



Trapping potentials controlled wave function distributions in BEC

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Abstract: This paper will focus on theoretical treatment of one-dimension harmonic oscillator potential HOP which is usually used in experiments that lead to produced Bose-Einstein condensation BEC in ultra-cold gases. This analysis will focus mainly on the anisotropy parameter and the role that this factor play in term of values and shapes of the trapping potential, initial wave function and final wave function. This specific study will give us the overall view of the region of confinement that the HOP has employed. The study is extended to the chemical potential and the energy of the working fluid.

Keywords: Laser cooled atom, BEC atom, Trapping, condensation, Atom Laser

I. Introduction

One of the most interesting properties of a system of bosons is that under certain conditions it is possible to have a phase transition at a critical value of the temperature in which all of the bosons can condense into the ground state. It is now well over eighty years since the phenomenon referred to as Bose-Einstein condensation (BEC) was first predicted for the ideal nonrelativistic Bose gas [1, 2]. BEC could occur in a real physical system, as suggested originally by London [3], and could occur also for exactions in certain types of non-metallic crystals (such as CuCl for example). There is now good evidence for this in a number of experiments [4-9]. the early BEC experiments achieving the condensed state around 100 nK. Their creation became possible after the development of appropriate experimental techniques needed to reach the necessary ultra-low temperatures (see, e.g., Ref. [10]). The required extreme cooling is achieved in two stages. First, the method of laser cooling (which was also rewarded with the Nobel Prize in Physics for 1997 [11]) is applied to the gas loaded into a magneto-optical trap, which makes it possible to create a moderately cool state, at temperature $\sim 100 \mu\text{K}$. Next, this state undergoes forced evaporative cooling, losing $\sim 90\%$ of atoms, and the remaining atomic cloud spontaneously forms the BEC. The applicability of the laser-cooling method to particular atomic species depends on the peculiarities of their electron configuration. As a result, this technique has made it possible to achieve the Bose-Einstein condensation in vapors of alkaline, alkaline-earth, and lanthanide metals: ^7Li , ^{23}Na , ^{39}K , ^{41}K , ^{85}Rb , ^{87}Rb , ^{133}Cs , ^{52}Cr , ^{40}Ca , ^{84}Sr , ^{86}Sr , ^{88}Sr , ^{174}Yb , ^{164}Dy , and ^{168}Er . The creation of BEC in the gases of chromium [12-14] and dysprosium [15] are more interesting because these atoms carry large magnetic moments, which makes it possible to predict and observe many effects produced by long-range dipole-dipole interactions [16]. BEC in the gas of spin-polarized hydrogen atoms has been also achieved, with a specially devised technique which made it possible to cool the gas to $50 \mu\text{K}$ [17]. The number of atoms involved in creation BEC is ranged from a few thousand to a few million, in potential wells that were to a good approximation anisotropic harmonic oscillator potentials. Such a spatial BEC gives rise to unique theoretical question, that is did these recent theoretical models give a true distribution of the wave function for the BEC state. The answer is, obviously, no, because these models unsuccessful to describe exactly the distribution of the BEC state. In this study we try to analysis the distributions of the wave function and the harmonic oscillator trapping potentials theoretically under the action of the anisotropy parameters. The relation between the chemical potentials and the energy is also taken into account.

II. Theory

The theoretical study of BEC develops its full richness only after realistic interatomic interactions are included. Although the density of atoms is extremely low, two-body collisions and two-body correlations play important roles in the detailed properties of the condensate [18]. By treating the two-body interaction as a contact interaction, the many-body mean Field theory reduces to the non-linear Gross-Pitaevskii (GP) equation [1].

$$\left[-\frac{\hbar^2}{2m} \sum_{i=1}^{N+1} \{\nabla_i^2 + V_{\text{ext}}(r_i)\} + \sum_{i<j=2}^{N+1} V(r_i - r_j) \right] \psi(r) = E\psi(r) \quad (1)$$

