

Few Excited State Energies and Chemical Potential Energy of ^{87}Rb Condensate by Many-Body Approach

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Abstract

We consider experimental ^{87}Rb condensate which is trapped by harmonic plus quartic trap [$V(r) = \frac{1}{2}m\omega^2 r^2 + \lambda r^4$]. Keeping similarity with experiments, the anharmonic parameter (λ) is considered as a controllable parameter. The excited state energies of stable Bose-Einstein condensate are strongly influenced by the presence of an anharmonic term, even when the interatomic interaction is repulsive. The necessary dependencies of excited state energies of the trapped condensate on λ are discussed in detail. In addition, the variation of chemical potential energy as a function of λ is also investigated to explore the role of interaction. The many-particle Schrödinger equation is solved by the potential harmonic expansion method, where all possible two-body correlations are considered by utilizing the correlated two-body basis function. Specifically, we present a clear physical explanation of excited state energies and chemical potential energy of the experimental repulsive condensate confined by the anharmonic trap.

Keywords: Bose-Einstein condensation; Anharmonic trap; Hyperspherical harmonics; Excited state energies; Chemical potential energy.

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1. Introduction

Bose-Einstein condensation (BEC) in trapped atomic gases is a typical topic of interest in the realm of ultra-low temperature [1]. The experimental situation is quite different from the ideal Bose gas [2], and the very crucial factor in the studies of BEC properties is the form of confinement. In most of the experiments on the ultra-cold atomic system, the trapping potential is harmonic [3-8]. As the actual experimental set is of a finite extent, the choice of harmonic potential is exceptional. In the control collapse experiments of BEC by Vincent Bretin *et al.* [9,10], the repulsive ^{87}Rb atomic cloud was trapped by non-harmonic confinement where the trapping potential was increased more rapidly than quadratically at a distance far away from the center of the cloud. They create laser tuned quadratic plus quartic confinement of the form $V_{trap} = 1/2 m\omega^2 r^2 + \lambda r^4$, where 'm' is

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the mass of the atom and ' λ ' is an anharmonic coefficient. Such trapping potential introduces many novel phases, and after that, many theoretical studies [11-28] of BEC have considered shallow anharmonic traps.

Motivated by these observations, we recently have studied [11] the variation of kinetic energy, interaction energy, trapping potential energy along with the total ground state energy of repulsive BEC, which is confined by trap potential $V_{trap} = 1/2 m\omega^2 r^2 + \lambda r^4$. The anharmonic parameter (λ) is considered as a controllable parameter and $|\lambda| \ll 0$ as used in experiments [9,10,29]. It is a fact that the size of the condensate gets reduced by increasing the strength of λ [11]. It possesses another window of study of excited state energies of repulsive BEC in an anharmonic well. One can expect that gap between excited states of energy will also depend on the value of an anharmonic distortion. In this direction, the study of excited-state energies of condensate in the anharmonic well is very significant to investigate the modification of monopole, quadrupole, and higher multipole frequencies. The primary intention is to observe how excited state energies change on increasing the strength of λ from a very low value up to the experimental order. In experiments [9,10], the quartic confinement was created by considering $\lambda \sim 10^{-3}$ and in our study, λ is tuned by keeping $\lambda \leq 1.0 \times 10^{-3}$. It is pointed that the gap between excited state energies increases on increasing the strength of λ and when $\lambda = 1.0 \times 10^{-3}$ the effect is very prominent. Further, to get a clearer picture of the effect of anharmonicity, we calculate the chemical potential energy for different values of λ but a fixed number of particles in the trap. The observation is again interesting to explore the role of an anharmonic effect in the formation of the BEC.

We solve the many-body linear Schrödinger equation for a large number of bosons (A) under certain approximations [30-34] by a method called the potential harmonic expansion method (PHEM). In PHEM, all two-body correlations are retained, and it is assumed that three and higher-body correlations are negligible. This choice is justified as a first approximation since the experimental condensate is very dilute. The use of the van der Waals interaction in the potential harmonic (PH) basis correctly describes the many-body system to give a realistic picture. As repulsive BEC, ^{87}Rb atom is considered with scattering length $a_{sc} = 0.000433$ o.u. and for a trap frequency of $\nu = 77.78$ Hz, which corresponds to the JILA trap experiment [35]. Throughout complete calculations, a harmonic oscillator unit (o.u.) is used where $\hbar\omega$ is the oscillator energy unit and $(\hbar/2\pi m\nu)^{1/2}$ is the oscillator length unit. The manuscript is organized as follows. The next section formulates the use of correlated potential basis function in the many-body calculation to solve the linear Schrödinger equation for a large number of trapped bosons. Section 3 discusses the numerical results and section 4 concludes the summary of the work.

