moving microscopic particle with an eigenenergy:

$$E = \frac{P^2}{2m} = \frac{1}{2m} (P_x^2 + P_y^2 + P_z^2),$$

$$(-\infty < P_x, P_y, P_z < \infty)$$

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

If a free particle can be confined in a small finite space, such as, a rectangular box of dimension  $a$ ,  $b$  and  $c$ , the solution of Eq. (1) is standing waves as follows:

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

where  $n_1$ ,  $n_2$  and  $n_3$  are three integers. In this case, the particle is still not localized, it appears also at each point in the box with a determinant probability. In this case the eigenenergy of the particle in this case is quantized as follows:

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

The corresponding momentum is also quantized. This means that the wave feature of microscopic particle has not been changed because of the variation of itself boundary condition

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

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

where

$$\psi = \psi'(\vec{r}) e^{-i E t/\hbar}$$

When  $V = \vec{F} \cdot \vec{r}$ , here  $\vec{F}$  is a constant field force, such as, a one dimensional uniform electric field  $E'$ , then

$$V(x) = -eE'x, \text{ thus its solution is } \psi' = A \sqrt{\xi} H_{1/2}^{(1)}\left(\frac{2}{3} \xi^{3/2}\right), \left(\xi = \frac{x}{l} + \bar{\lambda}\right)$$

where  $H^{(1)}(x)$  is the first kind of Hankel function,  $A$  is a normalized constant,  $l$  is the characteristic length, and  $\bar{\lambda}$  is a dimensionless quantity. The solution remains 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  $V(x) = ax^2$ , the eigenenergy and eigenwave function are

$$\psi'(x) = N_n e^{-a^2 x^2/2} H_n(\alpha x)$$

and

$$E_n = (n + 1/2) \hbar \omega, \quad (n=0,1,2,\dots),$$

respectively, here  $H_n(\alpha x)$  is the Hermite polynomial. The solution obviously has a decaying feature. If the potential fields are successively varied, we find that the wave nature of the solutions in Eq. (1) does not change no matter what the forms of interaction potential. This shows clearly that the wave nature of the particles is intrinsic in quantum mechanics.

(4) Simplicity. We can easily solve arbitrary complicated quantum problems or systems, only if their potential functions are obtained. Therefore, to solve quantum mechanical problems becomes almost to find the representations of the external potentials by means of various approximate methods.

(5) Quantization. The particles, which the matter is composed of, are quantized in the microscopic systems. Concretely, the eigenvalues of physical quantities of the particles are quantized. For instance, the eigenenergy of the

particles at  $V(\vec{r}, t) = 0$  in Eq. (1) is quantized, when  $V(x) = ax^2$ , its eigenenergy,  $E_n = (n + \frac{1}{2})\hbar\omega$ , is also

quantized as mentioned above, and so on. In practice, the momentum, moment of momentum, and spin of the microscopic particles are all quantized in quantum mechanics. These quantized effects refer to as microscopic quantum effects because they occur on the microscopic scale.

Because of the above nature of quantum mechanics, some novel results, such as the uncertainty relationship between the position and momentum and the mechanical quantities are denoted by some average values in any state, occur also. Meanwhile, the wave nature of the particles obtained from this theory is not only incompatible with de Broglie relation,  $E = \hbar\omega = \hbar k$  and  $\vec{p} = \hbar\vec{k}$ , of wave- corpuscle duality for microscopic particles and Davisson and Germer's experimental result of electron diffraction on double seam in 1927[12-13], but also contradictory to the traditional concept of particles. Thus a lot of difficulties and problems occur in the quantum mechanics, among them the central problem is how we represent and delineate the corpuscle feature of the microscopic particles. Aimed at this

issue, Born introduce a statistic explanation for the wave function, and use  $|\psi(\vec{r}, t)|^2$  to represent the probability of

the particles occurring the position  $\vec{r}$  at time t in the space-time. However, the microscopic particles have a wave

feature and can disperse over total system, thus the probability  $|\psi(\vec{r}, t)|^2$  has a certain value at every point, for

example, the probability of the particle denoted by Eq. (3) is same at all points. This means that the particle can occur at every point at same time in the space. In this case, a fraction of particle must appear in the systems, which is a very strange phenomenon and is quite difficult to understand. However, in physical experiments, the particles are always captured as a whole one not a fractional one by a detector placed at an exact position. Therefore, the concept of probability representing the corpuscle behavior of the particles cannot be accepted.

Due to the linearity of the theory and the dispersive effect of the microscopic particles, then the use of quantum mechanics is impossible to describe the corpuscle feature of microscopic particles. Thus some scientists suggest that using a wave packet, for example, a Gaussian wave packet, represents the corpuscle behavior of a particle. The wave packet is given by

$$\psi(x, t = 0) = A_0 \exp[-\beta_0^2 x^2 / 2]$$

at  $t = 0$ , where  $A_0$  is a constant. Although this wave packet is localized at  $t = 0$  because  $|\psi|^2 = |A_0|^2 \exp[-\beta_0^2 x^2] \rightarrow 0$  at  $x \rightarrow \infty$ , the wave packet is also inappropriate to denote the corpuscle feature of the particles because it disperses and attenuates always with time during the course of propagation, that is

$$\begin{aligned} \psi(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(k) \exp[i(kx - \hbar k^2 t / 2m)] dk \\ &= \frac{1}{\beta_0 \sqrt{\beta_0^{-2} + i\hbar t / m}} \exp[-x^2 (\beta_0^{-2} + i\hbar t / m) / 2] \end{aligned}$$

where

$$\Psi(k, t = 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x, t = 0) \exp[-ikx] dx$$

In this case,

$$|\psi(x, t)|^2 = \frac{1}{\sqrt{1 + (\beta_0^2 \hbar t / m)^2}} e^{-x^2 / \beta_t^2},$$

$$\beta_t = \frac{1}{\beta_0} \sqrt{1 + i\beta_0^2 \hbar t / m}$$

This indicates clearly that the wave packet is instable and dispersed as time goes by, and its position is also uncertain with the time, which is not the feature of corpuscle. The corresponding uncertainty relation is

$$\Delta x \Delta p = \frac{\hbar}{2} \sqrt{1 + \beta_0^4 \hbar^2 t^2 / m^2}$$

where

$$\Delta x = \frac{1}{2\beta_0} \sqrt{1 + \beta_0^4 \hbar^2 t^2 / m^2}, \Delta p = \frac{\hbar\beta_0}{\sqrt{2}}$$

Hence, the wave packet cannot be applied to describe the corpuscle property of a microscopic properties. How to solve this problem has always been a challenge in the quantum mechanics. This is just an example of intrinsic difficulties of the quantum mechanics.

On the other hand, we know from Eqs.(1)-(2) that the quantum mechanics requires to incorporate all interactions among particles or between particles and background field, such as the lattices in solids and nuclei in atoms and molecules, including nonlinear and complicated interactions, into the external potential by means of various approximate methods, such as, the free electron and average field approximations, Born-Oppenheimer approximation, Hartree-Fock approximation, Thomas-Fermi approximation, and so on. This is obviously incorrect. The method replacing these real interactions by an average field amounts to freeze or blot out real motions and interactions of the microscopic particles and background fields, which was often used in the quantum mechanics to study the properties of the particles in the systems of many-particles and many-bodies. This indicates that the quantum mechanics is only an approximate theory and therefore quantum mechanics cannot be used to solve the real properties of the microscopic particles, such as electrons in atoms. In contrast, since the electron denoting by  $\psi(\vec{r}, t)$  in atoms is a wave, then it does not have a determinant position in quantum mechanics, but the vector  $\vec{r}$  is use to denote the position of the electron with charge  $e$  and mass  $m$  in the wave function and the Coulomb potential,  $V(\mathbf{r}) = -Ze^2/\vec{r}$ . Thus it is difficult to understand correctly these contradictory representations in quantum mechanics.

These difficulties and problems of the quantum mechanics mentioned above inevitably evoked the contentions and further doubts about the theory among physicists. Actually, taking a closer look at the history of physics, we could find that not so many fundamental assumptions were required for a physical theory but the linear quantum mechanics. Obviously, these assumptions of linear quantum mechanics caused its incompleteness and limited its applicability. However, the disputations continued and expanded mainly between the group in Copenhagen School headed by Bohr representing the view of the main stream and other physicists, including Einstein, de Broglie, Schrödinger, Lorentz, etc[7-16]. The following is a brief summary of issues being debated and problems encountered in linear quantum mechanics.

The correctness and completeness of the linear quantum mechanics were challenged. Is linear quantum mechanics correct? Is it complete and self-consistent? Can the properties of microscopic particle systems be completely described by the linear quantum mechanics? Do the fundamental hypotheses contradict each other?

Is the linear quantum mechanics a dynamic or a statistical theory? Does it describe the motion of a single particle or a system of particles? The dynamic equation seems an equation for a single particle, but its mechanical quantities are determined based on the concepts of probability and statistical average. This caused confusion about the nature of the theory itself.

How to describe the wave-particle duality of microscopic particles? What is the nature of a particle defined based on the hypotheses of the linear quantum mechanics? The de Broglie relations established the wave-particle duality. Can statistical interpretation of wave function correctly describe such a property? There are also difficulties in using wave package to represent the particle nature of microscopic particles. Thus description of the wave-corpuscle duality was a major challenge linear quantum mechanics had to face.

Was the uncertainty principle due to intrinsic properties of microscopic particles or a result of uncontrollable interaction between the measuring instruments and the system being measured?

A particle appears in space in the form of a wave, and it has certain probability to be at a certain location. However, it is always a whole particle, rather than a fraction of it, being detected in a measurement. How can this be interpreted? Is the explanation of this problem based on wave package contraction in the measurement correct?

However, why does quantum mechanics have these questions? This is worth studying deeply and in detail. As is known, dynamic equation (1) describes the motion of a particle and Hamiltonian operator of the system, Eq.(2), consist only of kinetic and potential operator of particles; the potential is only determined by an externally applied field, and not related to the state or wavefunction of the particle, thus the potential can only change the states of MIP, and cannot change its nature and essence. Therefore, the natures and features of MIP are only determined by

the kinetic term. Thus there is no force or energy to obstruct and suppress the dispersing effect of kinetic energy in the system, then the MIP disperses and propagates in total space, and cannot be localized at all. This is the main reason why MIP has only wave feature in quantum mechanics. Meanwhile, the Hamiltonian in Eq.(2) does not represent practical essences and features of MIP. In real physics, the energy operator of the systems and number operator of particles are always associated with the states of particles, i.e., they are related to the wavefunction of MIP. On the other hand, Eq.(1) or (2) can describe only the states and feature of a single particle, and cannot describe the states of many particles. However, a system composed of one particle does not exist in nature. The simplest system in nature is the hydrogen atom, but it consists of two particles. In such a case, when we study the states of particles in realistic systems composed of many particles and many bodies using quantum mechanics, we have to use a simplified and uniform average- potential unassociated with the states of particles to replace the complicated and nonlinear interaction among these particles<sup>[10-11]</sup>. This means that the motions of the microscopic particles and background field as well as the interactions between them are completely freezed in such a case. Thus, these complicated effects and nonlinear interactions determining essences and natures of particles are ignored completely, to use only a simplified or average potential replaces these complicated and nonlinear interactions. This is obviously not reasonable. Thus nature of microscopic particles is determined by the kinetic energy term in Eq.(1). Therefore, the microscopic particles described by quantum mechanics possess only a wave feature, not corpuscle feature. This is just the essence of quantum mechanics. Then we can only say that quantum mechanics is an approximate and linear theory and cannot represent completely the properties of motion of MIPs. We here refer to it as linear quantum mechanics (LQM). Meanwhile, a lot of hypotheses or theorems of particles in quantum mechanics also do not agree with conventional understanding, and have excited a long-time debate between scientists. Up to now, there is no unified conclusion. Therefore, it is necessary to improve and develop LQM.

However, what is its direction of development? From the above studies we know that a key shortcoming or defect of LQM is its ignoring of dynamic states of other particles or background field, and the dependence of the Hamiltonian or energy operator of the systems on the states of particles and nonlinear interactions among these particles. As a matter of fact, the nonlinear interactions always exist in any realistic physics systems including the hydrogen atom, if only the real motions of the particles and background as well as their interactions are completely considered[17-30]. At the same time, it is also a reasonable assumption that the Hamiltonian or energy operator of the systems depend on the states of particles[17-30]. Hence, to establish a correct new quantum theory, we must break through the elementary hypotheses of LQM, and use the above reasonable assumptions to include the nonlinear interactions among the particles or between the particles and background field as well as the dependences of the Hamiltonian of the systems on the state of particles. Thus, we must establish nonlinear quantum mechanism (NLQM) to study the rules of motion of MIPs in realistic systems with nonlinear interactions by using the above new idea and method[18-25].

At present, to know the root problems generating the difficulties in quantum mechanics, it is very necessary to understand the basic tenets of the discipline. Obviously the roots relate closely to the fundamental postulates of the discipline [21-24]. From Eqs. (1.7) and (1.8) we see that the dynamic equation and Hamiltonian of the systems are composed of a kinetic energy term,  $(\hbar^2/2m)\nabla^2 = \hat{p}^2/2m$ , of particles, and an externally applied potential term,  $V(\vec{r})$ . As can be seen from the above analyses, the potential cannot change the nature of any of the particles, but only the shapes and outlines such as amplitude and velocity, and this is because it is not related to the wave function of the state of the particle. Too, the nature of particles is mainly determined by the kinetic energy term. But the latter has a dispersive effect and can make the particle dispersion in total system taking on the form of a wave. This means that there is not an interaction, which might balance and/or suppress the dispersive effect in the systems. Thus the microscopic particle have only a wave feature and cannot be localized in quantum mechanics. This is just one root generating the above difficulties in quantum mechanics. In this case we must incorporate all interactions, including nonlinear and complicated interactions; those among particles or between particles and the background field, into the external potential by means of various approximate methods, when quantum mechanics is applied to study motions of the microscopic particles [21-22]. This amounts to a freeze of the real motions of other particles and background fields as well as the interactions between them. According to basic theory, this is without reason. Therefore it is highly necessary to develop a new quantum mechanics theory that can truly describe and study the motion of the particles and background field as well as the interactions between them in these systems, especially in the examples of systems with many-particles and many-bodies.