Where m is the mass of each particle and $V_{\text{ext}} = \frac{1}{2}m\omega^2 r_i^2$ is the harmonic trapping field, ω being the frequency of the trap. The numerical solution of GP equation is fairly easy and a lot of work has already been done [18-21] to study the static, dynamic and thermodynamic properties of the condensate. However, the corresponding wave function does not include any correlations produced by the interaction when two atoms are close to each

other. In a mean-field approach the many-body wave function is taken as a product of single particle wave functions, which are obtained variationally. Clearly then the many-body wave function does not have any dependence on the relative separations of two or more particles. Thus to make the pictures easier one have to rewrite the nonlinear Gross-Pitaevskii in one-dimension as follows:

$$\left[-\frac{\hbar^2}{2m} \sum_{i=1}^{N+1} \{\nabla_i^2 + V_{ext}(x_i)\} + \sum_{i<j=2}^{N+1} V(x_i - x_j) \right] \psi(x) = E\psi(x) \quad (2)$$

$V_{ext} = \frac{1}{2} m \omega^2 x_i^2$ is the harmonic trapping field in one dimension. For simplicity we will drop the summation and moreover we will define H_0 as the Hamiltonian for an isolated atom in the trap, N_0 as the number of atoms in the condensate, U_0 represents the interaction between condensate atoms so we can write:

$$[H_0 + N_0 U_0 |\psi(x)|^2] \psi(x) = E\psi(x) \quad (3)$$

$$H_0 = -\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(x) \quad (4)$$

V_{trap} can be described by the anisotropic harmonic oscillator given above. Essentially the GPE is a Schrodinger equation with a total potential energy consisting of an external potential $V_{trap}(x)$ and also the additional nonlinear term $U_0 |\psi(x)|^2$ which represents the mean field produced by the interaction between the bosons. The time dependent GPE can be written as:

$$\left[i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(x) + N_0 U_0 |\psi(x,t)|^2 \right] \psi(x,t) \quad (5)$$

The equation determines the quantum wave function $\psi(x,t)$ of a gas of bosons in the limit in which thermal and quantum fluctuations are negligibly small. The three terms on the right side of the GPE derive from the condensate's kinetic energy T , the potential energy P_{ext} of interaction with the confining potential $V_{trap}(x)$, and the energy $G = N_0 U_0$ of mean field atom-atom interactions. For repulsive interactions ($G > 0$), the energy functional $E = T + P_{ext} + G$ is convex and its minimum delivers the gas's stable ground state. For $G < 0$, the gas is stable only at low coupling for limited numbers of bosons in the trap, as long as the zero-point energy balances the effect of attractions and prevents collapse. The wave equation's quantum nature requires more care than classical problems. As is well known, simple first-order time-marching schemes, such as forward Euler which are unconditionally unstable—that is, they break unitarily for any finite dt no matter how small. Several ways out of this difficulty exist. However The Crank-Nicolson (CN) method is the slogger for the numerical integration of quantum wave equations. The method's major advantage is that it ensures unitarity for an arbitrary size of the time step dt . This lets the wave function advance by large steps—that is, larger than the inverse of the highest eigen value $\omega_{MAX} = E_{max}/\hbar$. Only accuracy (at the second order) limits the time-step size, not stability or unitarity considerations. The CN method requires us to solve a matrix algebraic problem at each time step. This is a fairly expensive computational task. To solve the GPE several properties should be assign that are:

- A first property of the GPE is the time invariance. This means that the equation is time reversible: the equation is stable with respect to the time change of variable $t \rightarrow -t$.
- A second property is known as invariance by phase shift or gauge invariance: if $\tilde{\psi}$ is the solution to equation (5), then $\psi = \tilde{\psi} e^{-i\alpha t}$ is solution to (5) with $V \rightarrow V + \alpha$.
- Invariants: mass conservation The mass is defined by:

$$N(t) = N(\psi(t, \cdot)) = \int_x |\psi|^2 dx, \forall t > 0. \quad (6)$$

Then we can prove that we have the mass conservation $N(t) = N(0)$.

- Another conserved quantity is the energy: let us introduce the energy functional E_ψ as

$$E_\psi = \int_x \left\{ \frac{1}{2} |\psi|^2 + V(x) |\psi|^2 + \beta(|\psi|^2) \right\} dx, \forall t \geq 0. \quad (7)$$

where the primitive B of β is defined as:

$$B(\lambda) = \int_0^\lambda \beta(\lambda) d\lambda. \quad (8)$$

Then we have the energy conservation property $E_\psi = E_{\psi_0}$.