Here χ_{P0} is the P -th component of the column vector corresponding to the lowest eigenvalue $\omega_0(r)$. The excited states in this potential are the states with the l -th surface mode and n -th radial excitation, which is denoted by E_{nl} . Thus E_{00} is the ground state energy. The present calculation is performed for hyperradial excitations, which corresponds to the breathing mode with $l = 0$.

3. Numerical Results

3.1. Choice of the inter-atomic potential

As a realistic long-range interatomic potential, we choose the van der Waals potential. Here the short-range repulsion is characterized by a hard-core radius r_c and the long-range part is described by an attractive tail $1/r_{ij}^6$, viz. $V(r_{ij}) = \infty$ for $r_{ij} \leq r_c$ and $= C_6/r_{ij}^6$ for $r_{ij} > r_c$. C_6 is known for a specific atom, the value of r_c is adjusted to get the desired value of scattering length [45]. For Rb atoms, $C_6 = 6.4898 \times 10^{-11}$ o.u. The appropriate value of the hard-core radius is $r_c = 1.121054 \times 10^{-3}$ o.u. to get the experimental value of scattering length. It is noteworthy to mention that for a controlled collapse experiment of attractive BEC (^{85}Rb) [46,47], the required value of r_c are calculated and well documented [31].

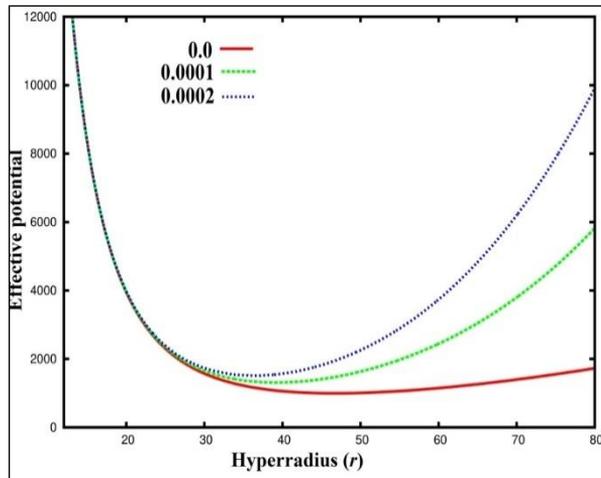


Fig. 1. Plot of effective potential $\omega_0(r)$ in o.u. of ^{87}Rb condensate against r (o.u.) for 500 number of bosons, confined by harmonic ($\lambda = 0$) and anharmonic trap with different values of anharmonic distortion (λ) as indicated in the figure.

3.2. Energies of BEC in an anharmonic trap

A very promising direction is to investigate the excitation energies of repulsive (stable) BEC in the anharmonic trap ($\lambda \neq 0$). In routine experiments [9,10], a blue detuned laser ray is directed along the axial direction to create the weak quartic term on the non-

harmonic trapping potential. The stable BEC is formed by gradually controlling the potential height by varying the laser intensity in the optical trap. In the present study, we are also interested in blue-shifted laser frequency ($\lambda > 0$), to show that the non-harmonic character of the trapping potential has a clear influence on the many-body effective potential (MBEP). As stated earlier, the collective motion of the condensate is considered in the effective MBEP ($\omega_0(r)$) in the hyperradial space. The reader should keep in mind that, in an actual experimental setup, the number of atoms is generally quite small; it ranges from even just a few to a few thousand atoms in the external trap. We first plot this effective potential in Fig. 1, for $A = 500$, as a function of hyperradius (r) for both harmonic ($\lambda = 0$) and anharmonically ($\lambda \neq 0$) trapped system. Repulsive BEC is always stable when a harmonic potential traps it. For an anharmonic trapping potential, the quartic term plays an important role, and the whole MBEP gets shifted upward. The upward shifting is very clear even when $\lambda = 1.0 \times 10^{-4}$ [Fig. 1] though the number of the particle is not so high [$A = 500$].

