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Exact solutions for nonlinear Schrödinger equation in phase space: applications to Bose–Einstein condensate

Lu Jun(陆 军)†

Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100080, *China*

Department of Computational Science, National University of Singapore, Singapore 117543, *Singapore*

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The stationary-state nonlinear Schrödinger equation, which models the dilute-gas Bose–Einstein condensate, is introduced within the framework of the quantum phase-space representation established by Torres-Vega and Frederick. The exact solutions of equation are obtained in the phase space, by means of the wave-mechanics method. The eigenfunctions in position and momentum spaces are obtained through the 'Fourier-like' projection transformation from the phase space eigenfunctions. The eigenfunction with a hypersecant part is discussed as an example.

Keywords: nonlinear equation, phase space, Bose–Einstein condensate
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1. Introduction

In any statistical distribution of two variables, such as position x and momentum p, an important question is whether or not the two variables are correlated. In classical physics, a particle is something that has simultaneously a definite position and a definite momentum. In quantum theory, however, a particle can show either a definite position or a definite momentum, but not both at the same time. As a central concept in classical mechanics, phase space cannot be utilized directly in quantum mechanics due to the limitation of the Heisenberg uncertainty principle. Nevertheless, quantum phase space theory has provided a method to describe a quantum state directly in classical phase space. To a first approximation, the effects of the quantum properties of matter can be pictured in terms of a classical particle of uncertain position and momentum, provided that we assume that $\Delta x \Delta p \geq \frac{\hbar}{2}$. This picture must be used with caution, because the wave properties of matter are not taken into account completely and correctly. Yet it is often very helpful, provided its limitations are understood.

Since the first quantum phase-space distribution function was introduced by Wigner [1] in 1932, a variety of phase-space theories for quantum mechanics have been proposed [2,3] and extensive uses have been found in many areas of physics and chemistry.[4−6] The most direct way to establish phase-space representations of quantum mechanics is to define quantum phase-space distribution functions. To date, the quantum phase-space distribution function most used in physics and chemistry is still the Wigner distribution function,[7] which is called the quasi-probability distribution function. There have been many attempts to improve the inadequacy that the Wigner distribution function is not always positive in phase space.[8]

The other way to establish phase-space representations is to define quantum state functions and corresponding Schrödinger equations. Thus, almost all the mathematical properties in the general position or momentum representation of quantum mechanics are retained for quantum state functions in phase space, and a variety of useful methods and results can be replanted to phase-space representation. The quantum phase-space theory established by Torres-Vega and Frederick (TF) in the 1990s reflects this idea.[9,10] In the TF phase-space representation, the principal operator of dynamic variables and the Schrödinger equations are defined directly, and the phase-space wavefunctions are determined by the Schrödinger equations solved. The mean values of dynamic variables may

†E-mail: lujun@itp.ac.cn

be computed just as those in position or momentum space.[11]

Since the TF phase-space representation of quantum mechanics was proposed, a variety of advances have been made in theory and applications to atomic and molecular systems. The harmonic oscillator in the phase space has been treated by Torres-Vega and Frederick in their initial papers.[9,10] The possibilities and limitations of utilizing wave mechanics in the phase space have been discussed by Møller *et al.*[12] The rigorous solutions of Morse oscillator, a particle in δ potential fields, and the one-dimensional (1D) hydrogen atom in the phase space have been obtained. The vibration theory of diatomic molecules with an empirical potential function in the phase space has been discussed.[13−16] The scattering theory in phase space has also been developed.[17,18]

On the other hand, there can be many kinds of equivalent quantum phase-space theories. In addition to the theory established by Torres-Vega and Frederick, the relative-state theory, the linear transformation theory, and the displacement-operator theory in phase space have also been established, and it has been proved that all these representations are equivalent to each other.[19−21]

Many physical phenomena can be described with the nonlinear Schrödinger equation (NLSE): for example, the behaviour of the Stokes wave near the state of modulational instability. The NLSE also has wide and important applications in nonlinear optics, plasma physics, and fluid dynamics. Some NLSEs can be solved exactly in position representation, and some numerical methods have been studied for solving the generalized NLSE.