How do we improve and develop the discipline of quantum mechanics? What is the direction of development? These problems are worth studying deeply. Looking back to the development and applications of quantum mechanics as well as the related disputes that have endured for almost a century, we see that it seems impossible to solve these problems and improve the theory within the framework of linear quantum mechanics. Therefore, to

further develop a new base theory we need to find alternatives beyond quantum mechanics. To do this, we must break through some fundamental postulates of the existing disciplinary base of quantum mechanics, such as the linearity of the theory and the independence of the Hamiltonian operator related to the system on the states of particles. The linearity of theory greatly limits the applicable scope and domain of the development of quantum mechanics and cannot be used to study the properties of the microscopic particles in the complex systems of many-body, many-particle examples in which there exist complicated interactions, such as the self-interaction and nonlinear interactions among particles and between particles and environment. The independence of the Hamiltonian operator on the states of particles erases the real relation of the energy of a system with the states of particles *and* blots out the nonlinear interactions among particles and between particles and background field. Therefore, these two postulates should be abandoned in the new theory. In other words, we must consider the *real* motions of all particles and the true interactions among particles and between particles and background field including the nonlinear interactions in the new theory. We expect that these nonlinear interactions among particles and between particles and background field can be involved in the Hamiltonian operator and dynamic equation to balance and suppresses the dispersive effect in systems and make eventually the particles the localization and wave-corpucle duality. The above is our concept of the direction and objective of development of quantum mechanics.

This paper is essentially composed of four parts. The first presents the fundamental principles of NLQM. The descriptions of essential features of microscopic particles, including the wave-particle duality of the solution of the nonlinear Schrödinger equation, the stability of microscopic particles described by NLQM, the invariances and conservation laws of motion of particles, the Hamiltonian principle of particle motion and corresponding Lagrangian and Hamilton equations, the classical rule of microscopic particle motion, the mechanism and rules of particle collision, the features of reflection and the transmission of particles at interfaces, and the uncertainty relation of particle's momentum and position, are covered in the second part. The resolution of difficulties and problems of quantum mechanics are stated in the third part, A conclusion of the investigation is finally given. These investigations are helpful for understanding the properties of MIPs in nonlinear systems and the essences of NLQM.

## 2. ESTABLISHMENT OF NONLINEAR QUANTUM MECHANICS

### 2.1 Basic principles of nonlinear quantum mechanics

Pang worked out the NLQM describing the properties of motion of MIPs in nonlinear systems [17-30]. The elementary principles, theory, calculated rules and applications of NLQM were described in Pang *et al.*'s books [25-27]. For the development of quantum mechanics from linear range to nonlinear domain in the basis of original quantum mechanics, Pang worked at and investigated this problem for about 20 years[17-30]. In this investigation, Pang first sought the roots of these problems existing in the LQM. Subsequently, Pang [23-30] broke through the restrictions of the elementary hypotheses for the independence of the Hamiltonian of the systems on the states of the particles and the linearity of the theory in the LQM, and proposed and established the elementary principles and theory of the NLQM, based on the relations among the nonlinear interaction and soliton motions and macroscopic quantum effect, and incorporating modern theories of superconductors, superfluids and solitons [23-27]. In these physical systems the Hamiltonian, free energy or Lagrangian functions of the systems are all nonlinear functions of the wave function of the microscopic particles which break down the hypotheses for the independence of the Hamiltonian of the systems on the states of the particles and the linearity of the theory in the LQM, the dynamic equations of microscopic particles, such as superconductive electrons and superfluid helium atoms which were depicted by a macroscopic wave function,

$$\phi(\vec{r}, t) = \varphi(\vec{r}, t)e^{i\theta(\vec{r}, t)},$$

are the time-independent and time-dependent Ginzburg-Landau equations,(G-L) and Gross- Pitaerskii (G-P) equation[31-36], which are in essece the nonlinear Schrödinger equation and have a soliton solution with a wave-corpucle duality because the nonlinear interactions balance and suppress the dispersive effect of the kinetic energy in these dynamic equations[23-27]. We demonstrated that the macroscopic quantum effects are in an ordered coherent state or a Bose-Einstein condensed state, the superconductivity and superfluidity are caused by motions of solitons of superconductive electrons and superfluid helium atoms under actions of nonlinear interactions, respectively. According to modern soliton theory, a soliton, which differs completely from a microscopic particle in the quantum mechanics, possesses the wave-particle duality. Therefore, the investigations of essences and properties of macroscopic quantum mechanics, superconductivity and superfluid provide direction and fundamental for establishing nonlinear quantum mechanics[23-27].

Based on the above discussions, the fundamental principles of nonlinear quantum mechanics (NLQM) proposed by Pang may be summarized as follows [18-30].

(1) Microscopic particles in a nonlinear quantum system are described by the following wave function,

$$\phi(\vec{r}, t) = \varphi(\vec{r}, t) e^{i\theta(\vec{r}, t)} \quad (4)$$

where both the amplitude  $\varphi(\vec{r}, t)$  and phase  $\theta(\vec{r}, t)$  of the wave function are functions of space and time, and satisfy different equation of motion.

(2) In the nonrelativistic case, the wave function  $\phi(\vec{r}, t)$  satisfies the generalized nonlinear Schrödinger equation (NLSE), i.e.,

$$i\hbar \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \phi \pm b |\phi|^2 \phi + V(\vec{r}, t) \phi + A(\phi), \quad (5)$$

or

$$\mu \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \phi \pm b |\phi|^2 \phi + V(\vec{r}, t) \phi + A(\phi) \quad (6)$$

where  $\mu$  is a complex number,  $V$  is an external potential field,  $A$  is a function of  $\phi(\vec{r}, t)$ , and  $b$  is a coefficient indicating the strength of nonlinear interaction.

In the relativistic case, the wave function  $\phi(\vec{r}, t)$  satisfies the nonlinear Klein-Gordon equation (NLKGE), including the generalized Sine-Gordon equation (SGE) and the  $\phi^4$ -field equation, i.e.,

$$\frac{\partial^2 \phi}{\partial t^2} - \frac{\partial^2 \phi}{\partial x_j^2} = \beta \sin \phi + \gamma \frac{\partial \phi}{\partial t} + A(\phi) \quad (j=1,2,3) \quad (7)$$

and

$$\frac{\partial^2 \phi}{\partial t^2} - \frac{\partial^2 \phi}{\partial x_j^2} \mp \alpha \phi \pm \beta |\phi|^2 \phi = A(\phi) \quad (j=1,2,3) \quad (8)$$

where  $\gamma$  represents a dissipative or frictional effects,  $\alpha$  is a constant,  $\beta$  is a coefficient indicating the strength of nonlinear interaction and  $A$  is a function of  $\phi(\vec{r}, t)$ .

These are the only two fundamental hypotheses of nonlinear quantum mechanics yet are quite different from linear quantum mechanics which is based on several hypotheses, as discussed above. However, the dynamic equations are just generalizations of the linear Schrödinger and linear Klein-Gordon equations in linear quantum mechanics to nonlinear quantum systems. These equations were also used to study the motion of superconducting electrons and helium atoms in the superfluid state.

It has been shown that Eqs. (5)–(8) indeed describe the law of motion and properties of microscopic particles in nonlinear quantum systems. This is the basis for having the two hypotheses as the principles of nonlinear quantum mechanics. Obviously, nonlinear quantum mechanics is an integration of superconductivity, superfluidity and modern soliton theories and its experimental foundation are the macroscopic quantum effects.

## II.2. The features of the fundamental Principles.

From the two above hypotheses, the following can be deduced.

(1). Equation (4) indicates the basic form of wave function of states of the microscopic particles, where  $\varphi(\vec{r}, t)$  is its amplitude and  $\theta(\vec{r}, t)$  is its phase, therefore, they all have a determinant physics significance and satisfy different dynamic equations. If by inserting Eq. (4) into Eq. (5) we can ascertain that they satisfy, in a one dimensional case, the following two equations

$$\frac{\partial^2 \varphi}{\partial x'^2} - \frac{\partial \theta}{\partial t'} \varphi - \left( \frac{\partial \theta}{\partial x'} \right)^2 \varphi + b \varphi^3 = V(x', t) \varphi \quad (9)$$

$$\varphi \frac{\partial^2 \theta}{\partial x'^2} + 2 \frac{\partial \varphi}{\partial x'} \frac{\partial \theta}{\partial x'} + \frac{\partial \varphi}{\partial t'} = 0 \quad (10)$$

respectively, where  $x' = x \sqrt{2m/\hbar}$ ,  $t' = t/\hbar$ .

From Eq. (10) we can easily find the relation of  $\theta(x', t')$  with  $\varphi(x', t')$ , then the solution,  $\varphi(x', t')$ , of Eq. (9) can also be found and, the  $b$  and  $V(x', t')$  known. In a bulk and uniform material,  $\theta(x', t')$  is a constant, then  $\theta(x', t')$  is independent with  $x'$  and  $t'$ , thus from Eq. (9) we can get

$$\frac{\partial^2 \phi}{\partial x'^2} + b\phi^3 - V(t')\phi = 0$$

It is a time-independent nonlinear Schrödinger equation and is same with time-independent G-L equation. This shows that the nonlinear Schrödinger equation in Eq. (5) depicting the states of microscopic particles has a good experimental foundation. This feature of wave function of the microscopic particles does not occur in quantum mechanics.

(2) We know from soliton theory that these equations in Eqs.(5)-(8) have all a soliton solution; therefore, the wave function  $\phi(\vec{r}, t)$  represents a soliton or a solitary wave. It is no longer a linear or dispersive wave in the linear quantum mechanics. This differs also from that in quantum mechanics.

(3) The absolute square of wave function  $\phi(\vec{r}, t)$  given in Eq.(4),  $|\phi(\vec{r}, t)|^2 = |\phi(\vec{r}, t)|^2 = \rho(\vec{r}, t)$  is no longer the probability of finding the microscopic particle at a given point in the space-time, but rather gives us the mass density of the microscopic particles at that point. Thus, the concept of probability or the statistical interpretation of wave function is no longer relevant in nonlinear quantum mechanics. The interpretation of Eq.(4) will be discussed in more detail in the following.

(4) The Lagrange density function, L, corresponding to Eq. (5) at  $A(\phi) = 0$  is given as follows:

$$L' = \frac{i\hbar}{2} (\phi^* \partial_t \phi - \phi \partial_t \phi^*) - \frac{\hbar^2}{2m} (\nabla \phi \cdot \nabla \phi^*) - V(x) \phi \phi^* + (b/2) (\phi \phi^*)^2 \quad (11)$$

where  $L' = L$ . The momentum density of the particle system is defined as  $P = \partial L / \partial \dot{\phi}$ . Thus, the Hamiltonian density, H, of the systems is as follows

$$H = \frac{i\hbar}{2} (\phi^* \partial_t \phi - \phi \partial_t \phi^*) - L = \frac{\hbar^2}{2m} (\nabla \phi \cdot \nabla \phi^*) + V(x) \phi \phi^* - (b/2) (\phi \phi^*)^2 \quad (12)$$

Equations.(11)-(12) clearly show that the Lagrange density function and Hamiltonian density of the systems are all related to the wave function of state of the particles and involve a nonlinear interaction,  $(b/2) (\phi \phi^*)^2$ .

The above, when compared to the linear quantum theory, thus shows that two major breakthroughs were made in the nonlinear quantum mechanics. One, the linearity of the dynamic equation and the other, the fundamental hypothesis of independence of the Hamiltonian operator on the wave function of the microscopic particles. In nonlinear quantum mechanics, the dynamic equations are nonlinear in the wave function,  $\phi(\vec{r}, t)$ , i.e., they are nonlinear partial differential equations. The Hamiltonian operators depend on the wave function  $\phi(\vec{r}, t)$ . In this respect, the nonlinear quantum mechanics is truly a breakthrough in the development of modern quantum theory. Then the natures of microscopic particles are simultaneously determined by the kinetic and nonlinear interaction terms in dynamic equations of nonlinear quantum mechanics. The balance each other between them results in the motion of soliton of microscopic particles, this means that the particles in nonlinear quantum mechanics have different properties from those in quantum mechanics, and no longer disperse and could may be localized.

(5) Obviously, the Lagrange density functions in Eq. (11) and the Hamiltonian density in Eq. (12) have space-time symmetry. That is, L and H remain unchanged under the transformations of  $t \rightarrow -t$  and  $\vec{r} \rightarrow -\vec{r}$  or  $x \rightarrow -x$ ,  $y \rightarrow -y$  and  $z \rightarrow -z$ . In the meanwhile, they also possess the  $U(1)$  symmetry, i.e., they are unchanged undergoing the transformations of

$$\phi(\vec{r}, t) \rightarrow \phi'(\vec{r}, t) = e^{-iQ_j \theta} \phi(\vec{r}, t)$$

due to the fact that the Hamiltonian density in Eq. (3.9) contains the product of the  $\phi_j(\vec{r}, t)$  and the invariance of charge of the system, i.e.,  $(Q_1 + Q_2 + \dots + Q_n) = 0$ , and the facts of  $\nabla\phi_j \rightarrow e^{-i\theta Q_j} \nabla\phi_j$  in this case, where  $Q_j$  is the charge of the particle,  $\theta$  is a phase independent of  $x$ .

(6) The concept of operator in linear quantum mechanics can still be used in nonlinear quantum mechanics. However, the majority of them are no longer linear operators, and thus certain properties of linear operators, such as the conjugate Hermitian of the momentum and the coordinate operators, are no longer required,  $i\hbar \frac{\partial}{\partial t}$  no longer corresponds to the energy operator. Instead, nonlinear operators are constructed and used in the nonlinear quantum mechanics. For example, Equation (5) may be written as

$$i\hbar \frac{\partial \phi}{\partial t} = \hat{H}(\phi)\phi \tag{13}$$

The Hamiltonian operator  $\hat{H}$  has a nonlinear dependence on  $\phi(\vec{r}, t)$  and is given by

$$\hat{H}(\phi) = -\frac{\hbar^2}{2m} \nabla^2 - b|\phi|^2 + V(\vec{r}, t) \tag{14}$$

for  $A(\phi) = 0$ .