- A last property of interest is related to the dispersion relation providing hence special solutions: the plane wave

$$\psi(t, x) = a e^{i(kx - \omega t)} \quad (9)$$

is solution to system (5) (with $V = 0$) if the following nonlinear dispersion relation holds

$$\omega = \|k\|^2 / 2 + \beta(|a|^2), \quad (10)$$

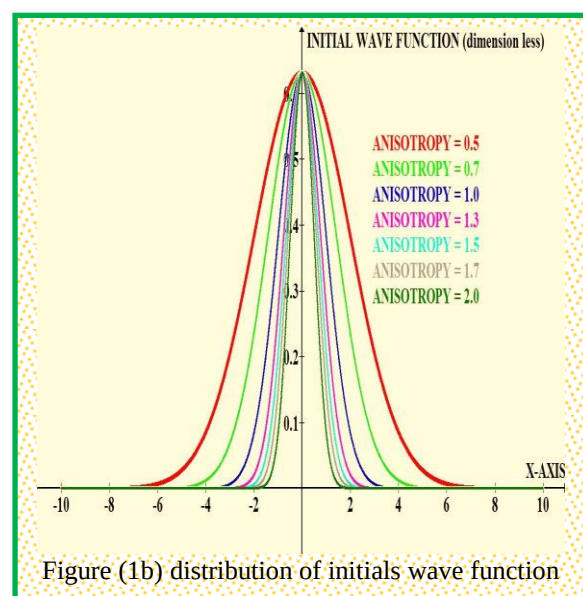
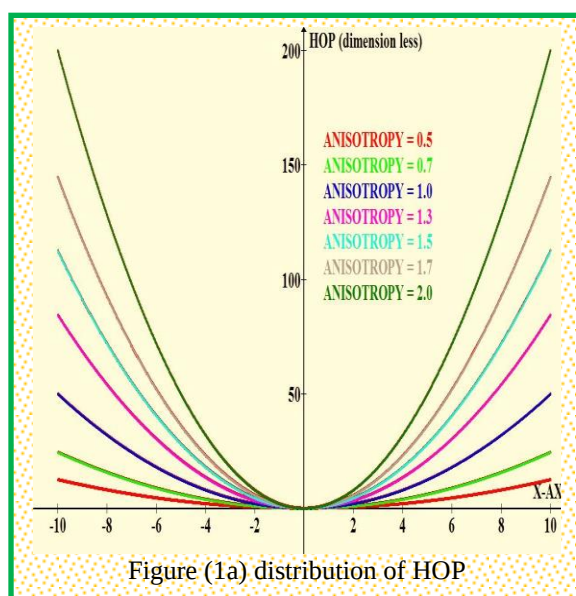
where $\|\cdot\|$ is the usual 2-norm for complex valued vector fields.

