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BAND ALIGNMENT OF ULTRATHIN GIZO/SiO2/Si HETEROSTRUCTURE DETERMINED BY ELECTRON SPECTROSCOPY

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CORRECTION OF THE GROUND STATE ENERGY
OF ONE-DIMENSIONAL GROSS-PITAEVSKII EQUATION
WITH GAIN-LOSS TERM

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Abstract

We consider the correction of ground state energy of one-dimensional Gross-Pitaevskii equation by adding a gain-loss term as a time-dependent external potential. The interesting purpose of this term is that it can be used to explain the experimental results especially in the nonlinear fiber optics regarding the pulse propagation and collapse-revival of the condensate in the Bose-Einstein condensation. In the Bose-Einstein condensation itself, the function can represent that condensate can interact with the normal atomic cloud. Some analytical solutions have been obtained by choosing an ansatz solution of the wave function and its solution can be dark or bright soliton. Since the Gross-Pitaevskii equation can be treated as a macroscopic quantum oscillator, we can use time-dependent perturbation theory as in ordinary quantum mechanics to find the ground state energy correction if we assume other terms to be very small. In addition, time-dependent potential allows a transition from one energy level to others. In this case, we expand the solution of nonstationary one-dimensional wave function as a linear superposition of harmonic oscillator normalized eigen functions. To get the recursive formulas, we suggest an option to formulate the coefficients after inserting the initial condition which must be satisfied such as in quantum mechanics.

Keywords: Bose-Einstein condensation, Gross-Pitaevskii, quantum oscillator

1. Introduction

The realization of Bose-Einstein condensation (BEC) in ultra cold atomic gases was initially verified by a sequence of experiments in 1995 by Anderson *et al*. (vapor of rubidium) and Davis *et al*. (vapor of sodium) that those atoms were confined in magnetic traps and cooled down to low temperatures at an order of microkelvins [1]. For the detail discussions see also [2-3]. On the other hand, cigar-shaped BEC has been considered as an interesting subject especially in the coherent atom optics [4-6]. In these verifications, theoretical exploration of characteristic of Bose gases needs a mathematical model describing those systems at very low temperatures. The first proposed model is the nonlinear Schrödinger equation, which is usually called Gross-Pitaevskii equation (GPE), which describes the dynamics of interacting condensed atomic clouds in three-dimensional, trapped in anisotropic external parabolic potential achieved by magnetic trap. Some discussions on the results of GPE have been considered by reducing it to one-dimensional model by assuming the case of cigar trap (highly anisotropic) of the axial symmetry [7-11]. This is observed as a classical

nonlinear equation that can be treated as a nonlinear generalization of a macroscopic quantum oscillator [9]. Although the model is considered as a valid model for analyzing BEC at $T \cong 0$ K, GPE has no analytical solution for cylindrical symmetry, except in the framework of Thomas Fermi approximation [7,9]. However, the general property of GPE equation is the existence of soliton solutions shown by their numerical result since GPE is a pure nonlinear Schrödinger equation if we only keep nonlinear potential and remove all the rest of external potential terms.

In literatures, many authors investigated the effect of gravitation [12] by adding the gravitational potential as an external interaction, gain or loss in the discussion of pulse propagation in nonlinear fiber optics and collapse-revival of the condensate by adding a time-dependent function [13-14]. Here, we are interested in discussing the effect of gain or loss as described by the time-dependent potential in GPE. In recent Letters [13-14], an analytical solution has been obtained by proposing an ansatz wave function solution. The ansatz solution is chosen by the recent inspiring experiments. The aim of this paper is to find the correction of ground state

energy of the macroscopic oscillator by extending the work done by Kivshar *et al.* [7], who suggested that physical features of eigen modes remain valid in the nonlinear case.

In this paper, we analyze the correction of nonlinear eigen energy of the macroscopic quantum oscillator ground state by using time-dependent perturbation theory. For this purpose, we extend a similar procedure proposed by Kivshar *et al.* [7] by assuming that a one-dimensional nonlinear nonstationary state is built by applying linear superposition of quantum oscillator normalized eigen functions. The rest of this paper is organized as follows. We derive the mathematical model of GPE in Sec. 2 by applying axial symmetry and transforming all coordinates into dimensionless ones in order to reduce 3D nonstationary GPE into 1D nonstationary GPE. In Sec. 3, we apply our nonstationary GPE equation to calculate the correction of ground state energy of macroscopic oscillator system represented by expansion coefficients. We close our discussion in Sec. 4 with conclusions based on our final results.