In general, equations (5)–(6) in one-dimensional case can be expressed as

$$\phi_t = \frac{d\phi}{dt} = K(\phi) \quad , \quad \phi = \phi(x', t') \tag{15}$$

according to the Lax method[28], where  $K(\phi)$  is a nonlinear operator or hereditary operator. In a one-dimensional case, a new operator  $Q(\phi)$ , which is obtained from the generator of the translation group, can be used to produce the vectorial field  $K(\phi)$ , i.e.

$$K(\phi) = Q(\phi)\phi_x \tag{16}$$

and the operator,  $Q(\phi)$ , is called a nonlinear recursion operator. The nonlinear Schrödinger equation (5) at  $A(\phi) = 0$  and can be generalized as

$$Q(\phi) = -iD + 4i\phi D^{-1} \text{Re}(\bar{\phi}) \tag{17}$$

where the operator  $D$  denotes the derivative with respect to  $x$ , and

$$D^{-1}f(x') = \int_{-\infty}^{x'} f(\xi) d\xi$$

From the hereditary property of  $K(\phi)$ , we can obtain the following vector field

$$K_n(\phi) = Q(\phi)^n \phi_x, \quad n=0,1 \tag{18}$$

The equation of motion of the eigenvalue  $\lambda'$  of the recursion operator  $Q(\phi)$  may be expressed as

$$\lambda'_t = \partial \lambda' / \partial t' = K'(\phi)[\lambda'] \tag{19}$$

where  $K'(\phi)$  is the variational derivative with respect to  $\phi$  and is given by

$$K'(\phi)[\lambda'] = \left. \frac{\partial}{\partial \varepsilon} K(\phi + \varepsilon \lambda') \right|_{\varepsilon=0} \tag{20}$$

The equation describing the time variation of the recursion operator can be obtained via;

$$\frac{\partial}{\partial t'} Q(\phi) = K'(\phi)Q(\phi) - Q(\phi)K'(\phi) = [K'(\phi), Q(\phi)] \tag{21}$$

This equation is very similar to the Heisenberg matrix equation in quantum mechanics. However, both  $K'(\phi)$  and  $Q(\phi)$  here are nonlinear operators. Therefore, we may refer to Eq. (21) as the Heisenberg equation of nonlinear operator in nonlinear quantum mechanics.

(7) The theory of nonlinear quantum mechanics describes an integral system. For a general nonlinear equation given in Eq.(15), we know that  $K(\phi)$  is a nonlinear operator of  $\phi$ . According to the Lax method [28], if two linear operators  $\hat{L}$  and  $\hat{B}$  corresponding to Eq. (15), which depend on  $\phi$ , satisfy the following Lax operator equation

$$iL_{t'} = \hat{B}\hat{L} - \hat{L}\hat{B} = [\hat{B}, \hat{L}] \tag{22}$$

where  $t' = t/\hbar$  and  $\hat{B}$  is a self-adjoint operator, then the eigenvalue  $k$  and eigenfunction  $\Psi$  of the operator  $\hat{L}$  satisfy the equation:

$$\hat{L}\Psi = k\Psi \tag{23}$$

with

$$\Psi(x', t') = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix},$$

but  $\hat{B}$  satisfies the equation:

$$\hat{B}\Psi = i\Psi_{t'} \tag{24}$$

For the following nonlinear Schrödinger equation in Eq. (5) at  $V(\vec{r}, t) = A(\phi) = 0$

$$i\phi_{t'} + \phi_{x'x'} + b|\phi|^2\phi = 0 \tag{25}$$

where  $x' = x\sqrt{2m}/\hbar$ , from Zakharov and Shabat et al. [29-30] we see that the concrete representations of  $\hat{L}$  and  $\hat{B}$  for Eq. (25), which are as follows

$$\hat{L} = i \begin{pmatrix} 1+s & 0 \\ 0 & 1-s \end{pmatrix} \frac{\partial}{\partial x'} + \begin{pmatrix} 0 & \phi^* \\ \phi & 0 \end{pmatrix}, \hat{B} = -s \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \frac{\partial^2}{\partial x'^2} + \begin{pmatrix} |\phi|^2 & i\phi_x^* \\ -i\phi_x & -|\phi|^2 \end{pmatrix} \tag{26}$$

where  $s^2 = (1 - 2/b)$ ,  $\phi(\vec{r}, t)$  and satisfies Eq.(25). This is just the Lax form for the nonlinear Schrödinger equation (25) or Equation(5).

In general, many nonlinear dynamic equations can be written either in the Lax form, or in the Hamilton form of a compatibility condition for overdetermined linear spectral problems. In the former, the nonlinear dynamic equations with soliton solutions are often expressed as Eq. (15), corresponding the eigenvectors and eigenvalues of the linear operator  $\hat{L}$  and its time evolution are determined by Eqs. (23) and (24), respectively.

We now assume that the eigenfunction of the operator  $\hat{L}$  satisfies the equation :

$$i\Psi_{t'} = \hat{B}\Psi + f(\hat{L})\Psi \tag{27}$$

where the function  $f(\hat{L})$  may be chosen according to convenience. In this case we can write the over-determined system of linear matrix equations as

$$\Psi_{x'} = U(x', t', \alpha)\Psi, \Psi_{t'} = G(x', t', \alpha)\Psi \tag{28}$$

where  $U$  and  $G$  are  $2 \times 2$  matrices. The compatibility condition of this system is obtained by differentiating the first equation of Eq.(28) with respect to  $t'$  and the second one with respect to  $x'$  and then subtracting one from the other

$$U_{t'} - G_{x'} - [U, G] = 0,$$

or

$$U_{t'} - G_{x'} = [U, G] \tag{29}$$

We emphasize that the operators  $U$  and  $G$  depend, not only on  $t'$  and  $x'$ , but also on some parameters,  $\alpha$ , which are called spectral parameters. Then the condition in Eq.(29) must be satisfied by  $\alpha$ . In this case Makhankov et al [31-32] gave the representations of the operators  $U$  and  $G$  by

$$\begin{aligned}
 U &= -i\alpha \begin{pmatrix} (1+s)^{-1} & 0 \\ 0 & (1-s)^{-1} \end{pmatrix} + \begin{pmatrix} 0 & i(1+s)^{-1}\phi^* \\ i(1+s)^{-1}\phi & 0 \end{pmatrix}, \\
 \hat{B} &= -i\alpha^2 \begin{pmatrix} s(1+s)^{-2} & 0 \\ 0 & s(1-s)^{-2} \end{pmatrix} + \\
 & i2\alpha \begin{pmatrix} 0 & \frac{s\phi^*}{(1+s)(1-s^2)} \\ \frac{s\phi}{(1-s)(1-s^2)} & 0 \end{pmatrix} + \\
 & \begin{pmatrix} \frac{i(\phi\phi^*)}{1-s^2} & \frac{\phi_x}{1+s} \\ \frac{\phi_x}{1-s} & -\frac{i|\phi|^2}{1-s^2} \end{pmatrix}
 \end{aligned}$$

The presence of a continuous time-independent parameter is a reflection of the fact that the nonlinear Schrödinger equation (25) describes a Hamiltonian system with a set of infinite number of conservation laws. In the case of a system with a finite number ( $N'$ ) of degrees of freedom one can sometimes succeed in finding  $2N'$  first integrals of motion between which the Poisson brackets are zero (in this case they are said to be in involution). Such a system is called completely integral. In such a case, equation (28) with Eq.(29) are referred to as the compatibility condition, and their consequence is the nonlinear Schrödinger equation (25).

This means that, for each solution,  $\phi(x', t')$  of Eq.(25), there is always a set of basis function  $\Psi$ , parameterized by  $\alpha$ , which can be obtained through solving the set of linear equations (27) – (29). Thus we can conclude that the nonlinear quantum systems described by nonlinear quantum mechanics is completely integrable. Zakharov and Faddeev [33]

generalized this concept in quantum field theory.

(8) Vector nonlinear Schrödinger equations. When a system is composed of  $n$  same particles in same condition, among which there are nonlinear interactions, the system of particles can be described by a vectorial nonlinear Schrödinger equation [31-32], which can often be written as

$$i\hbar \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \phi - b(\bar{\phi}\phi)\phi + V(\vec{r}, t)\phi \tag{30}$$

where

$$\phi = \begin{pmatrix} \phi^{(1)} \\ \cdot \\ \cdot \\ \phi^{(n)} \end{pmatrix},$$

$\phi$  is a column vector of  $n$ -components, describing the “isospace” state,  $\bar{\phi}$  is its complex conjugate vector. The corresponding Lagrangian and Hamiltonian densities of the system are given by

$$L' = \frac{i\hbar}{2} (\bar{\phi}\phi_t - \phi\bar{\phi}_t) -$$

$$\frac{\hbar^2}{2m} (\phi_x \cdot \bar{\phi}_x) - V(x)\phi\bar{\phi} + (b/2)(\phi\bar{\phi})^2$$

and

$$H' = -\frac{\hbar^2}{2m} (\phi_x \cdot \bar{\phi}_x) + V(x)\phi\bar{\phi} - (b/2)(\phi\bar{\phi})^2$$

where  $L'=L$  and  $H'=H$ ,  $\bar{\phi} = \phi^* \gamma_0$  and  $\gamma_0$  is a diagonal matrix, and the internal product  $(\bar{\phi}\phi) = \phi^\dagger \gamma_0 \phi$  is conserved. Such transformations also conserve  $L$  and  $H$ . That is, they are symmetrical transformations of the systems which do not change the vector nonlinear Schrödinger equation (30). When  $\gamma_0$  is also an  $n$ -component unit matrix, the transformations form a compact group  $U'(n)$ . On the other hand, if

$$\gamma_0 = \text{diag.}(1, 1 \dots 1, -1, -1 \dots -1),$$

which plays the role of isotropic space metric and the dagger sign ( $\dagger$ ) denotes a Hermitian conjugate, the iso-transformation belongs to the non-compact group  $U(i, j)$ , here “ $i$ ” is the number of “ $1$ ”,  $j$  is the number of “ $-1$ ” in  $\gamma_0$ . Zakharov and Shabat [29-30] showed that Eq. (30) is completely integrable in the case of  $U(1)$  group for both positive ( $b > 0$ ) (the  $U(1, 0)$  model) and negative ( $b < 0$ ) (the  $U(0, 1)$  model) coupling constants. Furthermore, Manakov [34] integrated the vector equation (30) for the  $U(2)$  group (the  $U(2, 0)$  model,  $b > 0$ ), and the integrability for the case of  $U(1, 1)$  group was shown by Makhankov [31]. These can be considered as special cases of the general system.

Based on the elementary principle Pang[23-27] established the theory of nonlinear quantum mechanics, which includes the superposition theorem of states of the particles, relation of nonlinear Fourier transformation, nonlinear perturbation theory, theory of nonlinear quantization, eigenvalue theory of nonlinear Schrödinger equation, calculated method of eigenenergy of Hamiltonian operator and relativistic theory of nonlinear quantum mechanics, collision and scattering theory of microscopic particles, and so on (please read Pang’s book[25-27]). Thus a complete nonlinear quantum mechanics was established. Then we can investigate the rules and properties of motion of microscopic particles in any physical systems using these principle and theories of nonlinear quantum mechanics. In the following we will discuss the natures and properties of microscopic particles described by nonlinear quantum mechanics.

### 3. THE WAVE-CORPUSCLE FEATURES OF MICROSCOPIC PARTICLES

#### 3.1 The wave-corpucle duality of solutions of dynamic equation

As it is known, the microscopic particles have only the wave feature, but not corpucle property in the quantum mechanics. Thus, it is very interesting what are the properties of the microscopic particles in the nonlinear quantum mechanics? We now study firstly the properties of the microscopic particles described by nonlinear Schrödinger equation in Eq. (5). In the one-dimensional case, the equation (5) at  $V(x,t) = A(\phi) = 0$  becomes as

$$i\phi_{t'} + \phi_{x'x'} + b|\phi|^2 \phi = 0 \tag{31}$$

where  $x' = x / \sqrt{\hbar^2 / 2m}$ ,  $t' = t / \hbar$ . We now assume the solution of Eq.(31) to be of the form

$$\phi(x', t') = \varphi(x', t') e^{i\theta(x', t')} \tag{32}$$

substituting Eq. (32) into Eq. (31) we get

$$\varphi_{x'x'} - \varphi\theta_{t'} - \varphi\theta_{x'}^2 - b\varphi^2\varphi = 0, (b > 0) \tag{33}$$

$$\varphi\theta_{x'x'} + 2\varphi_{x'}\theta_{x'} + \varphi_{t'} = 0 \tag{34}$$

If let

$$\theta = \theta(x' - v_e t'), \varphi = \varphi(x' - v_e t'),$$

$$\zeta = x' - v_e t', \zeta' = x' - v_e t',$$

then Equations (33) - (34) become

$$\varphi_{\zeta'\zeta'} + v_e \varphi\theta_{\zeta'} - \varphi\theta_{\zeta'}^2 - b\varphi^3 = 0 \tag{35}$$

$$\varphi\theta_{\zeta'\zeta'} + 2\varphi_{\zeta'}\theta_{\zeta'} - v_e \varphi_{\zeta'} = 0 \tag{36}$$

If fixing the time  $t'$  and further integrating Eq. (36) with respect to  $x'$  we can get

$$\varphi^2(2\theta_{\zeta'} - v_e) = A(t') \tag{37}$$

Now let integral constant  $A(t') = 0$ , then we can get  $\theta_{\zeta'} = v_e / 2$ . Again substituting it into Eq. (35), and further integrating this equation we obtain

$$\int_{\varphi_0}^{\varphi} \frac{d\varphi}{\sqrt{Q(\varphi)}} = x' - v_e t' \tag{38}$$

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

When  $c'=0$ ,  $v_e^2 - 2v_e v_c > 0$ , then  $\varphi = \pm\varphi_0$ ,  $\varphi_0 = [(v_e^2 - 2v_e v_c) / 2b]$  is the roots of  $Q(\varphi) = 0$  except for  $\varphi = 0$ . From Eq. (38) Pang obtained the solution of Eqs. (33)-(34) to be

$$\varphi(x', t') = \varphi_0 \operatorname{sech} h \left[ \sqrt{\frac{b}{2}} \varphi_0 (x' - v_e t') \right].$$

Pang<sup>[18,23-27]</sup> represented eventually the solution of nonlinear Schrödinger equation in Eq. (11) in the coordinate of (x,t) by