The NLSE can also be used to model dilute-gas Bose–Einstein condensate (BEC).[22] BEC is a ubiquitous phenomenon, which plays important roles in condensed matter, atomic, nuclear, and elementary particle physics, as well as in astrophysics. Many applications of NLSE to BECs have been found.[23,24] Some works on NLSE in the context of BECs have also been done in the phase-space representation.[25]

In this paper, we will solve the 1D NLSE which models the dilute-gas BECs in the quantum phase-space representation established by Torres-Vega and Frederick. We obtain the Jacobian elliptic function solution for the phase-space NLSE in Section 2. We discuss the properties of the solution in Section 3, and draw our conclusion in Section 4.

2. Nonlinear equation and its solution in phase space

The dilute-gas BEC can be modelled with NLSE in a three-dimensional (3D) mean-field theory. The NLSE that describes a BEC of N atoms of mass M is

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\Gamma,t)=\left[\frac{\hat{\boldsymbol{p}}^2}{2M}\pm g\,|\Psi(\Gamma,t)|^2+V(\hat{\boldsymbol{r}})\right]\Psi(\Gamma,t)\,. \tag{1}$$

Here the atoms are confined in the external potential $V(\hat{\boldsymbol{r}})$. $|\Psi(\Gamma,t)|^2$ is the single particle density function, $g>0$ is the coupling constant which is related to the nature and quantity of the atoms, and '+' and '−' correspond to the cases of repulsive and attractive interactions respectively.

On the other hand, if the BEC is in the situation that its transverse dimensions are on the order of the atomic interaction length or the actual atomic size, and its longitudinal dimension is much longer than its transverse ones, it can be defined in the quasi-1D regime.[26,27] Thus the 3D NLSE (1) will be reduces as a 1D NLSE, i.e.

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\Gamma,t)=\left[\frac{\hat{p}_x^2}{2M}\pm g\,|\Psi(\Gamma,t)|^2+V(\hat{x})\right]\Psi(\Gamma,t)\,. \tag{2}$$

The 1D NLSE (2) admits of considerable simplification when the potential energy $V(\hat{x})$ does not depend on time. It is then possible to express its solution as a product of functions of Γ and t, i.e.

$$\Psi(\Gamma,t)=\Psi(\Gamma)\exp\left(-\frac{\mathrm{i}E}{\hbar}t\right), \tag{3}$$

where E is the eigenenergy. We let the constant factors $M=\hbar=1$, as such constant factors make no difference in our results. Thus the 1D NLSE (2) will become a 1D stationary-state NLSE as follows:

$$\left[\frac{\hat{p}_x^2}{2}\pm g\,|\Psi(\Gamma)|^2+V(\hat{x})\right]\Psi(\Gamma)=E\,\Psi(\Gamma)\,. \tag{4}$$

In the TF quantum phase-space representation, the position and momentum operators can be written as the canonical form,[9,10] i.e.

$$\hat{x}\to\hat{X}=\frac{x}{2}+\mathrm{i}\frac{\partial}{\partial p_x}, \tag{5}$$

$$\hat{p}_x\to\hat{P}_x=\frac{p_x}{2}-\mathrm{i}\frac{\partial}{\partial x}. \tag{6}$$

Then Eq.(4), with the help of Eqs.(5) and (6), becomes

$$\left[\frac{1}{2}\left(\frac{p_x}{2}-\mathrm{i}\frac{\partial}{\partial x}\right)^2\pm g\,|\Psi(x,p_x)|^2+\hat{V}\left(\frac{x}{2}+\mathrm{i}\frac{\partial}{\partial p_x}\right)\right]\Psi(x,p_x)=E\,\Psi(x,p_x)\,. \tag{7}$$

By using the relations

$$\left(\frac{x}{2}+\mathrm{i}\frac{\partial}{\partial p_x}\right)^n = \exp\left(\frac{\mathrm{i}xp_x}{2}\right)\left(\mathrm{i}\frac{\partial}{\partial p_x}\right)^n \times \exp\left(-\frac{\mathrm{i}xp_x}{2}\right), \tag{8}$$

$$\left(\frac{p_x}{2}-\mathrm{i}\frac{\partial}{\partial x}\right)^n = \exp\left(-\frac{\mathrm{i}xp_x}{2}\right)\left(-\mathrm{i}\frac{\partial}{\partial x}\right)^n \times \exp\left(\frac{\mathrm{i}xp_x}{2}\right), \tag{9}$$

