Condensate wave function of neutral Bose atoms in power-law traps

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The macroscopic quantum states of a condensed neutral Bose gas in one-dimensional power-law traps are obtained by solving the Gross-Pitaevskii equation numerically. A suitable candidate for a trial wave function for the variational calculation of ground state energy is suggested, and shown that the suggested function produces a lower ground state energy than the conventional Gaussian trial wave function.

Key words: Bose-Einstein condensation, power-law traps

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Bose-Einstein condensation (BEC) is a first order phase transition of bosonic particles when the thermal de Broglie wavelength exceeds the mean spacing between particles. The first BEC was observed in a series of the landmark experiments in 1995 on alkali vapors in which the atoms were confined in magnetic traps and cooled down to sub μ-Kelvin temperatures. Some of the relevant features of these trapped Bose gases are that they are inhomogeneous, and a harmonic external potential is typically used to describe such a trapped system. However, due to the development of the experimental techniques of magnetic traps, the shape of the external trap can be managed intentionally, and power-law traps in the form of $V_{\text{trap}} \sim r^k (k > 0)$ are accessible now.

Bosonic atoms in optical lattices and periodic potentials often require non-harmonic traps such as elliptic or a trough type traps [1, 2]. Therefore, it is necessary to predict the condensate wave functions in arbitrary power traps since it has related with theoretical study of BEC such as the variational calculation of the ground state energy of the condensed atoms. In harmonic traps a Gaussian trial function of $psi(r,t) = exp(-r^2/2)$ is generally applied to the variational calculation, but the form is not guaranteed the adequate low energy in the power-law traps. Surprisingly, the shape of the condensate function at power-law traps has not been investigated in spite of many studies of power-law traps [3, 4]. Most of the previous works reported mainly transition temperatures and condensate fractions.

At zero temperature, the condensate wave function of the typical model can be described by a non-linear Schrödinger equation, named as the Gross-Pitaevskii equation (GPE). It is a mean-field approximation for the macroscopic wave function of weakly interacting bosons.

In this short note we’ll solve the one-dimensional GPE at a few power-law traps numerically, and suggest the shapes of the new condensate wave functions that lowers the ground state energy than the Gaussian form. Then, we will follow the three steps to compare the three energies: 1) Apply the above numerical wave functions to the Hamiltonian directly and obtain the ground state energy numerically. 2) Apply the new trial function to the Hamiltonian, and obtain the lowest state energy analytically. 3) Apply the conventional Gaussian trial function to the hamiltonian and obtain the lowest state energy analytically.

The GPE for $N$ interacting bosons confined by an external trap potential $V_{\text{trap}}$ and under delta-type interaction is written as

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}}(r) + g|\Psi(r,t)|^2 \right\} \Psi(r,t),$$

where $g$ is the interaction strength given by $g = 4\pi\hbar^2a/m$. The $a$ is the s-wave scattering length and $m$ is the mass. The $\Psi(r,t)$ is real and normalized to the total number of particles, $N$. We choose the power-law potential for the external trap of the form $V_{\text{trap}}(r) = cr^k$ where $c$ is a positive constant that satisfies the dimensionality condition, and $k = 1, 2, 3, \ldots$. Note that $k = 1$ corresponds to a linear trap, and $k = 4$ to a quadratic trap, and so on.

A scaling of variables such as $a_{ho} = \sqrt{\hbar/m\omega}$ for the length, and $\hbar\omega$ for the energy reduces Eq. (1) to a dimensionless form [3, 4]. It corresponds to $\hbar = m = \omega = 1$ in Eq. (1). We consider the one dimensional case because it is good enough for the comparison.

$$\frac{\partial \psi}{\partial t} = \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} x^k + P|\psi|^2 \right] \psi(x,t),$$

For convenience we chose $c = 1/2$ with an adjusted dimension of energy. The $P$ is the dimensionless number parameter defined by $P = 4\pi N|a|/a_{ho}$, which is

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FIG. 1: Density profile of condensed bosons at one-dimensional power-law traps. (a) for linear trap, $k = 1$, (b) for harmonic trap, $k = 2$, and (c) for quadratic trap, $k = 4$. Solid line for $P = 0.1$, long dashed lines for $P = 1$, short dashed line for $p = 10$, and dotted lines for $P = 100$.

the only variable that differentiate each atoms. Note that $|a|/a_{ho}$ is order of $10^{-3}$ for alkali atoms, and then, $P = 1$ corresponds approximately to $N = 10^2$. $\psi(x,t) = \psi(x)\exp(-i\mu t/\hbar)$ is normalized to unity, and $\mu$ is the chemical potential.