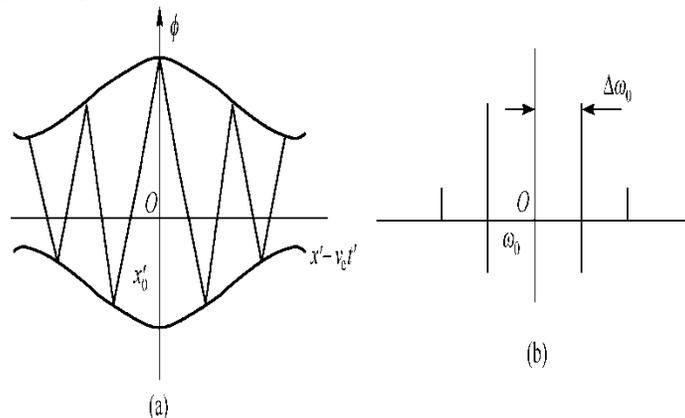
$$\phi(x, t) = A_0 \operatorname{sech} h \left\{ \frac{A_0 \sqrt{bm}}{\hbar} [(x - x_0) - vt] \right\} e^{i[mv(x-x_0) - Et]/\hbar} \tag{39}$$

where  $A_0 = \sqrt{(mv^2 / 2 - E) / 2b}$ ,  $v$  is the velocity of motion of the particle,  $E = \hbar\omega$ . This solution is completely different from Eq. (3), and consists of an envelop and carrier waves, the former is

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

and a bell-type non-topological soliton with an amplitude  $A_0$ , the latter is  $\exp\{i[mv(x - x_0) - Et] / \hbar\}$ . This solution is shown in Fig.1a. Therefore, the particles described by nonlinear Schrödinger equation (31) are solitons. The envelop  $\varphi(x, t)$  is a slow varying function and is a mass centre of the particles; the position of the mass centre is just at  $x_0$ ,  $A_0$  is its amplitude, and its width is given by  $W' = 2\pi\hbar / A_0\sqrt{2m}$ . Thus, the size of the particle is

$A_0 W' = 2\pi\hbar / \sqrt{2m}$  and a constant. This shows that the particle has exactly a determinant size and is localized at  $x_0$ . Its form resemble a wave packet, but differ in essence from both the wave solution in Eq. (1) and the wave packet mentioned above in linear quantum mechanics due to invariance of form and size in its propagation process. According to the soliton theory [37-38], the bell-type soliton in Eq. (39) can move freely over macroscopic distances in a uniform velocity  $v$  in space-time retaining its form, energy, momentum and other quasi-particle properties. However, the wave packet in linear quantum mechanics is not so and will be decaying and dispersing with increasing time. Just so, the vector  $\vec{r}$  or  $x$  in the representation in Eq.(39) has definitively a physical significance, and denotes exactly the positions of the particles at time  $t$ . Thus, the wave- function  $\phi(\vec{r}, t)$  or  $\varphi(x, t)$  can represent exactly the states of



**Fig.1.** The solution of Eq. (31) and its features.

the particle at the position  $\vec{r}$  or  $x$  at time  $t$ . These features are consistent with the concept of particles. Thus the microscopic particles depicted by Eq. (31) display outright a corpuscle feature.

Using the inverse scattering method Zakharov and Shabat[39-40] obtained also the solution of Eq. (31), which was represented as

$$\begin{aligned} \varphi(x', t') = & 2 \left( \frac{2}{b} \right)^{1/2} \eta \operatorname{sech} [2\eta(x' - x'_0) + 8\eta\xi t'] \times \\ & \exp \left[ -4i(\xi^2 - \eta^2)t' - i2\xi x' - i\theta \right] \end{aligned} \quad (40)$$

in the coordinate of  $(x', t')$ , where  $\eta$  is related to the amplitude of the microscopic particle,  $\xi$  relates to the velocity of the particle,

$$\theta = \arg \gamma, \lambda = \xi + i\eta, x'_0 = (2\eta)^{-1} \log \left( \frac{|\gamma|}{2\eta} \right),$$

$\gamma$  is a constant.. We now re-write it as following form<sup>[23-27]</sup>:

$$\phi(x', t') = 2\sqrt{\frac{2}{b}} k \operatorname{sech} \left\{ 2k \left[ (x' - x'_0) - v_e t' \right] \right\} e^{i v_e [(x' - x'_0) - v_e t'] / 2} \quad (41)$$

where  $v_e$  is the group velocity of the electron,  $v_c$  is the phase speed of the carrier wave in the coordinate of  $(x', t')$ . For a certain system,  $v_e$  and  $v_c$  are determinant and do not change with time. We can obtain

$$2^{3/2} k / b^{1/2} = A_0, \quad A_0 = \sqrt{\frac{v_e^2 - 2v_c v_e}{2b}}.$$

According to the soliton theory, the soliton shown in Eq. (41) has determinant mass, momentum and energy, which can be represented by<sup>[23-27]</sup>

$$\begin{aligned} N_s = \int_{-\infty}^{\infty} |\phi|^2 dx' = 2\sqrt{2} A_0, \quad p = -i \int_{-\infty}^{\infty} (\phi^* \phi_{x'} - \phi \phi_{x'}^*) dx' = 2\sqrt{2} A_0 v_e = N_s v_e = \text{const}, \\ E = \int_{-\infty}^{\infty} \left[ |\phi_{x'}|^2 - \frac{1}{2} |\phi|^4 \right] dx' = E_0 + \frac{1}{2} M_{sol} v_e^2 \end{aligned} \quad (42)$$

where  $M_{sol} = N_s = 2\sqrt{2} A_0$  is the effective mass density of the particles, which is a constant. Thus we can confirm that the energy, mass and momentum of the particle cannot be dispersed in its motion, which embodies concretely the corpuscle features of the microscopic particles. This is completely consistent with the concept of classical particles. This means that the nonlinear interaction,  $b|\phi|^2 \phi$ , related to the wave function of the particles, balances and suppresses really the dispersion effect of the kinetic term in Eq. (31) to make the particles become eventually localized. Thus the position of the particles,  $\vec{r}$  or  $x$ , has a determinately physical significance. However, the envelope of the solution in Eqs. (39)- (41) 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. Its feature of propagation depends on the concrete nature of the particles. Figure 1(b) shows the width of the frequency spectrum of the envelope  $\varphi(x, t)$  which has a localized distribution around the carrier frequency  $\omega_0$ . This shows that the particle has also a wave feature<sup>[23-27]</sup>. Thus we believe that the microscopic particles described by nonlinear quantum mechanics have simultaneously a wave-corpuscle duality. Equations (39) - (41) and Figure 1.a are just the most beautiful and perfect representation of this property, which consists also of de Broglie relation,  $E = \hbar\omega$  and  $\vec{p} = \hbar\vec{k}$ , wave-corpuscle duality and Davisson and Germer's experimental result of electron diffraction on double seam in 1927 as well as the traditional concept of particles in physics [11-13]. Thus we have reasons to believe the correctness of nonlinear quantum mechanics proposed by Pang.<sup>[23-27]</sup>

### III.2. The feature of Newton's motion of microscopic particles

Since the microscopic particle described by the nonlinear Schrödinger equation (5) at  $A(\phi) = 0$  has a corpuscle feature and is also quite stable as mentioned above. Thus its motion in action of a potential field in space-time should have itself rules of motion. Pang<sup>[41-43]</sup> studied deeply this rule of motion of microscopic particles in such a case.

Let now  $\phi(x, t)$  represent the field of the particle, and assume that it has derivatives of all orders, and all integrations, and is convergent and finite. The Lagrange and Hamiltonian density function corresponding to the nonlinear Schrödinger equation (5) at  $A(\phi) = 0$  are represented by Eqs. (11) and (12), respectively, which involve all the nonlinear interactional energy,  $b(\phi\phi^*)^2$ , which can obstruct and suppress the dispersive effect of kinetic

energy of microscopic particles. In the general case, the total energy of the particles is a function of  $t'$  and is represented by

$$E(t') = \int_{-\infty}^{\infty} \left[ \left| \frac{\partial \phi}{\partial x'} \right|^2 - \frac{b}{2} |\phi \phi^*|^2 + V(x') |\phi|^2 \right] dx' \tag{43}$$

However, in this case,  $b$  and  $V(x')$  are not functions of  $t'$ . So, the total energy of the systems is a conservative quantity, i.e.,  $E(t') = E = \text{const.}$ . We can demonstrate<sup>[46-47]</sup> that when  $x' \rightarrow \pm\infty$ , the solutions of Eq. (5) at  $A(\phi) = 0$  and  $\phi(x', t')$  should tend to zero rapidly, i.e.,

$$\lim_{|x'| \rightarrow \infty} \phi(x', t') = \lim_{|x'| \rightarrow \infty} \frac{\partial \phi}{\partial x'} = 0$$

Then

$$\int_{-\infty}^{\infty} \phi^* \phi dx' = \int_{-\infty}^{\infty} \rho(x') dx' = \text{constant, or}$$

$$\frac{\partial}{\partial t'} \int_{-\infty}^{\infty} \phi^* \phi dx' = 0$$

which is the mass conservation of the microscopic particle. Therefore,  $\phi^* \phi dx' = \rho(x') dx'$  can be regarded as the mass in the interval of  $x'$  to  $x'+dx'$ . Thus the position of mass centre of a microscopic particle at  $x'_0 + v_g t'$  in nonlinear quantum mechanics can be represented by

$$\langle x' \rangle = x'_g = x_0 = \frac{\int_{-\infty}^{\infty} \phi^* x' \phi dx'}{\int_{-\infty}^{\infty} \phi^* \phi dx'} \tag{44}$$

since

$$v = v_g = \frac{d}{dt'} \left\{ \frac{\int_{-\infty}^{\infty} \phi^* x' \phi dx'}{\int_{-\infty}^{\infty} \phi^* \phi dx'} \right\} =$$

$$\frac{\int_{-\infty}^{\infty} (\phi_t^* x' \phi + \phi^* x' \phi_t) dx'}{\int_{-\infty}^{\infty} \phi^* \phi dx'}$$

then from Eq. (31) and its conjugate equation we can get that the velocity of mass centre of microscopic particle can be denoted by

$$v_g = d \langle x' \rangle / dt' = -2i \frac{\int_{-\infty}^{\infty} \phi^* \phi_x dx'}{\int_{-\infty}^{\infty} \phi^* \phi dx'} \tag{46}$$

Otherwise, we know that the solution Eq. (41), shown in Fig.1, of the nonlinear Schrödinger equation (5) with different potentials at  $A(\phi) = 0$ , has the behavior of  $\frac{\partial \phi}{\partial x'} = 0$  at  $x' = x'_0$ . Thus we can infer that the position of

the soliton is localized at  $x' = x'_0$  at  $t'=0$ , which is just the position of the mass center of microscopic particle, and is defined by Eq. (44). Its velocity is represented in Eq. (45). We now determine the acceleration of the mass center of the microscopic particles and its rules of motion in an externally applied potential.

Now utilizing Eq. (5) at  $A(\phi) = 0$  and its conjugate equation as follows

$$-i\hbar \frac{\partial \phi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \phi^* \pm b |\phi|^2 \phi^* + V(\vec{r}, t) \phi^* \tag{47}$$

we can obtain

$$\frac{d}{dt'} \int_{-\infty}^{\infty} \phi^* \phi_x dx' = \int_{-\infty}^{\infty} \phi_t^* \phi_x dx' + \int_{-\infty}^{\infty} \phi^* (\phi_t)_x dx'$$

$$= i \int_{-\infty}^{\infty} \left\{ \phi^* \frac{\partial}{\partial x'} [\phi_{xx'} + b \phi^* \phi^2 - V \phi] - V \phi^* \phi_x \right\} dx' \tag{48}$$

$$= i \int_{-\infty}^{\infty} \phi^* \frac{\partial V}{\partial x'} \phi dx'$$

where  $x' = x / \sqrt{\hbar^2 / 2m}$ ,  $t' = t / \hbar$ . We here utilize the following relations and the boundary conditions:

$$\int_{-\infty}^{\infty} (\phi^* \phi_{x'x'} - \phi_{x'x'}^* \phi) dx' = 0, \int_{-\infty}^{\infty} b(\phi^{*2} \phi \phi_x + \phi^* \phi^2 \phi_x^*) dx' = 0 \quad \int \phi^* \phi dx' = \text{constant (or a function of } t') \text{ and}$$

$$\lim_{|x'| \rightarrow \infty} \phi^* x' \frac{\partial \phi}{\partial x'} = \lim_{|x'| \rightarrow \infty} \frac{\partial \phi^*}{\partial x'} x' \phi = 0,$$

$$\lim_{|x'| \rightarrow \infty} \phi(x', t') = \lim_{|x'| \rightarrow \infty} \phi_{x'}(x', t') = 0$$

where  $\phi_x = \frac{\partial \phi}{\partial x}$ ,  $\phi_{x'x'x'} = \frac{\partial^3 \phi}{\partial x'^3}$ . Thus, we can get

$$\frac{d}{dt} \int_{-\infty}^{\infty} \phi^* x' \phi dx' = \int_{-\infty}^{\infty} \left( \frac{\partial \phi^*}{\partial t'} x' \phi + \phi^* x' \left( \frac{\partial \phi}{\partial t'} \right) \right) dx' = -2i \int_{-\infty}^{\infty} \phi^* \phi_x dx' \tag{49}$$

In the systems, the position of mass centre of microscopic particle can be represented by Eq. (44), thus the velocity of mass centre of microscopic particle is represented by Eq. (45). Then, the acceleration of mass centre of microscopic particle can also be denoted by

$$\begin{aligned} \frac{d^2}{dt^2} \langle x' \rangle &= -2i \frac{d}{dt} \left\{ \int_{-\infty}^{\infty} \phi^* \phi_x dx' / \int_{-\infty}^{\infty} \phi^* \phi dx' \right\} \\ &= -2 \int_{-\infty}^{\infty} \phi^* V_x \phi dx' = -2 \left\langle \frac{\partial V}{\partial x'} \right\rangle \end{aligned} \tag{50}$$

If  $\phi$  is normalized, i.e.,  $\int_{-\infty}^{\infty} \phi^* \phi dx' = 1$ , then the above conclusions also are not changed.

where  $V=V(x')$  in Eq. (50) is the external potential field experienced by the microscopic particles. We expand  $\frac{\partial V}{\partial x'}$

at the mass centre  $x' = \langle x' \rangle = x'_0$  as

$$\begin{aligned} \frac{\partial V(x')}{\partial x'} &= \frac{\partial \langle V(x') \rangle}{\partial \langle x' \rangle} + (x' - \langle x' \rangle) \frac{\partial^2 V(\langle x' \rangle)}{\partial \langle x' \rangle^2} + \\ &\quad \frac{1}{2!} (x' - \langle x' \rangle)^2 \frac{\partial^3 V(\langle x' \rangle)}{\partial \langle x' \rangle^3} + \dots \end{aligned}$$