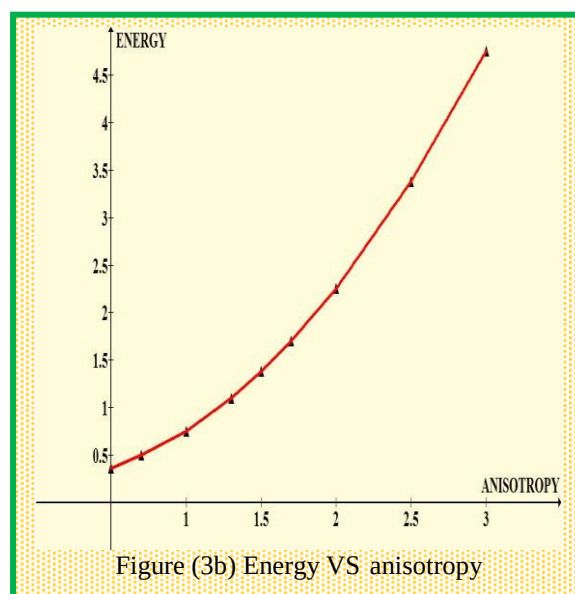
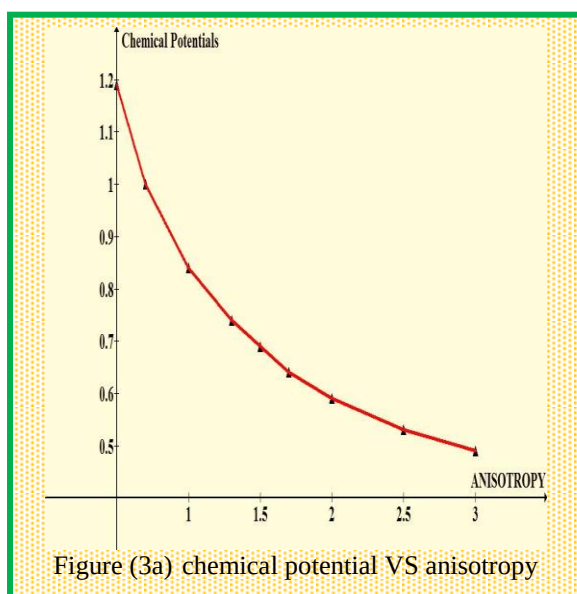
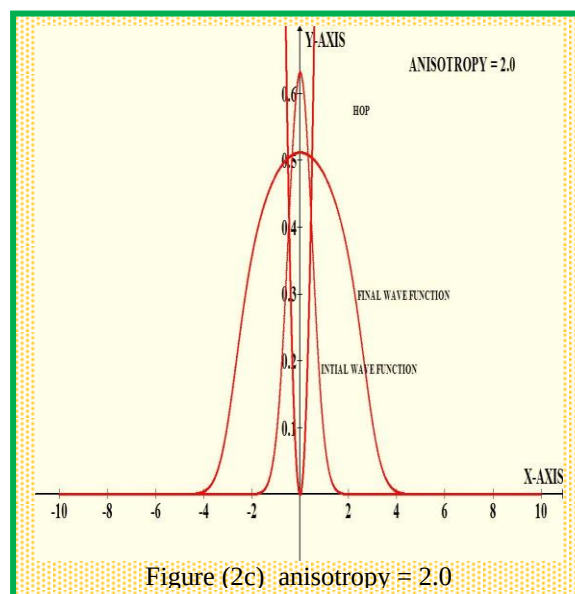
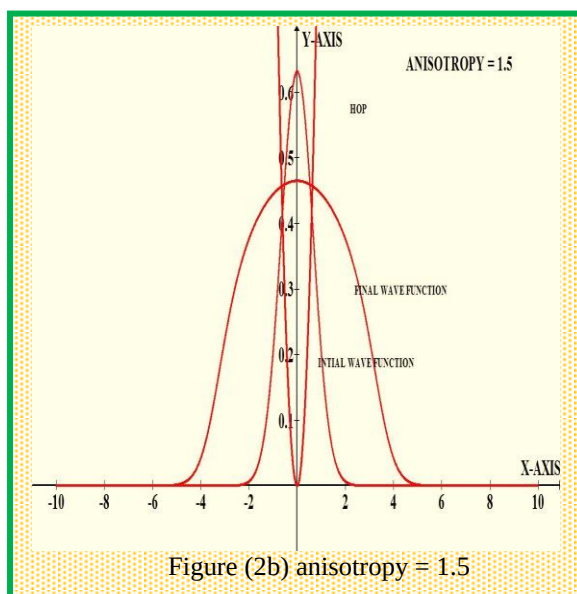
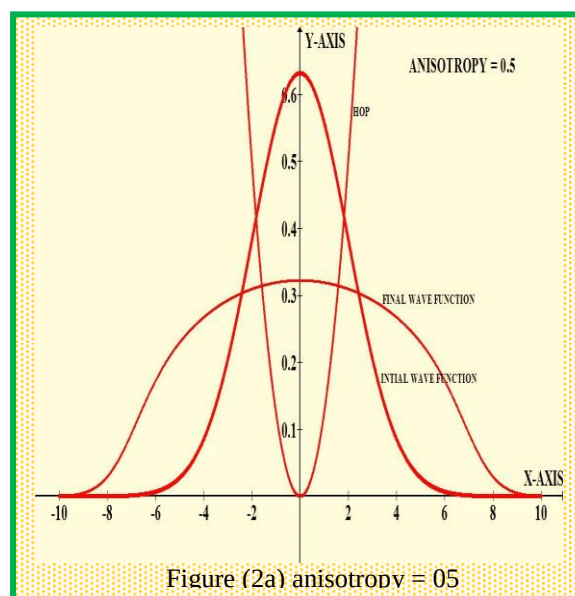
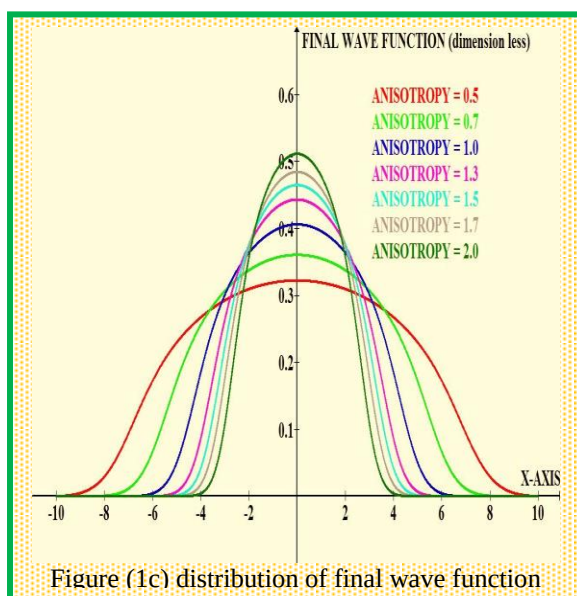
III. Result and Discussion