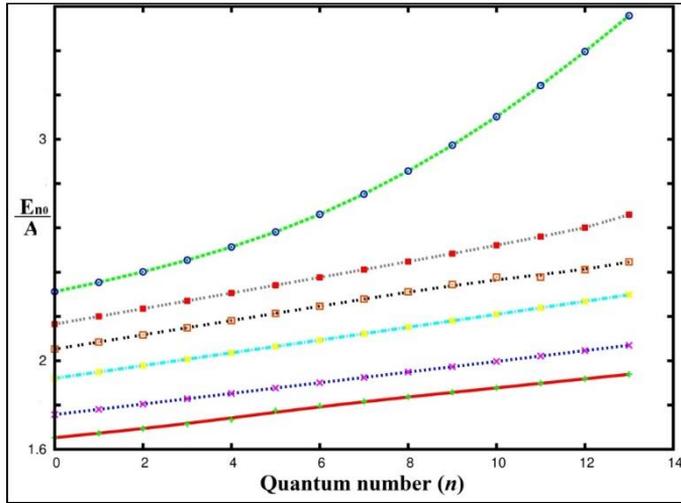


Fig. 2. Plot of excited state energies ($E_{n,0}$) per particle for $n = 0$ to 13 of ^{87}Rb condensate containing 100 number of trapped atoms having scattering length $a_{sc} = 0.000433 \text{ o.u.}$ The lower most line is for harmonic trap ($\lambda=0$) and from bottom to top curves are showing for anharmonic coefficient $\lambda = 0.0, 1.0 \times 10^{-4}, 3.0 \times 10^{-4}, 5.0 \times 10^{-4}, 7.0 \times 10^{-4}, 1.0 \times 10^{-3}$.

The outcome is visible more on increasing the strength of anharmonicity slightly [$\lambda = 2.0 \times 10^{-4}$]. Due to the extreme diluteness of the condensate, the effect of trapping is so dominating. The anharmonic term causes stronger binding than the harmonic trapping potential, and naturally, all energy states get shifted. Observation is more striking when we take a look at Fig. 2, where few radial excited state energies ($E_{n,0}$) are displayed for harmonic ($\lambda = 0$) and different anharmonic parameters. Fig. 2 is plotted for the fixed number of bosons ($A = 100$) in the trap and fourteen consecutive values of n ($n = 0$ to 13). It can be seen that gap between energies enhances on increasing the value of λ . For

$\lambda = 0$ (lowermost line) and 1.0×10^{-4} (the second lower line) excited-state energies per particle increase almost linearly with n . But when the value of the anharmonic parameter is high ($\lambda = 1.0 \times 10^{-3}$), the excited state energies per particle (E_{n0}/A) increases very rapidly (top most line). The observation is expected as the anharmonic effect is very clear.

Table 1. Different radial ($l = 0$) excited state energies of 100, 200 and 500 number of trapped ^{87}Rb atoms for harmonic ($\lambda=0$) and different anharmonic condensate with scattering length $a_{sc} = 0.000433$ o.u. Energy values are in o.u. of energy.

| A | λ | E_{00} | E_{10} | E_{20} | E_{30} | E_{40} | E_{50} | E_{60} |
|-----|-----------|----------|----------|----------|----------|-----------|----------|----------|
| 100 | 0.0 | 165.3372 | 167.2753 | 169.3230 | 171.3703 | 173.4173 | 175.4603 | 177.5105 |
| | 0.0001 | 175.6623 | 178.0527 | 180.4463 | 182.8431 | 185.2429 | 187.6460 | 190.0521 |
| | 0.0005 | 205.2477 | 208.4570 | 211.6743 | 214.8997 | 218.1329 | 221.3738 | 224.6226 |
| | 0.001 | 231.2039 | 235.4202 | 240.1532 | 245.4311 | 251.3510 | 258.1684 | 266.1097 |
| 200 | 0.0 | 348.9653 | 351.0439 | 353.1230 | 355.2055 | 357.3058 | 359.4603 | 361.7236 |
| | 0.0001 | 393.1857 | 395.9435 | 398.8664 | 402.0927 | 405.8134 | 410.1863 | 415.3045 |
| | 0.0005 | 500.6533 | 504.8079 | 509.3172 | 514.3679 | 520.1726 | 526.9835 | 534.9617 |
| | 0.001 | 587.4823 | 592.7036 | 598.4473 | 604.750 | 611.5175 | 618.6531 | 626.0862 |
| 500 | 0.0 | 997.5801 | 999.791 | 1002.183 | 1004.809 | 1007.6739 | 1010.831 | 1014.394 |
| | 0.0001 | 1313.749 | 1317.405 | 1321.310 | 1325.558 | 1330.141 | 1335.043 | 1340.342 |
| | 0.0005 | 1927.093 | 1932.804 | 1938.517 | 1944.234 | 1949.963 | 1955.731 | 1961.601 |
| | 0.001 | 2385.750 | 2392.912 | 2400.078 | 2407.247 | 2414.421 | 2421.611 | 2428.848 |