Taking the expectation value on the above equation, we can get

$$\left\langle \frac{\partial V(x')}{\partial x'} \right\rangle = \frac{\partial V(\langle x' \rangle)}{\partial \langle x' \rangle} + \frac{1}{2!} \langle (x' - \langle x' \rangle)^2 \rangle \frac{\partial^3 V(\langle x' \rangle)}{\partial \langle x' \rangle^3}$$

where

$$\begin{aligned} \Delta_{ij} &= \langle ((x' - \langle x' \rangle)^2) \rangle = \langle (x'_i - x'_0)(x'_j - x'_0) \rangle = \\ &\quad \langle (x'_i - \langle x'_i \rangle)(x'_j - \langle x'_j \rangle) \rangle \end{aligned}$$

For the microscopic particle described by Eq. (5) at  $A(\phi) = 0$  or Eq. (31), the position of the mass center of the particle is known and determinant, which is just  $\langle x' \rangle = x'_0 = \text{constant}$ , or 0. Since we here study only the rule of motion of the mass centre  $x_0$ , which means that the terms containing  $x'_0$  in  $\langle x'^2 \rangle$  are considered and included, then

$\langle (x' - \langle x' \rangle)^2 \rangle = 0$  can be obtained. Thus

$$\left\langle \frac{\partial V(x')}{\partial x'} \right\rangle = \frac{\partial V(\langle x' \rangle)}{\partial \langle x' \rangle}$$

Pang[20-21] finally obtained the acceleration of mass center of microscopic particle in the nonlinear quantum mechanics, Eq. (49), which is denoted as

$$\frac{d^2}{dt'^2} \langle x' \rangle = -2 \frac{\partial V(\langle x' \rangle)}{\partial \langle x' \rangle} \quad (51)$$

Returning to the original variables, the equation (51) becomes

$$m \frac{d^2 x_0}{dt^2} = - \frac{\partial V}{\partial x_0} \quad (51)$$

where  $x'_0 = \langle x' \rangle$  is the position of the mass centre of microscopic particle. Equation (51) is the equation of motion of mass center of the microscopic particles in the nonlinear quantum mechanics. It resembles quite the Newton-type equation of motion of classical particles, which is a fundamental dynamics equation in classical physics. Thus it is not difficult to conclude that the microscopic particles depicted by the nonlinear quantum mechanics have a property of the classical particle.

### III.3. The properties of solution of nonlinear Schrödinger equation under influence of weak potential energy

We now find the properties of solution of nonlinear Schrödinger equation (5) at  $A(\phi) = 0$  and small  $V(x')$  by the linear perturbed theory. In such a case Pang [23-27] introduced a small parameter  $\varepsilon$  to denote the small external perturbation potential  $V(x)$ . Thus equation (5) with  $A(\phi) = 0$  can now be written as:

$$i \frac{\partial \phi}{\partial t'} + \frac{\partial^2 \phi}{\partial x'^2} + b |\phi|^2 \phi = \varepsilon V(x') \phi, \quad (52)$$

where  $t' = t/\hbar$ ,  $x' = \sqrt{2m/\hbar^2} x$ . Pang [44-48] assumed the following form for the linear perturbed solution of Eq. (52)

$$\phi = \phi_0 + \phi_1 = (f + \varepsilon F(x)) e^{i\theta(x', t')} \quad (53)$$

where  $\phi_0 = f(x', t') e^{i\theta(x', t')}$  which is an unperturbed solution of Eq. (52) with  $\varepsilon = 0$ . This is the same as Eq.(40), where  $2\eta$  and  $4\xi'$  are respectively the amplitude and group velocity of the microscopic particle. Inserting Eq. (53) into Eq. (52) and neglecting terms higher than the second order in  $\varepsilon$ , we obtain the following equation for  $F(x', t')$ :

$$i \frac{\partial F}{\partial t'} + \frac{\partial^2 F}{\partial X'^2} - v^2 [1 - 4 \operatorname{sech}^2(vX')] F + 2v^2 \operatorname{sech}^2(vX') F^* = v \sqrt{\frac{2}{b}} \operatorname{sech}(vX') V(X' + v_e t') \quad (54)$$

where

$$X' = x' - v_e t', v^2 = (v_e^2 - 2v_e v_e) / 4 = (v_e / 2)^2 \delta, \delta = 1 - 2v_e / v_e \quad (55)$$

Performing the transformation  $y = vX'$  and  $v^2 t' = \tau$ , we let

$$F(y, \tau) = F_1(y, \tau) + iF_2(y, \tau) \quad (56)$$

and by inserting it into Eq. (3.90) we can get

$$\frac{\partial F_1}{\partial \tau} + \frac{\partial^2 F_2}{\partial y^2} - (1 - 2 \operatorname{sech}^2 y) F_2 = 0 \quad (57)$$

$$\frac{\partial F_2}{\partial \tau} + \frac{\partial^2 F_1}{\partial y^2} = (1 - b \operatorname{sech}^2 y) F_1 = \frac{1}{v} \sqrt{\frac{2}{b}} \operatorname{sech} y V(y, \tau) \quad (58)$$

Differentiating Eqs.(57)-(58) with respect to  $\tau$  results in the following equation:

$$\frac{\partial^2 F_2}{\partial \tau^2} + \hat{M}_2 F_2 = A_2(y, \tau), \quad \frac{\partial^2 F_1}{\partial \tau^2} + \hat{M}_1 F_1 = A_1(y, \tau)$$

with

$$A_2 = -\frac{v^2}{v_e^2} \sqrt{\frac{2}{b}} \sec hy \frac{\partial v}{\partial y}$$

$$A_1 = -\frac{1}{v} \sqrt{\frac{2}{b}} \left( 2 \sec hy \tan y \frac{\partial V}{\partial y} - \sec hy \frac{\partial^2 V}{\partial y^2} \right)$$

$$\hat{M}_1 = \frac{d^4}{dy^4} - 2(1 - 4 \sec h^2 y) \frac{d^2}{dy^2} - 24 \sec h^2 y \tanh y \frac{d}{dy} + (1 + 16 \sec h^2 y - 24 \sec h^4 y)$$

$$\hat{M}_2 = \frac{d^4}{dy^4} - 2(1 - 4 \sec h^2 y) \frac{d^2}{dy^2} - 8 \sec h^2 y \tanh y \frac{d}{dy} + 1$$

Clearly,  $A_2$  possesses the properties of a force. The operator  $\hat{M}_1$  and  $\hat{M}_2$  satisfy the following eigenequations:

$$\hat{M}_2 g_2(vX') = \left(\frac{\omega}{v^2}\right)^2 g_2(vX') \tag{59}$$

$$\hat{M}_1 g_1(vX') = \left(\frac{\omega}{v^2}\right)^2 g_1(vX') \tag{60}$$

We can easily show that  $\hat{M}_1$  and  $\hat{M}_2$  are not Hermitian operators, but are Hermite conjugates to each other, i.e.,  $\hat{M}_1^+ = \hat{M}_2$ , and  $\hat{M}_2^+ = \hat{M}_1$ . Their eigenfunctions are also orthogonal to each other, i.e.

$$\int g_2^*(X', \omega) g_1(X', \omega') dX' = \delta(\omega - \omega').$$

The eigenfunctions belong to the eigenvalues  $\omega = \pm(vk^2 + v^2)$  and  $\omega = 0$  in Eqs. (59)-(60) can be obtained easily,  $k$  taking any value,  $-\infty < k < \infty$ , when  $\omega = 0$ . The eigenfunctions are:

$$g_1(x') = c_1 \sec h(vX') \tanh(vX'),$$

$$g_2(x') = c_2 \sec h(vX'). \tag{61}$$

where  $c_1 = c_2 = \sqrt{2v}$ .

Pang showed that Eq. (61) provides only *some* local solutions to Eqs. (57) - (60) when  $\omega = 0$ .

We now seek a power-series solution for  $\hat{M}_2$ . Pang considers first the asymptotic behavior of  $\hat{M}_2$  when  $y \rightarrow \infty$ , i.e.,

$$\hat{M}_2 \xrightarrow{y \rightarrow \infty} \frac{d^4}{dy^4} - 2 \frac{d^2}{dy^2} + 1.$$

The characteristic equation of  $\hat{M}_2$  is

$$-\frac{\omega^4}{v^4} + k^4 + 2k^2 + 1 = 0,$$

or

$$\omega^2 = (v^2 k^2 + v^2)^2.$$

We assume the following trial solution to it

$$g_2(y, k) = h_a \cos(ky) + h_b \sin(ky). \tag{62}$$

Substituting Eq. (62) into Eq. (60), and using the fact that  $\cos(ky)$  and  $\sin(ky)$  are linearly independent, we obtain:

$$\begin{aligned} & \frac{d^4 h_a}{dy^4} - [6k^2 + 2(1 - 4 \sec h^2 y)] \frac{d^2 h_a}{dy^2} - \\ & 8 \sec h^2 y \tanh y \frac{dh_a}{dy} - 8k^2 \sec h^2 y h_a \\ & + 4k \left[ \frac{d^3 h_b}{dy^3} - (k^2 + 1 - 4 \sec h^2 y) \frac{dh_b}{dy} - 2 \sec h^2 y \tanh y h_b \right] = 0, \end{aligned}$$

and

$$\begin{aligned} & \frac{d^4 h_b}{dy^4} - [6k^2 + 2(1 - 4 \sec h^2 y)] \frac{d^2 h_b}{dy^2} - \\ & 8 \sec h^2 y \tanh y \frac{dh_b}{dy} - 8k^2 \sec h^2 y h_b \\ & - 4k \left[ \frac{d^3 h_a}{dy^3} - (k^2 + 1 - 4 \sec h^2 y) \frac{dh_a}{dy} - 2 \sec h^2 y \tanh y h_a \right] = 0. \end{aligned}$$

A further transformation,  $z = \tan y$ , was made by Pang. Under this transformation, equation (60) becomes

$$\begin{pmatrix} N_1 & N_2 \\ -N_2 & N_1 \end{pmatrix} \begin{pmatrix} h_a \\ h_b \end{pmatrix} = 0, \tag{63}$$

where

$$\begin{aligned} N_1 &= (1 - z^2)^3 \frac{d^4}{dz^4} - 12z(1 - z^2) \frac{d^3}{dz^3} - \\ & 2(1 - z^2)(3k^2 + 1 - 14z^2) \frac{d^2}{dz^2} - 4z(3k^2 - 1) \frac{d}{dz} - 8k^2. \end{aligned} \quad N_2 = 4k \left[ (1 - z^2)^2 \frac{d^3}{dz^3} - 6z(1 - z^2) \frac{d^2}{dz^2} - (k^2 - 1 - 2z^2) \frac{d}{dz} - 2z \right].$$

with the following unitary transformation

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}, \quad S^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix},$$

equation (63) becomes

$$\begin{pmatrix} N_1 - iN_2 & 0 \\ 0 & N_1 + iN_2 \end{pmatrix} \begin{pmatrix} h_a + ih_b \\ i(h_a - ih_b) \end{pmatrix} = 0. \tag{64}$$

Equation (64) is equivalent to two equations. Their solutions can be assumed to take the form:

$$h_a = z^p \sum_{n=0}^{\infty} c_n z^n, \quad h_b = z^r \sum_{m=0}^{\infty} b_m z^m. \tag{65}$$

The solution of Eq. (64) can be obtained by substituting Eq. (65) into it. Since we desire a finite solution in the complete range of interest, the series in Eq. (65) must be truncated. It can be shown that this truncation is only a kind of case. Besides a constant coefficient, in such a case, it has a group of solutions taking the following form:

$$h_a(z) = (k^2 - 1) + 2kz,$$

$$h_b(z) = (k^2 - 1) - 2kz$$

The solutions  $g_1$  and  $g_2$  can be then be expressed as

$$g_1(x') = c_1 \operatorname{sech}(vX') \tanh(vX'), \quad g_2(x') = c_2 \operatorname{sech}(vX'),$$

when  $\omega = 0$ , and

$$\left. \begin{aligned} g_1(X', k) &= \frac{1}{k^2 + 1} \sqrt{\frac{v}{2\pi}} \left\{ \begin{aligned} & \left[ k^2 - 1 + 2k \tanh(vX') + 2 \operatorname{sech}^2(vX') \right] \cos(kvX') + \\ & \left[ k^2 - 1 + 2k \tanh(vX') + 2 \operatorname{sech}^2(vX') \right] \sin(kvX') \end{aligned} \right\} \\ g_2(X', k) &= \frac{1}{k^2 + 1} \sqrt{\frac{v}{2\pi}} \left\{ \begin{aligned} & \left[ k^2 - 1 + 2k \tanh(vX') \right] \cos(kvX') + \\ & \left[ k^2 - 1 + 2k \tanh(vX') \right] \sin(kvX') \end{aligned} \right\} \end{aligned} \right\} \text{ when } \omega = \pm(v^2 k^2 + v^2), \text{ where } g_1 \text{ and } g_2 \text{ satisfy the}$$

following orthogonality and normalization conditions:

$$\begin{aligned} \int_{-\infty}^{\infty} g_1(X', k) g_2(X', k) dX' &= 0, \quad \int_{-\infty}^{\infty} g_1(X', k) g_2(X', k') dX' = \delta(k - k'), \\ \int_{-\infty}^{\infty} g_1(X', k) g_1(X') dX' &= \frac{\pi k}{3\sqrt{2}} \operatorname{sech}\left(\frac{\pi k}{2}\right), \quad \int_{-\infty}^{\infty} g_2(X', k) g_1(X') dX' = \sqrt{\frac{\pi}{2}} \operatorname{sech}\left(\frac{\pi k}{2}\right), \\ \int_{-\infty}^{\infty} g_1^2(X') dX' &= 2/3, \quad \int_{-\infty}^{\infty} g_2(X') g_1(X', v) = 0, \quad \int_{-\infty}^{\infty} g_2^2(X') dX' = 2 \end{aligned} \tag{66}$$

Thus  $F_1$  and  $F_2$  can be expanded using the eigenfunction  $g_1$  and  $g_2$ , i.e.,

$$\begin{aligned} F_1(y, \tau) &= \varphi_{10}(\tau) g_1(y) + \int_{-\infty}^{\infty} dk \varphi_{1k}(\tau) g_1(y, k) \\ F_2(y, \tau) &= \varphi_{20}(\tau) g_2(y) + \int_{-\infty}^{\infty} dk \varphi_{2k}(\tau) g_2(y, k) \end{aligned} \tag{67}$$