$$\hat{V}\left(\frac{x}{2}+\mathrm{i}\frac{\partial}{\partial p_x}\right) = \exp\left(-\frac{\mathrm{i}xp_x}{2}\right)\hat{V}\left(x+\mathrm{i}\frac{\partial}{\partial p_x}\right) \times \exp\left(\frac{\mathrm{i}xp_x}{2}\right), \tag{10}$$

and by putting

$$\Psi(x,p_x) = \exp\left(-\frac{\mathrm{i}xp_x}{2}\right)\Phi(x,p_x), \tag{11}$$

we can transform Eq.(7) into

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} \pm g\left|\Phi(x,p_x)\right|^2 + \hat{V}\left(x+\mathrm{i}\frac{\partial}{\partial p_x}\right)\right]\Phi(x,p_x) = E\Phi(x,p_x). \tag{12}$$

The harmonic oscillator is one of the models most used for the dilute-gas BEC. The NLSE with the harmonic potential has been discussed, and the existence of the bound states has been proved for the equation.[28] Despite having less accuracy than with the harmonic potential, the NLSE with a constant potential is useful for describing the dilute-gas BEC.[26−30] The long-time exact solutions of the 1D NLSE with the constant potential have been obtained by the inverse scattering method.[31] Here we consider Eq.(12) in the regions of constant potential. Without loss of generality, we put $V(\hat{x}) = 0$, then the 1D phase-space NLSE (12) becomes

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} \pm g\left|\Phi(x,p_x)\right|^2\right]\Phi(x,p_x) = E\Phi(x,p_x). \tag{13}$$

2.1. Repulsive nonlinearity

The case of repulsive interactions considered here corresponds to '+' in Eq.(13), i.e.

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + g\left|\Phi_{\mathrm{R}}(x,p_x)\right|^2\right]\Phi_{\mathrm{R}}(x,p_x) = E\Phi_{\mathrm{R}}(x,p_x). \tag{14}$$

Equation (14) is similar to the standard form of the NLSE in Ref.[32], and admits an infinite number of exact solutions. The complicated solutions can be regarded as the nonlinear superposition of simple solutions. The most general form of the solutions is

$$\Phi_{\mathrm{R}}(x,p_x) = B\,\mathrm{sn}\left[k(x-x_0)+\delta\,|m\right]\exp\left[\mathrm{i}C(p_x)\right], \tag{15}$$

where $\mathrm{sn}(x\,|m)$ is the Jacobian elliptic function,[33] x_0 is the eigenvalue of the position operator, and $C(p)$ is an arbitrary reasonable real function satisfying the following condition:

$$\int_{-\infty}^{+\infty}\mathrm{d}p_x\left|\frac{\mathrm{d}^n}{\mathrm{d}p_x^n}\exp\left[\mathrm{i}C(p_x)\right]\right| < \infty \quad (n=0,1,2,\cdots). \tag{16}$$

The parameters B, k, δ and m will be determined by substitution of Eq.(15) into Eq.(14), the boundary conditions and normalization.

Inserting Eq.(15) into Eq.(11), we obtain

$$\Psi_{\mathrm{R}}(x,p_x) = \exp\left(-\frac{\mathrm{i}xp_x}{2}\right)B\,\mathrm{sn}\left[k(x-x_0)+\delta\,|m\right] \times \exp\left[\mathrm{i}C(p_x)\right]. \tag{17}$$

This is the phase-space eigenfunction of dilute-gas BEC modelled with a NLSE for the case of repulsive interactions.

2.2. Attractive nonlinearity

The attractive interactions correspond to '−' in Eq.(13), i.e.

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} - g\left|\Phi_{\mathrm{A}}(x,p_x)\right|^2\right]\Phi_{\mathrm{A}}(x,p_x) = E\Phi_{\mathrm{A}}(x,p_x). \tag{18}$$

Equation (18) also admits an infinite number of exact solutions like Eq.(14), and the most general form of the solutions is

$$\Phi_{\mathrm{A}}(x,p_x) = B\,\mathrm{cn}\left[k(x-x_0)+\delta\,|m\right]\exp\left[\mathrm{i}C(p_x)\right], \tag{19}$$

where $\mathrm{cn}(x\,|m) = \sqrt{1-\mathrm{sn}^2(x\,|m)}$ is also the Jacobian elliptic function,[33] $C(p_x)$ satisfies the same condition as Eq.(16), and the parameters B, k, δ and m will be determined by substitution of Eq.(19) into Eq.(18), the boundary conditions and normalization.