Our calculations are for the ideal gas. In the thermodynamic limit the density becomes infinite at the origin in a harmonic potential. It is easy to extend the ideal gas calculations to include a mean-field interaction. Because the actual experiments are done with just a few particles, the ideal gas should become a fair approximation to the real experiments, and the density divergence of the ideal gas should never become an issue. We re-examine and extend the analysis of Bose-Einstein condensation in an external harmonic potential here. The one-dimensional

system of N non-interacting Bosons with the particles contained in an isotropic one-dimensional harmonic potential are analysis in this work. In this paper we have examined several features of BEC in harmonic potentials for the ideal gas theoretically which we are going to explain it as follow: First of all it's worth to mention that the working field is divide into 8000 point in space coordinates, and divide into 200000 point in time coordinates, the space interval is $DX = 0.0025$ and the time interval is $DT = 0.0002$, the nonlinearity is fixed to the value of 62.742, the total number of runs for each case is 20000.

- 1) Figure (1a) shows a one dimensional distribution of harmonic oscillator potential along the working field which is the X-axis, for different values of an isotropy (0.5, 0.7, 1.0, 1.3, 1.5, 1.7, 2.0). One can see from this figure that the distribution of the HOP is symmetric and has a shape of parabola, the an isotropy has no influences on this shape of this distribution, but the distribution become narrow as the values of an isotropy increases. Moreover the values of the HOP increase as the isotropy increases.
- 2) Figure (1b) shows the corresponding normalized distribution of the initial wave function for same values of the HOP. The normalized distribution look like Gaussian shape profile. The main conclusion of this figure is that the maximum values of the wave function has not affected by anisotropy values, but one can see clearly that the distribution become more narrow when the an isotropy increase.
- 3) Figure (1c) shows the distribution of the normalized final wave function after 20000 runs. One can conclude from this figure that the maximum values of the wave function are change as the anisotropy parameters of the HOP change. As the anisotropy parameters increase the wave function increase, the Gaussian like distribution of the final wave function is not affected by the anisotropy parameter.
- 4) For more analysis of figures (1), one can plot a judgement figures for specific values of anisotropy this is done by figures (2). Figure (2a) shows the distribution of the trapping HOP together with the normalize distribution of the initial and final wave function for the specific value of the anisotropy that is 0.5. This plot shows that the distribution of the HOP around the X-axis is cover the area almost from -2.0 to 2.0, whereas the initial wave function distribution extended almost from -4.0 to 4.0 along the X-axis, and the maximum value exceed 0.6. The final wave function distribution are well behind this picture, this wave function is cover the area along the X-axis extended from -0.9 to 0.9 with the maximum value of the final wave function almost greater than 0.3. As the anisotropy increase to the value of 1.5 or 2.0 one can see the difference which are quite clear in figures (2b) and (2c) for the distributions of the HOP, initials and final wave functions.
- 5) Figure (3a) shows the chemical potentials as a function of anisotropy. The chemical potentials are decreases exponentially as the anisotropy increases. This picture is true because the chemical potential is connected with the final wave function, and we have shown that the maximum value of the final wave function is decrease as the anisotropy increase. One knows from the basics physics that the particles tend to move from higher chemical potential system to the lower chemical potential. In our case one can say that as the anisotropy increase the atoms in higher or excitation energy state ten to move to the lower or ground energy state which in turn forms what is called BEC.
- 6) Finally figure (3b) shows the energy is plotted as a function of the anisotropy. The energy is increase almost exponentially as the anisotropy increase which mean that the force exerted on the gas atom will increase which tend to confine the atom in a very small area at the center of the working field.





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