Applying the conditions in Eq. (66), Pang finally arrived at:

$$\hbar \frac{d^2 \varphi_{1k}(\tau)}{d\tau^2} + (k^2 + 1)^2 \varphi_{1k}(\tau) = A_1(\tau, k), \quad \hbar \frac{d^2 \varphi_{2k}(\tau)}{d\tau^2} + (k^2 + 1)^2 \varphi_{2k}(\tau) = A_2(\tau, k) \tag{68}$$

and

$$\begin{aligned} \frac{d^2 \varphi_{10}(\tau)}{d\tau^2} &= \frac{3}{2} A_1(\tau) - \sqrt{\frac{\pi}{8}} \int_{-\infty}^{+\infty} dk A_1(\tau, k) k \operatorname{sech}\left(\frac{\pi k}{2}\right) = H_1(\tau), \\ \frac{d^2 \varphi_{20}(\tau)}{d\tau^2} &= \frac{1}{2} A_2(\tau) - \sqrt{\frac{\pi}{8}} \int_{-\infty}^{+\infty} dk A_2(\tau, k) k \operatorname{sech}\left(\frac{\pi k}{2}\right) = H_2(\tau), \end{aligned} \tag{69}$$

where  $A_1(\tau) = \int_{-\infty}^{+\infty} A_1(\tau, y) g_1(y) dy$ ,  $A_2(\tau) = \int_{-\infty}^{+\infty} A_2(\tau, y) g_2(y) dy$ ,

$$\begin{aligned} A_1(\tau, k) &= \int_{-\infty}^{+\infty} A_1(\tau, y) g_1(y, k) dy, \quad A_2(\tau, k) \\ &= \int_{-\infty}^{+\infty} A_2(\tau, y) g_2(y, k) dy. \end{aligned} \tag{70}$$

Once the external potential  $V(x')$  is known, then we can find the solutions of Eqs. (68)-(69), and can determine as  $\varphi_{1k}$ ,  $\varphi_{2k}$ ,  $\varphi_{10}$  and  $\varphi_{20}$ . Inserting them into Eq. (67) gives us  $F_1$  and  $F_2$ . From Eqs. (56)-(58) and Eq. (53) we can then obtain  $\phi$  of Eq. (52). Obviously, the solution has soliton characters.

Also, from Eqs. (68)-(69), we can see that the amplitudes of the “classical modes”,  $\varphi_{10}(\tau)$  and  $\varphi_{20}(\tau)$  in Eq. (69), which possess discrete eigenvalues, satisfy the Newton-type of motion equation.

The amplitudes of the “quantum modes”,  $\varphi_{1k}(\tau)$  and  $\varphi_{2k}(\tau)$  in Eq.(68), which possesses continuous eigenvalues, satisfy the wave equations. There is a gap,  $\delta$ , between the “classical modes” and the “quantum

modes”, of size  $\Delta E = v^2$ . When the system is quantized, *i.e.*,  $\delta \rightarrow 0$ , the “quantum mode” is near the “classical mode”, and the gap approaches zero.

When  $\delta = 0$ , the “classical modes” disappears, and only the “quantum mode” remains. However, when the classical condition is satisfied, *i.e.*,  $v_e \rightarrow \infty$ , the gap approaches infinity. The two “quantum modes” are separated at  $\pm\infty$ . Now there is only a “classical mode”. In this case the system shows pure classical behavior, a Newton-type of motion equations is sufficient. Therefore, for external potential field  $V(x')$ , the solutions of the nonlinear Schrödinger equation possess, not only classical mechanical properties, but also quantum mechanical properties. This is a very interesting result and worth studying deeply.

#### 4. THE APPLICATIONS OF NONLINEAR QUANTUM MECHANICS IN MOLECULAR CRYSTALS

We now study a concrete example, *i.e.*, the nonlinear properties of the exciton occurred in molecular crystal by the above nonlinear quantum –mechanical theory.

##### 4.1 The structure of molecular crystals and nonlinear excitation of the exciton

The acetanilide ( $CH_3COHNC_4H_5$ )<sub>x</sub>, or CAN is a typ-

ical molecular crystal, in which the two close chains of hydrogen-bonded amide-I groups which consists of atoms of carbon, oxygen, nitrogen and hydrogen (CONH) run through the acetanilide crystal [44-48]. This crystal structure has been determined and a unit cell of ACN is shown in Fig. 2. The space group is  $D_{2h}^{15}(P_{bca})$  and the unit cell or factor group is  $D_{2h}$  for this crystal. The average lattice constants are  $a = 1.9640$  nm,  $b = 0.9483$  nm, and  $c = 0.7979$  nm. There are eight molecules in an unit cell and at the amide- I frequency, each of these has one degree of freedom (d.f.). Thus, there are three infrared-active modes ( $B_{1u}$ ,  $B_{2u}$ , and  $B_{3u}$ ), four Raman-active modes ( $A_g$ ,  $B_{1g}$ ,  $B_{2g}$  and  $B_{3g}$ ), and one inactive mode ( $A_u$ ). However, at low frequency ( $< 200\text{ cm}^{-1}$ ), each molecule exhibits 6 d.f. (three translations and three rotations. This gives 48 low-frequency modes: 24 Raman active modes ( $6A_g + 6B_{1g} + 6B_{2g} + 6B_{3g}$ ), 18 infrared-active modes ( $6B_{1u} + 6B_{2u} + 6B_{3u}$ ) and six ( $A_u$ ) modes corresponding to acoustic modes of translation and rotation). All of these active modes are seen in infrared absorption and Raman experiments. Meanwhile, in ACN, the nearly planar amide-I groups have bond lengths, which are close to those found in polypeptide (see Fig. 3). Since the physical properties of such hydrogen bonded amide-I systems are very sensitive to bond lengths, hence, studies of ACN can reveal new phenomena. For example, in experiments of infrared absorption and Raman scattering, a new amide-I band red-shifted from the main peak at  $1666\text{ cm}^{-1}$  by about  $16\text{ cm}^{-1}$ , when the crystalline acetanilide is cooled from 320 to 10 K, but no other major changes occur from  $4000$  to  $800\text{ cm}^{-1}$ .

The intensity of this new band increases steadily from room temperature to 70 K. The band at  $1650\text{ cm}^{-1}$  is not present in amorphous materials or ACN methylated at the position where hydrogen-bonded distances occur, but it is recovered after annealing. Similar phenomena can be observed in Raman scattering experiments[49-55]. As it is known, the characteristic feature of amide-I group, CONH, in polypeptides is amide-I mode, which mainly involves the stretching of C=O bond.

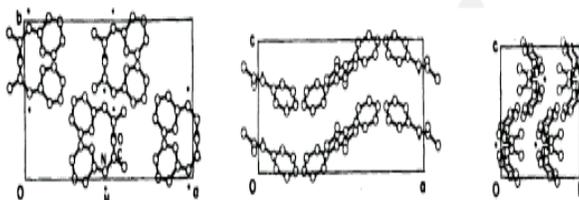


Fig. 2. Various views of the cell unit of ACN, with cell parameters  $a = 19.640\text{ \AA}$ ,  $b = 9.483\text{ \AA}$ , and  $c = 7.979\text{ \AA}$ .

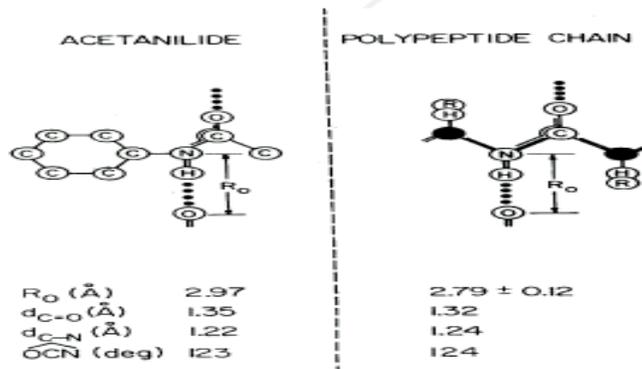


Fig.3. Comparisons between of ACN and a protein molecule.

This mode is observed as an infrared absorption peak at  $1666\text{ cm}^{-1}$  in ACN and near this value in a wide variety of materials, including the amide-I groups. The corresponding spectroscopic evidence of the new band at  $1650\text{ cm}^{-1}$  has been mentioned earlier, but detailed measurements of the crystal structure and specific heat as a function of temperature peptide groups preclude assignment of the new band to (1) a conventional amide-I mode, (2) crystal defect states, (3) Fermi resonance or (4) frozen kinetics between two different subsystems. The correct assignment is the self-trapping of the amide-I vibrational energy. These conclusions are based on the following experimental facts: (1) the  $^{15}\text{N}$  substitution induces a small shift to the amide-I at  $1666\text{ cm}^{-1}$ , and the new band is also shifted by the same amount; (2) deuterium substitution at the NH position strongly affects both the amide-I and the new band in a complicated way; (3) upon cooling a decrease in the integrated absorption of the normal amide-I and a corresponding increase in the integrated absorption of the  $1650\text{ cm}^{-1}$  band are observed; (4) the  $1650\text{ cm}^{-1}$  band and the amide-I band show the same dichroism over the temperature range integrated; and (5) the measurements of specific heat, the dielectric constant and the volume expansion as a function of temperature rule out the occurrence of rotational isomerism or polymorphic transition which would affect some other infrared and Raman absorption bands, but not the new band. The self-trapping mechanism of amide-I vibrational energy used by Scott and Eilbeck et al [49-57] comes from the Davydov model of vibration energy transport in alpha-helix protein molecules [58-64]. They have given a good account of the properties of first excited state in this model. Scott and co-workers, Alexander and Krumbansl have also obtained an exponential dependence of the absorption intensity on temperature,  $\exp(-\beta T^2)$  [55-57], and explained the experimentally observed intensity change of the new band with decreasing temperature in terms of a complementary polaron or soliton of the self-trapping state of exciton on the basis of the Davydov model (Davydov referred to the intramolecular excitation occurred in the systems as exciton in such a case). However, the red shift of a few  $\text{cm}^{-1}$  given by this model is much smaller than the experimental value of  $16\text{ cm}^{-1}$ . This indicates that these models need further improvement and development.

#### 4.2. Theory of nonlinear excitation of excitons

Pang et al [65-73] also proposed that the new band of amide-I is caused by the self-trapping of amide-I vibrational quanta (exciton) in their soliton model (the vibrational quantum is referred to as exciton, in accordance with the exciton theory by Davydov). But this model is different from Davydov's soliton model or Alexander's complementary polaron model, where it is nonlinear interaction between the localized amide-I vibrational-quantum and low frequency vibrations of the lattice (phonons) that result in self-trapping of the exciton as a soliton. The mechanism of this soliton model can be described as follows: Through their intrinsic nonlinear interaction, an amide-I vibrational quantum acts as a source of low-frequency phonons and causes shifts in the average positions of the lattice molecules in ground state. These shifts, or lattice distortions, in turn, react through the same nonlinear interaction, as a potential well to trap the amide-I vibrational quantum, resulting in the soliton, and preventing the energy dispersion of the amide-I vibrational quantum via the dipole-dipole interaction that occurs in neighboring peptides with certain electric moments. Evidently, the soliton is formed by the self-trapping of excitons interacting with low frequency lattice phonons, and is a dynamic self-sustaining entity. This entity propagates, together with the lattice deformation along the molecular chains. The main property of the soliton is that it can move over macroscopic distances at velocity  $v$  and retain its wave form, energy, momentum, and other quasi-particle properties. Using this model, Pang and coworkers also assigned an exponential dependence of the infrared-absorption intensity to the temperature which is consistent with experimental result [65-73].

From these studies, we know that collective excitations can result from a localized fluctuation of the amide-I vibrational quanta and structural deformation of peptide groups due to photon-excitation in molecular crystals. The Hamiltonian of the systems given by Pang[65-73] is as follows:

$$\begin{aligned}
 H = H_{ex} + H_{ph} + H_{int} = & \frac{1}{2m} \sum_n p_n^2 + \\
 & \frac{m\omega_0^2}{2} \sum_n r_n^2 + \frac{m\omega_1^2}{2} \sum_n r_n r_{n+1} \\
 & + \frac{1}{2M} \sum_n P_n^2 + \frac{\beta}{2} \sum_n (R_n - R_{n-1})^2 + m\chi_1 \sum_n (R_{n+1} - R_{n-1}) r_n^2 \\
 & + m\chi_2 \sum_n (R_{n+1} - R_n) r_{n+1} - m\chi \sum_n (R_{n-1} - R_n) r_n r_{n-1}
 \end{aligned} \quad (71)$$

This Hamiltonian includes vibrational excitation of amide-I caused by localized fluctuation and vibration of the peptide groups. This is, in turn, caused by structural deformation of molecular chains, and the interaction between the two modes of motion in the respective crystals. Here  $m$  is the mass of amide-I vibrational quantum (exciton),  $\omega_0$  and  $\omega_1$  are diagonal and off-diagonal elements of the dynamic matrix of vibrational quantum,  $\omega_0$  is also a Einstein vibrational frequency of the exciton, and  $m\omega_1^2 r_n r_{n+1} / 2$  is the interaction between the nearest neighboring excitons caused by the dipole-dipole interaction in molecular chains. Likewise  $r_n$  and  $p_n = m(\dot{r}_n)$  are the normal coordinates of the  $n$ th excitons and its canonical conjugate momentum, respectively,  $M$  the mass of a peptide group in the unit cell,  $\chi_1 = \partial\omega_0^2 / \partial R_n$  and  $\chi_2 = \partial\omega_1^2 / \partial R_n$  are the change of energy of exciton and of coupling interaction between the excitons for an unit extension of molecular chain, respectively.  $R_n$  and  $P_n = M$

$\dot{R}_n$  are the canonically conjugate operators of displacement and the momentum of peptide group and  $\beta$  the elastic constant of molecular chains.  $H_{ex}$  in  $H$  is the Hamiltonian of harmonic vibration of amide-I including the off-diagonal factor,  $H_{ph}$  is the Hamiltonian of harmonic vibration of the peptide group and  $H_{int}$  is the interaction Hamiltonian between the two modes of motion.