Inserting Eq.(19) into Eq.(11), we obtain

$$\Psi_{\mathrm{A}}(x,p_x) = \exp\left(-\frac{\mathrm{i}xp_x}{2}\right)B\,\mathrm{cn}\left[k(x-x_0)+\delta\,|m\right] \times \exp\left[\mathrm{i}C(p_x)\right]. \tag{20}$$

This is the phase-space eigenfunction of dilute-gas BEC modelled with a NLSE for the case of attractive interactions.

3. Discussion

The eigenenergy E in the quantum phase-space representation will be determined by substitution of Eq.(15) or (19) into Eq.(14) or (18) and the boundary conditions. It can be predicted that the eigenenergy obtained in the phase space is the same as those obtained in the position space. This is easy to understand, because the values of dynamic variables are independent of mathematical representation for a physical system.

Equations (17) and (20) describe the eigen-states of a dilute-gas atom in the BECs within the framework of the quantum phase-space representation for the cases of repulsive and attractive interactions respectively. It is well known that the wavefunctions in position or momentum representation are unique, differing at most by a phase factor. However, the eigenfunctions (17) and (20) are not unique in the phase space due to the arbitrariness of function $C(p_x)$. This is not surprising. Although the choice of operators in Eqs.(5) and (6) seems to determine a Schrödinger equation, and there should be the corresponding unique eigenfunction in the phase space, as we know, the states of a physical system are determined by the eigen-equation and the corresponding boundary conditions. For the phase-space NLSE (7), if the boundary conditions of the position (momentum) part in its eigenfunctions are completely certain, those of momentum (position) parts could not be certain due to the limitation of the Heisenberg uncertainty principle. Since the position and momentum variables are now used simultaneously in phase space, the forms of eigenfunctions must be uncertain in order to incorporate the uncertainty principle. In fact, this is the same in nature as the eigenfunctions of the position and momentum operators, the solutions of the harmonic oscillator, the Morse oscillator, the oscillator with an empirical potential function, the 1D hydrogen atom, and the δ potential fields in the phase space.[9,10,13−16]

If the phase-space eigenfunctions (17) and (20) are projected into position or momentum space through the 'Fourier-like' projection transformation,[9−11] it should be expected that the unique eigenfunctions in position or momentum space can be obtained, since the eigen-equations and the boundary conditions are completely certain in position or momentum space.

As an illustration, we put

$$C(p_x) = x_0 p_x. \tag{21}$$

Strictly speaking, the integral in Eq.(16) does not converge if taken over an infinite limit for Eq.(21); as we know, however, in any real problem, the wavefunction must take the form of a packet, rather than the plane wave, since the particle always exist in a limited position with a finite momentum. We may think of the region of phase space in which such a wavefunction is defined as being arbitrarily large but finite; then the integral in Eq.(16) is over the finite limit of this region and converges.

If $C(p_x)$ is defined as Eq.(21), the phase-space eigenfunctions (17) and (20) will become

$$\begin{aligned}\Psi_{\mathrm{R}}(x,p_x) =& \exp\left(-\frac{\mathrm{i}xp_x}{2}\right) B\,\mathrm{sn}\left[k(x-x_0)+\delta\,|m\right] \\ &\times \exp(\mathrm{i}x_0p_x)\end{aligned} \tag{22}$$

and

$$\begin{aligned}\Psi_{\mathrm{A}}(x,p_x) =& \exp\left(-\frac{\mathrm{i}xp_x}{2}\right) B\,\mathrm{cn}\left[k(x-x_0)+\delta\,|m\right] \\ &\times \exp(\mathrm{i}x_0p_x)\end{aligned} \tag{23}$$

respectively. By using the 'Fourier-like' projection transformation [9−11]

$$\psi(x) = \int_{-\infty}^{+\infty} \mathrm{d}p_x \exp\left(\frac{\mathrm{i}xp_x}{2}\right) \Psi(x,p_x), \tag{24}$$

$$\varphi(p_x) = \int_{-\infty}^{+\infty} \mathrm{d}x \exp\left(-\frac{\mathrm{i}xp_x}{2}\right) \Psi(x,p_x), \tag{25}$$