2. Methods

In this section, our concern is to reduce 3D nonstationary GPE into 1D nonstationary GPE by applying axial symmetry. We start with considering condensed atomic clouds confined in a three-dimensional anisotropic parabolic potential and contained loss or gain term $\eta(t)$ [13-14]

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

where $\psi(\vec{r},t)$ is the macroscopic wave function of condensate, $V(\vec{r})$ is the three-dimensional anisotropic parabolic trap given by

$$V(\vec{r}) = \frac{1}{2}m\omega^2\left(\lambda_x^2 x^2 + \lambda_y^2 y^2 + \lambda_z^2 z^2\right) \quad (2)$$

$U = 4\pi\hbar^2 a/m$ (a is the s-wave scattering length) describes two-particle interaction in the condensate which can be repulsive ($a > 0$) or attractive ($a < 0$), and $\eta(t)$ is the arbitrary function which is phenomenologically related by a gain or loss term. The wave function itself is assumed to be normalized by defining the number of particles in condensate

$$N = \int|\psi|^2 d^3\vec{r} \quad (3)$$

To discuss cigar-shaped BEC of the axial symmetry, we imply the condition on parabolic trap $\lambda_x = \lambda_y = 1$ and define the parameter λ_z as the quotient between frequency propagating along z direction (ω_z) and radial one (ω), $\lambda_z = \omega_z/\omega$, is very small $\lambda_z \ll 1$. After that, it is convenient to transform cylinder coordinate to

dimensionless coordinate in order to make easier our discussion (some authors have their conventions, for comparison see [7-9])

$$\tau = \frac{1}{2}\omega\lambda_z t , \quad (4)$$

$$z = a_0 s , \quad (5)$$

$$r = a_0\rho , \quad (6)$$

where $r = \sqrt{x^2 + y^2}$ and $a_0 = \sqrt{\hbar/m\omega\lambda_z}$ is the harmonic oscillator length with frequency ω_z. In addition, we also define new functions by the following transformations

$$g(t) = \frac{i}{2\hbar\omega\lambda_z}\eta(t) , \quad (7)$$

$$u(\rho, s, \tau) = \psi(r, z, t)\sqrt{\frac{a_0^3}{N}} , \quad (8)$$

and the quantity

$$Q = -\frac{8\pi Na}{a_0} \quad (9)$$

With these changes, the GPE in Eq. (1) becomes

$$i\frac{\partial u}{\partial\tau} = -\nabla^2 u + \left(\frac{\rho^2}{\lambda_z^2} + s^2\right)u - Q|u|^2 u + g(\tau)u \quad (10)$$

Now, our purpose is to simplify Eq. (10) in order to make separated variables by defining the wave function $u(\rho, s, \tau)$ under the transformation

$$u(\rho, s, \tau) = \phi(\rho)\varepsilon(s, \tau)e^{-2i\gamma\tau} \quad (11)$$

After substituting Eq. (11) into Eq. (10), one obtains two expressions in the left and right hand side. To make equations consistent both sides should be constant. For simplicity we choose the constant value to be zero. By this condition, one of those two expressions should be quantum harmonic oscillator in two dimensions written in polar coordinate as

$$\frac{1}{\rho}\frac{d}{d\rho}\left(\rho\frac{d\phi}{d\rho}\right) + 2\gamma\phi - \frac{\rho^2}{\lambda_z^2}\phi = 0 \quad (12)$$

One of the simple solutions is the ground state solution which can be chosen as

$$\phi(\rho) = C\exp\left(-\gamma\rho^2/2\right) \quad (13)$$

For this choice, the arbitrary parameter γ in Eq. (11) can be related to λ_z by substituting Eq. (13) into Eq. (12), then one will obtain $\gamma = 1/\lambda_z$. On the other hand, C can be determined by imposing the normalization condition

$$\int_{\rho=0}^{\infty}\int_{\theta=0}^{2\pi}|\phi|^2\rho\,d\rho\,d\theta = 1 \quad (14)$$

and one will also get $C = \sqrt{\gamma/\pi}$

Since the last expression still contains ϕ term, we have to eliminate the dependence of ϕ by multiplying both sides by $|\phi|^2$, integrating over the space and absorbing the resulting constant into Q, thus one will obtain one-dimensional nonstationary GPE

$$i\frac{\partial\varepsilon}{\partial\tau}+\frac{\partial^2\varepsilon}{\partial s^2}-s^2\varepsilon+Q|\varepsilon|^2\varepsilon-g(\tau)\varepsilon=0 \qquad (15)$$