This Hamiltonian is significantly different from that of the Davydov model used by Scott and co-workers. As far as the vibration of amide-I is concerned, we adopt a harmonic oscillator model with optical vibration that includes an off-diagonal factor, which comes from the interaction between excitons, and interaction with displacement of peptide groups. Thus, vibrational frequencies of amide-I are related to displacements of peptide groups, which shows the occurrence of the interaction between amide-I vibrations and displacement of peptide groups. Their relationship is described by:

$$\omega_0^2(R_n) \approx \omega_0^2 - \frac{\partial\omega_0^2}{\partial R_n}(R_n - R_{n-1}) = \omega_0^2 + \chi_1(R_n - R_{n-1}), \quad \omega_1^2(R_n) \approx \omega_1^2 + \chi_2(R_n - R_{n-1}).$$

Inserting the above into the vibrational Hamiltonian of amide-I, and taking into account the effect of the neighboring peptide groups on the excitons in both sides, the result seen in equation (71) can be obtained. Therefore, the Hamiltonian given above has a one-to-one correspondence for the interactions.

However, the Hamiltonian in the Davydov model does not have such a one-to-one correspondence. In other words, there is no interaction between the amide-I vibrational quantum and displacement of the peptide groups resulting from the interaction between the neighboring excitons in the Davydov model. Thus, the Davydov model[58-63] has encountered many difficulties in the study of the dynamics of energy transport in the systems.

The Hamiltonian given above does not include only the optical vibration of amide-I, but also the resonant interaction caused by the dipole-dipole interaction between neighboring excitons; and it also takes into account both the change of the relative displacement of neighboring peptide groups resulting from the vibration of amide-I and the correlation interaction between neighboring excitons. Therefore, the Hamiltonian given above has a one-to-one correspondence in  $H_{ex}$  and  $H_{int}$ . Thus it can give a more complete description on the dynamics of systems compared to Davydov model and other models.

Since amide-I vibration and vibration of peptide groups are all quantized, we here introduce the following canonical second quantization transformation,

$$r_n = \sqrt{\frac{\hbar}{2m\omega_0}} (b_n^+ + b_n), p_n = -i\sqrt{\frac{2m\omega_0}{\hbar}} (b_n - b_n^+) \tag{72}$$

$$R_n = \sum_q \left[ \frac{\hbar}{2NM\omega_q} \right]^{1/2} e^{iqnr_0} (a_{-q}^+ + a_q), \tag{73}$$

$$P_n = i \sum_q \left[ \frac{M\hbar\omega_q}{2N} \right]^{1/2} e^{iqnr_0} (a_{-q}^+ - a_q)$$

where  $i = \sqrt{-1}$ ,  $\omega_q = 2(\beta/M)^{1/2} \sin(r_0q/2)$  is the frequency of the phonon with wave vector  $q$ ,  $N$  the number of unit cells in the molecular chain,  $r_0$  the distance between the molecules,  $b_n^+(b_n)$  and  $a_q^+(a_q)$  are the creation (annihilation) operator of the exciton and phonon, respectively.

Using Eqs. (72) and (73), equation (71) becomes

$$H = \sum_n \varepsilon_0 \left( b_n^+ b_n + \frac{1}{2} \right) - J \sum_n (b_n^+ b_{n+1} + b_n b_{n+1}^+) + \sum_{n,q} [g(q)(b_n^+ b_n + b_n b_n^+) + g_1(q)(b_n^+ b_{n+1} + b_n b_{n+1}^+) - \sum_q \hbar\omega_q \left( a_q^+ a_q + \frac{1}{2} \right) + g_2(q)(b_n^+ b_{n-1} + b_n b_{n-1}^+)] (a_q + a_{-q}^+) e^{inr_0q} \tag{74}$$

where

$$\varepsilon_0 = \hbar\omega_0, J = \hbar\omega_1^2/4\omega_0,$$

$$g(q) = \left( \frac{\hbar}{2NM\omega_q} \right)^{1/2} \left( \frac{\hbar\chi_1}{2\omega_0} \right) [e^{ir_0q} - e^{-ir_0q}],$$

$$g_1(q) = \left( \frac{\hbar}{2NM\omega_q} \right)^{1/2} \left( \frac{\hbar\chi_2}{2\omega_0} \right) [e^{ir_0q} - 1],$$

$$g_2(q) = \left( \frac{\hbar}{2NM\omega_q} \right)^{1/2} \left( \frac{\hbar\chi_2}{2\omega_0} \right) [e^{-ir_0q} - 1].$$

Because the collective excitations generated by the localized fluctuation of the excitons and structural deformation of the peptide groups have a coherent feature, thus Pang [65-73] represented the excitation states of the excitons and vibrations of peptide group (phonons) by the following wave function:

$$|\Phi\rangle = |\varphi(t)\rangle U(t) |0\rangle_{ph} = \frac{1}{\rho} \left( 1 + \sum_n \varphi_n(t) b_n^+ \right) |0\rangle_{ex} \cdot U(t) |0\rangle_{ph} \tag{75}$$

with

$$U(t) = \exp \left\{ \sum_n \frac{1}{i\hbar} [u_n(t) P_n - \pi_n(t) R_n] \right\} \tag{76}$$

or

$$U(t) = \exp \left\{ \sum_q [\alpha(t) a_q^+ - \alpha_q^*(t) a_q] \right\}$$

where  $|0\rangle_{ex}$  and  $|0\rangle_{ph}$  are the excitonic and

phononic ground-states, respectively. The  $\rho$  is the normalization factor. We assume hereafter that  $\rho=1$  for convenience of calculation unless it is explicitly noted otherwise. The  $\varphi_n(t)$ ,  $u_n(t)=\langle\Phi|R_n|\Phi\rangle$  and  $\pi_n(t)=\langle\Phi|P_n|\Phi\rangle$  are three unknown functions.

In Eq. (75) the wave function of the excitons is  $|\varphi\rangle=\frac{1}{\rho}\left(1+\sum_n\varphi_n(t)b_n^+|0\rangle_{ex}\right)$ , which is different from  $|\varphi_D\rangle=\sum_n\varphi_n(t)B_n^+|0\rangle_{ex}$  in the Davydov wave function  $|D_2\rangle$ , and it is not an excitation state of a single particle, but rather a coherent state, or more accurately, a quasi-coherent state. In the case of small  $\varphi_n(t)$  (i.e.,  $|\varphi_n(t)|\ll 1$ ) and it can be approximately written as

$$|\varphi\rangle \approx \frac{1}{\rho} \exp\left[-\frac{1}{2}\sum_n|\varphi_n(t)|^2\right] \exp\left[\sum_n\varphi_n(t)b_n^+\right]|0\rangle_{ex} = \frac{1}{\rho} \exp\left[\sum_n\varphi_n(t)b_n^+ - \varphi_n^*(t)b_n\right]|0\rangle_{ex}$$

in which the final representation is a standard coherent state, which is normalized.

Since the condition  $\sum_n|\varphi_n(t)|^2=1$ , is required in this calculation, then the condition,  $|\varphi_n(t)|\ll 1$ , is naturally satisfied for the acetanilide consisting of several hundreds peptide groups. Therefore, the above representation is correct. Thus, the wave function in Eq. (75) is also normalized at  $\rho=1$ .

In fact, the wave function of the exciton state in Eq. (75) should be viewed as an effective truncation of a standard coherent state, in which the aforementioned two terms are retained. Thus it is referred to as a quasi-coherent state. However, it is not an eigenstate of the number operator  $\hat{N}=\sum_n b_n^+b_n$  since

$$\hat{N}|\varphi\rangle = \sum_n b_n^+b_n|\varphi\rangle = |\varphi\rangle - |0\rangle_{ex} \neq |\varphi\rangle.$$

Hence,  $|\varphi\rangle$  represents a coherent superposition of the one-quantum amide-I vibrational state and the ground state of the exciton. But, the number of quantum are determinate in this state and it contains only one exciton because:

$$N = \langle\varphi|\hat{N}|\varphi\rangle = \langle\varphi|\sum_n b_n^+b_n|\varphi\rangle = \sum_n|\varphi_n(t)|^2 = 1.$$

Therefore,  $|\varphi\rangle$  given in Eq.(75) not only exhibits coherent feature of collective excitations of the excitons caused by the nonlinear interaction generated by means of the exciton-phonon interaction, which makes the wave functions of the states of the exciton and phonon symmetrical (because the wave function of the phonon was already a standard coherent sate), but it can also make the number of the excitons conserved for the Hamiltonian in Eq. (74) as well.

Meanwhile, the wave function given above has another advantage, i.e., the equation of motion of the exciton can be obtained from the following Heisenberg equations for the creation and annihilation operators in Eqs. (74) – (76)

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\langle\Phi|b_n|\Phi\rangle &= |\Phi\rangle[b_n, H]|\Phi\rangle, \\ i\hbar\frac{\partial}{\partial t}\langle\Phi|a_q|\Phi\rangle &= |\Phi\rangle[a_q, H]|\Phi\rangle \end{aligned} \tag{77}$$

From these equations we can obtain the following equations of  $\varphi_n(t), \alpha_q(t)$  and  $\alpha_{-q}^*(t)$

$$\begin{aligned} i\hbar\dot{\varphi}_n &= \hbar\omega_0\varphi_n - J(\varphi_{n+1} + \varphi_{n-1}) + \\ &\sum_q\{2g(q)(\alpha_q + \alpha_{-q}^*)\varphi_n + \end{aligned}$$

$$(g_1(q) - g_2(q)) \left[ (\alpha_q + \alpha_{-q}^*) \varphi_{n+1} + (\alpha_q + \alpha_{-q}^*) \varphi_{n-1} \right] \} e^{ir_0qn}, \tag{78}$$

$$i\hbar \dot{\alpha}_q = \hbar \omega_q \alpha_q + \sum_n \left\{ 2g(q) |\varphi_n(t)|^2 + [g_1(q) - g_2(q)] (\varphi_n^* \varphi_{n+1} + \varphi_n^* \varphi_{n-1}) \right\} e^{-ir_0qn} \tag{79}$$

$$i\hbar \dot{\alpha}_{-q}^* = -\hbar \omega_q \alpha_{-q}^* - \sum_n \left\{ 2g(q) |\varphi_n(t)|^2 + [g_1(q) - g_2(q)] (\varphi_n^* \varphi_{n+1} + \varphi_n^* \varphi_{n-1}) \right\} e^{-ir_0qn} \tag{80}$$

From Eqs. (6.9) and (6.10), we can get:

$$\ddot{\alpha}_{-q}^* + \ddot{\alpha}_q = -\omega_q^2 (\alpha_q + \alpha_{-q}^*) - \sum_n \left\{ \frac{4g(q)\omega_q}{\hbar} |\varphi_n|^2 + \frac{2g_1(q) - 2g_2(q)}{\hbar} \omega_q (\varphi_n^* \varphi_{n+1} + \varphi_n^* \varphi_{n-1}) \right\} e^{-ir_0qn}.$$

Also, from Eq. (73) we get the Fourier transformation

of the variable,  $u_n = \langle \Phi | R_n | \Phi \rangle$ , as:

$$u_n = \frac{1}{\sqrt{N}} \sum_q u_q(t) e^{iqx},$$

where  $x = n r_0$  and  $u_q(t) = \sqrt{\frac{\hbar}{2M\omega_q}} (\alpha_q + \alpha_q^*)$ .

Thus we get in the long-wave length approximation

$$\ddot{u}_q + v_0^2 q^2 u_q = \frac{1}{\sqrt{N}} \sum_n \left\{ \frac{2iq\hbar r_0 \chi_1}{M\omega_0} |\varphi_n|^2 + \frac{iq\hbar r_0 \chi_2}{M\omega_0} (\varphi_n^* \varphi_{n+1} + \varphi_n^* \varphi_{n-1}) \right\} e^{-ir_0qn} \text{ where } \omega_q = v_0 q, v_0 = r_0 (\beta/M)^{1/2}.$$

Now, multiplying the above equation by  $\exp(ir_0qn) / \sqrt{N}$ , summing over the wave number,  $q$ , and making the continuum approximation, we [65-73] get:

$$\frac{\partial^2 u(x,t)}{\partial t^2} - v_0^2 \frac{\partial^2 u(x,t)}{\partial x^2} = \frac{2\hbar r_0 (\chi_1 + \chi_2)}{M\omega_0} \frac{\partial |\varphi(x,t)|^2}{\partial x}. \tag{81}$$

At the same time, equation (77) becomes:

$$i\hbar \frac{\partial \varphi(x,t)}{\partial t} = (\hbar \omega_0 - 2J) \varphi(x,t) - J r_0^2 \frac{\partial^2 \varphi(x,t)}{\partial x^2} + \frac{2\hbar r_0 (\chi_1 + \chi_2)}{\omega_0} \varphi(x,t) \frac{\partial u(x,t)}{\partial x} \tag{82}$$

Inserting Eq. (81) into Eq. (82), we can get the following nonlinear Schrödinger equation for motion of the exciton:

$$i\hbar \frac{\partial \varphi(x,t)}{\partial t} = (\hbar \omega_0 - 2J) \varphi(x,t) - J r_0^2 \frac{\partial^2 \varphi(x,t)}{\partial x^2} + \frac{4\hbar^2 r_0^2 (\chi_1 + \chi_2)^2}{M\omega_0 (v^2 - v_0^2)} |\varphi(x,t)|^2 \varphi(x,t) \tag{83}$$

where  $\hbar^2 / 2m = Jr_0^2$ . Here  $m$  is the effective mass of the exciton. Equation (83) is a nonlinear Schrödinger equation, its solution is a soliton and can be represented by:

$$\varphi(x,t) = \sqrt{\frac{\mu}{2}} \operatorname{sech} h[\mu'(x-x_0-ut)] \exp \left\{ \frac{i}{\hbar} \left[ \frac{\hbar^2 v(x-x_0)}{2Jr_0^2} - E_{sol}t \right] \right\}, \tag{84}$$

$$u(x,t) = -\frac{\hbar(x_1+x_2)}{2\omega_0\beta(1-s^2)} \tanh [\mu'(x-x_0-ut)] \tag{85}$$

where

$$\mu = \frac{G}{4J}, G = \frac{4\hbar^2 r_0^2 (\chi_1 + \chi_2)^2}{M v_0^2 \omega_0^2 (1-s^2)}, \mu' = \frac{\mu}{r_0}, \tag{86}$$

$$s = \frac{v}{v_0}, \varepsilon = \hbar\omega_0 - 2J, \varepsilon_0 = \hbar\omega_0,$$

Using

$$\alpha_q = \sqrt{\frac{M\omega_q}{2\hbar}} u_q + i \sqrt{\frac{1}{2M\hbar\omega_q}} \pi_q,$$

and the results given above, we found that  $\alpha_q(t)$  in Eq. (73) is given by:

$$\alpha_q(t) = \frac{1}{\sqrt{N}} \sum_n \alpha_n(t) e^{-iqx} = \frac{i\hbar(\chi_1 + \chi_2)\pi M(\omega_q + vq)}{2Mv_0^2\omega_0(1-s^2)\hbar N\omega_q} \sinh\left(\frac{\pi r_0 q}{2\mu}\right) e^{iqvt} = \alpha_q e^{iqvt}. \tag{87}$$

These results clearly show that the excitation, and motion of the excitons in the ACN, are a nonlinear quantum mechanical problem, and can satisfy or obey the laws of nonlinear quantum mechanics. Thus the exciton-soliton has the properties of microscopic articles.