Next, to quantify the anharmonic effect, the excited state energies are investigated by changing the trapped particle number (A). For $A = 100, 200$, and 500 trapped bosons, we calculate different radial excited state energies by tuning the strength of anharmonic distortion (λ) and present them in Table 1. The way of increase of anharmonic effect is two-fold. First, the effect increases by increasing the strength of anharmonicity (λ) when the number of particles within the trap is fixed. On the other hand, for a fixed value of anharmonic distortion (λ), the effect can also be enhanced by increasing the number of particles (A) in the trap. The result is very interesting as there is a competition to increase anharmonic consequences if both A and λ are controlled simultaneously. For a more specific understanding, we calculate chemical potential energy for the same number of bosons (viz. $A = 100, 200$, and 500) by considering the different values of λ . The variation of chemical potential energy as a function of λ for a different number of particles within the trap is displayed in Fig. 3. The chemical potential energy is calculated as the difference between the ground state energy (E_{00}) of $(A + 1)$ particle system and that of A particle system. It is visible from Fig. 3 that chemical potential energy increases by increasing the strength of λ . But, the rate of increase is very prominent when the number of particles is high ($A = 500$). As stated earlier, the many body effective potential becomes tighter on increasing the value of an anharmonic distortion. This causes the rise of interatomic interaction. This anharmonic effect is very sensitive, and as a result, the chemical potential energy is raised to increase the strength of the anharmonic distortion.

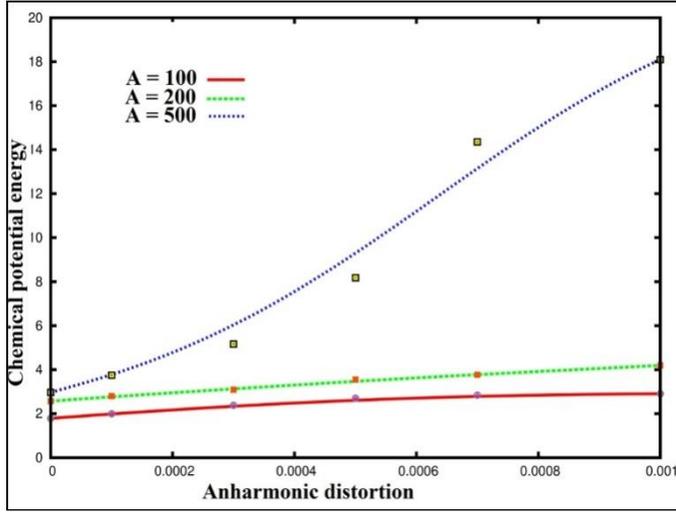


Fig. 3. Plot of chemical potential energy per particle in o.u. of ^{87}Rb condensate as a function of the anharmonic parameter (λ) for different indicated values of particles (A).

4. Conclusion

The critical behavior of excited state energies and the chemical potential energy of the ^{87}Rb repulsive condensate ($a_{sc} > 0$) of the JILA experiment [35] have been studied by an approximate many-body calculation. Our method is one step ahead of the Gross-Pitaevskii (GP) equation as the interatomic correlation is calculated. The van der Waals interaction is considered as a realistic interatomic interaction, which correctly produces pragmatic results. We paid attention to the study of excitation energies of the condensate when it is confined by experimental [9,10] quadratic plus quartic external trap viz. $V_{trap}(r) = 1/2 m\omega^2 r^2 + \lambda r^4$. Keeping similarity with experiments, the blue-shifted Lasser tuned ($\lambda > 0$) quartic term is considered. For this type of fine extent trap and for very small anharmonic distortion ($\lambda \approx -1 \times 10^{-4}$), the effective many-body potential becomes tighter due to the rapid growth of the quartic term. The strength λ is responsible for remodeling the many-body effective potential. As a result, we observe the significant change of the gap of excited state energies by tuning the strength of anharmonicity (λ). The investigation is very interesting by finding a close interplay between the number of particles in the trap and anharmonic interaction as it reflects in the significant increase of excited state energies of the condensate within the trap. In this direction, the study of the chemical potential energy of the condensate for a different number of particles and by varying the anharmonic parameter (λ) is very significant to explore the role of anharmonicity. The anharmonic effect can be enhanced by increasing the number of particles within the trap (keeping λ fixed) and increasing the value of λ (when number of bosons are fixed). The present investigation is restricted mainly to the anharmonic trap where the coefficient of anharmonicity can easily be varied to vary the shape of the many-body effective potential. So, the study is significant as it is concerned with the present-day

experiments, where the shape of the finite external confining potential is controlled by controlling the laser trap frequency.

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