3. Results and Discussion

In Sec. 2, we have derived the one-dimensional nonstationary GPE which can be considered as the propagating nonlinear wave along s direction. If we remove the nonlinear and gain-loss term, the problem should be the one-dimensional eigenvalue equation of quantum harmonic oscillator. By this fact, we can apply perturbative solution which 1D nonstationary GPE solutions in Eq. (15) should be an expansion of a set normalized eigenfunctions of harmonic oscillator. Before discussing the solution method, we should review some useful expressions of 1D quantum harmonic oscillator in dimensionless unit. The eigenvalue equation in ordinary quantum mechanics can be written as

$$-\frac{d^2\Omega_n}{ds^2}+s^2\Omega_n=E_n\Omega_n \qquad (16)$$

where $E_n=2n+1$ are discrete energies and $\Omega_n(s)$ should be normalized eigenfunctions of harmonic oscillator in quantum mechanics written in dimensionless unit

$$\Omega_n(s)=\sqrt{\frac{1}{2^n n!\sqrt{\pi}}}e^{-s^2/2}H_n(s) \qquad (17)$$

Here, $H_n(s)$ are Hermite polynomials written in Rodrigues formula

$$H_n(s)=(-1)^n e^{s^2}\frac{d^n}{ds^n}\left(e^{-s^2}\right) \qquad (18)$$

Finally, the perturbative GPE solution can be supposed in the form

$$\varepsilon(s,\tau)=e^{-iE\tau}\sum_{n=0}A_n(\tau)\Omega_n(s) \qquad (19)$$

where E is the total energy of system. After inserting the expansion (19) into Eq. (15), multiplying by Ω_m^* on both sides, and integrating over the space, we obtain the following equation

$$A_m(\tau)(E-E_m-g(\tau))+\dot{A}_m(\tau)$$
$$+Q\sum_{nlk=0}A_n^*(\tau)A_l(\tau)A_k(\tau)V_{mnlk}=0 \qquad (20)$$

where $\dot{A}_m=dA_m/d\tau$ and

$$V_{mnlk}=\int_{-\infty}^{\infty}\Omega_m^*(s)\Omega_n^*(s)\Omega_l(s)\Omega_k(s)ds \qquad (21)$$

For the ground state case ($m=0$), we assume that $A_0 >> A_m$ for $m\neq 0$, we find the expression

$$\dot{A}_0(\tau)=-A_0(\tau)(E-E_0-g(\tau))$$
$$-Q|A_0(\tau)|^2 A_0(\tau)V_{0000} \qquad (22)$$

To include the initial condition to the expansion coefficients and gain-loss term, we propose one suggestion at $\tau=0$, according to the time-dependent perturbation theory in quantum mechanics system should be in the particular state. However, we can choose the state as the ground state since we only concern at that state

$$\varepsilon(s,0)=\Omega_0(s). \qquad (23)$$

By this assumption, we conclude that the initial condition satisfied by A_0 should be written as

$$A_0(0)=\delta_{00} \text{ and } \dot{A}_0(0)=0 \qquad (24)$$

In addition, we also apply the initial condition for $g(\tau)$, let us say $g(\tau=0)=g(0)$. Finally, after inserting all the conditions into Eq. (22) simultaneously, we obtain the correction of the ground state energy as

$$E=E_0+g(0)-Q|A_0(0)|^2 V_{0000} \qquad (25)$$

By observing that sets of Ω_n are even functions for even n, $\Omega_n(s)=\Omega_n(-s)$, it is possible to construct the formulation of all even coefficients via Eq. (20) by solving linear differential equation

$$\dot{A}_{2p}(\tau)+A_{2p}(\tau)(E-E_{2p}-g(\tau))$$
$$=-Q|A_0(\tau)|^2 A_0(\tau)V_{(2p)000}, \quad p\neq 0 \qquad (26)$$

Note that one could also solve first-order linear differential equation by using Frobenius method to obtain the coefficients, should the explicit functions have been known.

4. Conclusion

We have obtained the correction of ground state energy of one-dimensional GPE with gain-loss term by applying time-dependent perturbation theory and assuming that physical entities of eigen modes remain valid in the nonlinear case. The gain-loss term itself can be considered as a time-dependent potential describing the interaction between the condensate and normal atomic cloud. To obtain the solution, we have reduced the three-dimensional GPE into one-dimensional GPE by transforming all quantities in the equation and applying the axial symmetry. In this case, we suggest an alternative perturbative solution to obtain the correction by expanding the coefficients and applying the conditions.

The extension of GPE by including gain-loss term is inspired by a series of experimental results of

propagation of pulse in nonlinear fiber optics and collapse-revival of the condensate [14]. Both of them describe the propagating soliton which can be dark or bright. Specially, we can determine the appropriate function of gain-loss term to explain the experiment result. Some specific functions have been considered, for example in Ref. [13-14] in order to analyze special cases, discussion about nonlinear fiber optics in Ref. [13] and soliton trains of BEC in Ref. [14]. However, in some literatures BEC is also used as a model to study the cosmological aspects [15-17], for example for the description of dark matter [18].

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