We have carried out a numerical procedure for Eq. (2), and have obtained the static solution $\psi(x)$ at various powers. Fig. 1(a) is for the linear trap ($k = 1$), and Fig. 1(b) is for the well-known harmonic trap ($k = 2$), and Fig. 1(c) is for the quadratic trap ($k = 4$). For small number of particles there is little dependence of the traps, and the wave function is close to the Gaussian. However, for large number of particles the wave function does not resemble the Gaussian any more, and it depends seriously on the power of the traps.

In the strongly repulsive limit of $P \gg 1$, the kinetic energy term in Eq. (2) is neglected and then the solution becomes $\psi^2(x) = (\mu - \frac{1}{2}x^k)/P$. However, it is not applicable for most of large realistic $P$'s. Therefore, we need to propose an alternative trial function for a large number of particles. We suggest it as $\psi(x) \sim \exp(-x^k)$ at the $k$-th power-law traps where $k = 1, 2, 3, \ldots$. Then, the Gaussian trial function is a special case for the harmonic traps.

To check the effectiveness of the new trial function, we need to compare the ground state energy densities produced by the new ones with two others: One from the direct numerical calculation by the Fig. 1, and the other from the analytic calculation by the conventional Gaussian trial functions. Similar to Eq. (2), the ground state energy per particle at one-dimension can be written in the dimensionless form [7, 8]

$$\frac{E}{N} = \frac{1}{2} \int_{-\infty}^{\infty} dx \left[ \left( \frac{\partial \psi}{\partial x} \right)^2 + x^k \psi^2(x) + P \psi^4(x) \right]. \quad (3)$$

One can minimize the energy densities in Eq. (3) using the variational ansatz with the new trial function

$$\psi_K(x) = A_k e^{-\frac{d}{2}(x)^k}, \quad (4)$$

and with the Gaussian trial function

$$\psi_G(x) = A_2 e^{-\frac{1}{2}(x)^2}. \quad (5)$$

The $d$ is the variational parameter which fixes the width of the condensate. $A_k$ is determined from the constraint $\int_{-\infty}^{\infty} \psi^2(x) dx = 1$. Then, $A_k = \sqrt{k/4\pi \Gamma(3/k)d^3}$.

Substituting $\psi_{K,G}$ in Eqs. (4) and (5) into Eq. (3), we obtain the energies per particle $E_{K,G}/N = f_{K,G}$ respec-
tively as
\[
f_K(d) = \frac{(k+1)\Gamma \left(\frac{1}{k}\right)}{8\Gamma \left(\frac{2}{k}\right) d^2} + \frac{3}{2k} d^k + \frac{kP}{2^{k+\frac{3}{2}} \pi \Gamma \left(\frac{2}{k}\right) d^3},
\]
and
\[
f_G(d) = \frac{3}{4d^2} + \frac{\Gamma \left(\frac{k+2}{2}\right)}{\sqrt{\pi}} d^k + \frac{P}{4\pi \sqrt{2\pi d^3}},
\]
where \(\Gamma\) is the Gamma function. It is clear that \(f_K = f_G\) when \(k = 2\).

We have determined the minimum of the energy densities by solving \(df_{K,G}/dd_c|_{d_c} = 0\) numerically, and plotted \(f_{K,G}(d_c)\) as a function of \(\log P\). Fig. 2(a) is for the linear trap, and Fig. 2(b) is for the quadratic trap. At small number of atoms such as \(\log P < 1\), the lowest energies by the two trial functions show similar values with the numerical calculation. On the other hand, for large number of atoms the trial function does not always guarantee an effective approximation for the ground state. It depends strongly on the power of the trap. At the quadratic trap the two trial functions are still good enough for the ground state even for large number of atoms, but at the linear trap it is not effective anymore. However, as we see, the new trial functions always produce the lower energies than the Gaussian.

We studied the solution of the one-dimensional GPE of neutral Bose atoms under power-law traps numerically, and suggested a better trial wave function, \(exp(-r^k)\), beyond Gaussian. We showed that the new trial function produce lower energy densities than the Gaussian. It can be applicable effectively for condensed wave functions at any non-harmonic traps.

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