Obviously, in this model the motions of the exciton and phonon and their interaction were all considered, the nonlinear interactions for the exciton and phonon occur simultaneously. In this case the nonlinear interaction energy ( $G$ ), is provided by the coupling between the excitons and phonons. Just so, the exciton is a self-trapped as a soliton in this case.

### 4.3. The effects of nonlinear interactions

The energy of the soliton can be found by using Eqs. (84) and (85) and is given by:

$$E_{sol} = \int_{-\infty}^{\infty} Hd\xi = \varepsilon_0 - 2J + \frac{\hbar^2 v^2}{4Jr_0^2} - \frac{\mu^2 J}{3} = E_0 + \frac{M_{sol} v^2}{2}, \text{ where}$$

$$E_0 = \varepsilon_0 - 2J - \frac{\hbar^4 (\chi_1 + \chi_2)^4}{3\beta^2 J\omega_0^4}$$

is the rest energy of the soliton. The mass of the soliton is given by:

$$M_{sol} = m + \frac{4\hbar^4 (\chi_1 + \chi_2)^4 (1 - 3s^2/2 - s^4/2)}{3\beta^2 J \omega_0^4 v_0^2 (1 - s^2)^2} > m$$

Therefore, the energy and the rest energy of the soliton are  $\hbar^4 (\chi_1 + \chi_2)^4 / 3\beta^2 J \omega_0^4 (1 - s^2)$  and  $\hbar^4 (\chi_1 + \chi_2)^4 / 3\beta^2 J \omega_0^4$ , respectively, both of which are lower than those of the exciton,  $E' = \varepsilon_0 - 2J + \frac{1}{2}mv^2$  and  $E_0 = \varepsilon_0 - 2J$ , respectively.

Therefore, the exciton-soliton is stable. But the mass of the soliton is greater than that of the exciton,  $m$ . Pang et al. [26-31] also studied the influence of anharmonic vibration of the peptide groups on the soliton. The peptide group's Hamiltonian in Eq. (71) is replaced by

$$H'_{ph} = \frac{1}{2M} \sum_n P_n^2 + \sum_n \left[ \frac{\beta}{2} (R_n - R_{n-1})^2 + \frac{1}{3} \lambda_1 (R_n - R_{n-1})^3 \right] \quad (88)$$

It was found that only terms such as  $(\hbar\omega_0 - 2J)\varphi(x, t)$  in Eq. (83) are changed. Thus only the phase, velocity, energy, amplitude and width of the soliton are affected.

From the above studies we know that exciton-soliton or localization of exciton occurs due to nonlinear exciton-phonon interaction. In such a case, the phonon is also localized at the same time, and moves in a soliton in the systems. This can be verified from Eqs.(81)–(82). In such a case, from Eqs. (84)–(85) and

$$\mu = (\chi_1 + \chi_2)^2 \hbar^2 / JM v_0^2 \omega_0^2 (1 - s^2)^2,$$

where  $s = v / v_0$ , we can get

$$\frac{\partial}{\partial x} |\varphi(\chi, t)|^2 = \frac{2(\chi_1 + \chi_2)^3 \hbar^3}{r_0^3 \beta J^2 (1 - s^2) \omega_0^3} \left[ u - \frac{4\omega_0^2 (1 - s^2)^2 \beta^2}{\hbar^2 (\chi_1 + \chi_2)^2} u^3 \right] \quad (89)$$

Substituting Eq. (89) into Eq. (81), we obtain

$$u_{tt} - v_0^2 u_{xx} = \frac{4(\chi_1 + \chi_2)^4 \hbar^4}{Mr_0^2 \beta J^2 (1 - s^2) \omega_0^4} \left[ u - \frac{4\omega_0^2 (1 - s^2)^2 \beta^2}{\hbar^2 (\chi_1 + \chi_2)^2} u^3 \right] \quad (90)$$

This is a  $\phi^4$ -equation for  $u(x, t)$ . It has a soliton solution given in Eq. (85). Thus phonon has been localized in this case. Obviously, the localization of phonon is due to the nonlinear exciton-phonon interaction in ACN. If  $\chi_1 = \chi_2 = 0$ , then Eq.(90) reduces to a linear wave equation,  $u_{tt} - v_0^2 u_{xx} = 0$ , which has a solution of plane wave,  $u = A \sin(\omega t - \theta_0)$ . This manifests that the peptide groups performs harmonic vibration in this case, which is dispersive. Then, the localization or soliton excitation of phonons is carried out by virtue of exciton-phonon coupling, which results in nonlinear interaction  $B'u^3$  in Eq.(90) because  $B' = 16(\chi_1 + \chi_2)^2 \hbar^2 \beta (1 - s^2) / Mv_0^2 \omega_0^2 J$ . Thus, its motion should be described by nonlinear quantum mechanics, instead of linear quantum mechanics.

These results show that the nonlinear interactions are acted to both microscopic particles (or excitons) and background field (or phonons). In other words, in such a case, the microscopic particles (excitons) and vibration of background field (or phonons) are localized and possess the wave-corpucle duality simultaneously. This also confirms the validity of the conclusion, i.e., the nonlinear action and counteraction exist simultaneously for interacting particles in nonlinear quantum mechanics.

## 5. CONCLUSIONS, DIFFICULTIES OF QUANTUM MECHANICS AND ITS RESOLUTION

### 5.1. The essences and limitations of the quantum mechanics

As known, the states and properties of microscopic particle were described by the linear Schrödinger equation (1) in the quantum mechanics. As far as quantum mechanics is concerned, we should affirm that its birth was a revolution of physics or science, it was the foundation of modern science, it triggered great successes in applications, especially on hydrogen atom and molecule as well as helium atom and molecule, in which the theoretical results obtained were

basically consistent with experimental data due to small nonlinear interaction. However, this theory makes only the microscopic particle display a wave feature and no corpuscle nature. This brings just about an uncertainty description for the microscopic particles, such as the existence of particles at a point in time-space is represented by a probability, the sizes of mechanical quantities are expressed by some average values, conjugate physical quantities, such as coordinate and momentum, cannot be determined simultaneously and meet an uncertainty relation, and so on. These features do not fit the traditional concept of particles and are contradictory with the experimental results of electronic diffraction on double seam by Davisson and Germer in 1927 and de Broglie's relation of wave-corpuscle duality[11-13]. Therefore, the probability description of the microscopic particles brings also about plenty of difficulties and troubles to understand the natures and essences of the linear quantum mechanics and results in intense controversies in physics, which elongate and continue a century. Very surprisingly, these difficulties and controversies have not been solved up to now as described in section 1. This displays sufficiently the limitations of the linear quantum mechanics. These limitations and shortages are embodied concretely in the basic hypotheses of linear quantum mechanics. The linearity of the theory, containing the linear superposition principle, linearity of dynamic equation and the independence of Hamiltonian operator of the systems on states of microscopic particles, and so on, are its great fault and defect. This feature is inconsistent with practical cases. In the applications it cannot be used to give the true properties and rules of the microscopic particles in the systems of many particles and many bodies. When the quantum mechanics is used to study the properties of motion of microscopic particles in these complicated systems, we have to use an average potential to replace the complicated and real nonlinear interaction among these particles, or between the particle and backgrounds through using some approximate methods, such as, the signal and free electronic approximations, compact-binding approximation and average field approximation, and so on. In such a case we obtained only some approximate results from linear quantum mechanics[1-13,25-27]. Therefore the linear Schrödinger equation is a linear dynamic equation. Quantum mechanics is also only a linear and approximate theory, and can be used to describe the motions of microscopic particles in simple systems, such as hydrogen atom and molecules as well as helium atom, in which the nonlinear interaction is very small.

Another great defect of linear quantum mechanics is to neglect the truthful motions of each microscopic particle, of which the physical systems are composed, and true interactions of the particle with other particles or background field, in other words, the motions of other particles and background field are fully frozen, plenty of complicated and nonlinear interactions among the particles or between the particle and background field have been completely blotted out, an average interaction unrelated to the states of particles is used to contain some interactions in the systems. This results necessarily in the independence of the Hamiltonian operator of the system on the states of particles, then the dispersed effect of kinetic energy cannot be canceled, finally the microscopic particles have only a wave feature in linear quantum mechanics. Thus it can only describe the properties and states of a single microscopic particle in the system of fewer bodies. Therefore linear quantum mechanics is an approximate theory, it cannot obtain in truth the properties and states of motion of microscopic particles in complicated systems, and is only correct in some simple atoms. This is just the essence and limitation of linear quantum mechanics.

## 5.2. Successes of nonlinear quantum mechanics and resolution of difficulties of linear quantum mechanics

On the contrary, we have broken through the hypothesis of independence of Hamiltonian operator of the systems on states of microscopic particles, forsaken the above linearity hypothesis of linear quantum mechanics and taken into account the true motions of each particle and background field and the interactions between them, thus the microscopic particles accepted a nonlinear interaction and their laws of motion are then described by Eqs. (5)-(8).

Finally we built a new nonlinear quantum mechanics based on these results. This means that the significance of the wave function displays essential variations, thus natures and properties of the microscopic particles show also considerable changes when compared with those in linear quantum mechanics. The changes can be summarized as follows<sup>[17-37]</sup>.

(1) In this new theory although the states of microscopic particles are still represented as a wave function  $\phi(\vec{r}, t)$  in Eq. (4), its absolute square,  $|\phi(\vec{r}, t)|^2 = |\phi(\vec{r}, t)|^2 = \rho(\vec{r}, t)$ , denotes no longer the probability of finding the microscopic particle at a given point in the space-time, and give just the mass density of the microscopic particles at that point. Thus we can find out the particle number or the mass of the particle from  $\int_{-\infty}^{\infty} |\phi|^2 d\tau = N$ , the concept of probability is abandoned thoroughly in nonlinear quantum mechanics. Then the difficulty of statistical interpretation for the wave function of microscopic particle in quantum mechanics is solved.

(2) The dynamic equations the particles satisfy are not the linear Schrödinger equation in Eq. (1) and linear Klein-Gordon equation, but nonlinear Schrödinger equations in Eqs. (5)- (6) and nonlinear Klein-Gordon equations in Eqs. (7)-(8). Their solutions have a wave-corpucle duality, which is embedded by organic combination of envelope and carrier wave as shown in Fig.1. In such a case the particle has not only wave features, such as a certain amplitude, velocity, frequency, and wavevector, but also corpucle natures, such as, a determinant mass centre, size, mass, momentum and energy. This is the first time to clearly explain physically the wave- corpucle duality of microscopic particles in quantum systems. This is a great advance of modern quantum theory, thus nonlinear quantum mechanics solved a most great difficulty of one century existed in quantum mechanics.

At the same time, we proved that the wave-corpucle duality of microscopic particles is quite stable, even though in an externally applied potential fields. Meanwhile we obtained that the corpucle feature of microscopic particles differs from the classical particles, the wave feature differs also from those of both linear wave, such as de Broglie wave in linear quantum mechanics and KdV solitary wave. It is a special solitary wave, which can embody both wave feature and corpucle feature of microscopic particles. Therefore, it has nontrivial physics significances and is the goal sought by physicists.

(3) In nonlinear quantum mechanics,  $\int_{-\infty}^{\infty} \phi^* x \phi d\tau$ ,  $\frac{\partial}{\partial t} \int_{-\infty}^{\infty} \phi^* x \phi d\tau$ ,  $\frac{\partial^2}{\partial t^2} \int_{-\infty}^{\infty} \phi^* x \phi d\tau$  and  $\int \phi^* \hat{H} \phi dx$  or  $\langle \phi | \hat{H} | \phi \rangle$  (please see chapter 4) are no longer some average values of the physical quantities in linear quantum mechanics, but represent the position, velocity and acceleration of the mass center and energy of the microscopic particles, respectively, and have determinant values. Thus, the presentations of physical quantities in the nonlinear quantum mechanics appear considerably the variations relative to those in linear quantum mechanics. This has solved the difficulty arising from the average values, which represent the physical quantities in linear quantum mechanics.

(4) The microscopic particles have determinant mass, momentum and energy, and obey universal conservation laws of mass, momentum, energy and angular momentum. Their motions satisfy not only nonlinear Schrödinger equations but also Newtonian law, Lagrangian equation and Hamilton equation. This amount to bridge over the gap between the classical mechanics and linear quantum mechanics.

(5) The microscopic particles meet also the classical collision rule, when they collide with each other. Although these particles are deformed in the collision process, which denotes its wave feature, they can still retain their form and amplitude to move towards after collision, where a phase shift occurs only. This feature denotes that the microscopic particles in nonlinear quantum mechanics possess both corpucle and wave property, but the corpucle property differs from classical particles.

(6) The position and momentum of the mass centre of microscopic particles are determinant, but their uncertainties obey only to a minimal uncertainty relation due to the wave-corpucle duality, which differs from those in linear quantum mechanics. This means that the coordinate and momentum of microscopic particles may be simultaneously determined at a certain degree. This amount also to bridge over the gap between the classical mechanics and linear quantum mechanics.

These new and interesting natures and properties of the microscopic particles are completely different from those of the linear quantum mechanics, thus nonlinear quantum mechanics solved and eliminated all difficulties and problems in linear quantum mechanics. These show clearly the necessity, validity and importance of establishing nonlinear quantum mechanics, and make us see clearly the essences and limitations of linear quantum mechanics. Thus the difficulties of linear quantum mechanics can be also solved thoroughly by nonlinear quantum mechanics. Therefore, to develop and to establish NLQM can solve problems disputed by scientists in the LQM field for about a century<sup>[7-9]</sup>, can promote the development of physics and enhance and raise the knowledge and recognition levels to the essences of microscopic matter. We can predict that nonlinear quantum mechanics has extensive applications in physics, chemistry, biology, polymers, and so on.

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