we project Eqs.(22) and (23) into position and momentum spaces respectively. The results are

$$\psi_{\mathrm{R}}(x) = B\,\mathrm{sn}(kx+\delta\,|m), \tag{26}$$

$$\varphi_{\mathrm{R}}(p_x) = \int_{-\infty}^{+\infty} \mathrm{d}x \exp(-\mathrm{i}xp_x) B\,\mathrm{sn}(kx+\delta\,|m), \tag{27}$$

for Eq.(22), and

$$\psi_{\mathrm{A}}(x) = B\,\mathrm{cn}(kx+\delta\,|m), \tag{28}$$

$$\varphi_{\mathrm{A}}(p_x) = \int_{-\infty}^{+\infty} \mathrm{d}x \exp(-\mathrm{i}xp_x) B\,\mathrm{cn}(kx+\delta\,|m), \tag{29}$$

for Eq.(23), in which the following formula has been used:

$$\begin{aligned}\int_{-\infty}^{+\infty} \mathrm{d}p_x \exp(\mathrm{i}x_0p_x) &= \lim_{L\to\infty} \int_{-L/2}^{L/2} \mathrm{d}p_x \frac{2\pi}{L} \exp\left(\mathrm{i}\frac{2\pi j p_x}{L}\right) \\ &= \delta_{j,0} \quad (j = 0, \pm 1, \pm 2, \cdots).\end{aligned} \tag{30}$$

It is clear that Eqs.(26) and (28) are the same as the eigenfunctions obtained in position representation, while Eqs.(27) and (29) are just the Fourier integrals

of Eqs.(26) and (28) respectively, if the constant factors can be omitted. This means that Eqs.(27) and (29) are also the eigenfunctions in momentum representation.

For Eq.(23), if we let m=1, we can also obtain the hypersecant solution in the position direction. We put $x_0 = 1$ and $\delta = 0$, thus Eq.(19) will be written as

$$\Phi_{\mathrm{A}}(x, p_x) = B \operatorname{sech} k(x-1), \tag{31}$$

therefore Eq.(23) becomes

$$\Psi_{\mathrm{A}}(x, p_x) = B \operatorname{sech} k(x-1) \exp\left[-\frac{\mathrm{i}}{2}(x-2)\, p_x\right]. \tag{32}$$

Inserting Eq.(31) into Eq.(18), we can obtain the relations among the parameters B, k, and the eigenenergy E as follows:

$$gB^2 = k^2, \tag{33}$$

$$2E + k^2 = 0. \tag{34}$$

On the other hand, the eigenfunction (32) should be normalized, i.e.

$$\int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}p_x \left|\Psi_{\mathrm{A}}(x, p_x)\right|^2 = 1, \tag{35}$$

then we can obtain the relation

$$k = 2B^2. \tag{36}$$

From Eqs.(33), (34), and (36), it follows at once that

$$E = -\frac{g^2}{8}, \tag{37}$$

$$B = \frac{\sqrt{g}}{2}, \tag{38}$$

$$k = \frac{g}{2}. \tag{39}$$

Inserting Eqs.(38) and (39) into Eq.(32), we obtain the eigenfunction

$$\Psi_{\mathrm{A}}(x, p_x) = \frac{\sqrt{g}}{2} \operatorname{sech} \frac{g}{2}(x-1) \exp\left[-\frac{\mathrm{i}}{2}(x-2)\, p_x\right], \tag{40}$$

which corresponds to the eigenenergy equation (37).

4. Conclusion

In this paper, we have considered the stationary-state NLSE, which modelled the dilute-gas BEC within the framework of the quantum phase-space representation established by Torres-Vega and Frederick, and obtained the exact solutions of the equation in the phase space. We have also discussed the relationships of eigenfunctions between the phase-space representation and position or momentum representation, and given an instance in which there is a hypersecant part in the phase-space eigenfunction.

The present analysis shows that the wave-mechanics method in TF phase-space representation, which has been developed by many authors, could be extended to the NLSE. The phase-space wavefunctions can describe the dilute-gas BECs; therefore, they provide the foundation for approximate calculation in the future.

For a physical problem, the arbitrary function, $C(p_x)$, in the function by using wave-mechanics method could be chosen as some suitable form in order to simplify the mathematical treatment in phase space.

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