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Study of Zero Temperature Ground State Properties of the Repulsive Bose-Einstein Condensate in an Anharmonic Trap

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Abstract

The zero-temperature ground state properties of experimental ⁸⁷Rb condensate are studied in a harmonic plus quartic trap $[V(r) = \sqrt{2}m\omega^2 r^2 + \lambda r^4]$. The anharmonic parameter (λ) is slowly tuned from harmonic to anharmonic. For each choice of λ , the many-particle Schrödinger equation is solved using the potential harmonic expansion method and determines the lowest effective many-body potential. We utilize the correlated two-body basis function, which keeps all possible two-body correlations. The use of van der Waals interaction gives realistic pictures. We calculate kinetic energy, trapping potential energy, interaction energy, and total ground state energy of the condensate in this confining potential, modelled experimentally. The motivation of the present study is to investigate the crucial dependency of the properties of an interacting quantum many-body system on λ . The average size of the condensate has also been calculated to observe how the stability of repulsive condensate depends on anharmonicity. In particular, our calculation presents a clear physical picture of the repulsive condensate in an anharmonic trap.

Keywords: Bose-Einstein condensation; Anharmonic trap; Hyperspherical harmonics; Potential harmonics.

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1. Introduction

The investigation of properties of Bose-Einstein condensation (BEC) is important for understanding the dynamics of the atomic quantum fluids in an ultra-low temperature (very close to absolute zero) regime. The very crucial factor in these studies is the form of confinement. Most experimental [1-7] and theoretical studies have been performed for the condensate trapped in a harmonic (parabolic) trap. The description of the wave function dynamics in such a trap has many simplifying properties both for repulsive and attractive interactions between atoms. However, it is interesting that the harmonic trapping is special in many respects as in actual experimental setup, BEC is observed with a finite extent trap.

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734 Repulsive Bose-Einstein Condensate

For this reason, different theoretical studies [8-26] have considered traps with other functional forms, in which the trapping potential grows more rapidly than quadratically at a distance far away from the center of the cloud. In the control collapse experiment of achieving BEC [27-29], the trapping potential is well approximated by a superposition of quadratic and a small quartic potential resulting in confinement of the form $V(r) = 1/2 m\omega^2 r^2 + (k/4)r^4$, where *m* is the mass of the atom. In the experiments of Stock and co-workers [28,29] the repulsive ⁸⁷Rb condensate is formed by radio-frequency evaporation in a combination of magnetic and laser trap. The pure magnetic trap provides harmonic confinement along with the three directions with a superimposition of the tuned laser along the *z*-direction, which provides the quartic term in confinement. The nice feature of this potential is the centrifugal force, varying as $\Omega^2 r$ can always be compensated by the trapping force varying as- $(m\omega^2 r + kr^3)$. Practically, one can easily increase the rotation frequency (Ω) of the gas above the trap frequency (ω) , which allows one to study the various phases of the gas and dramatic change in the appearance of the quantum gas.

In the present study, keeping similarity with experiments, the external potential is modelled as $V_{trap}(r) = 1/2 m\omega^2 r^2 + \lambda r^4$. We think that the study of zero-temperature ground state properties of Bose-Einstein condensation (BEC) is a very effective tool for exploring the role of interaction in the theoretical scheme. Our previous studies [30,31] of zero-temperature ground state properties of BEC were limited to harmonic trapping potential $[1/2 m\omega^2 r^2]$ only. However, in this study, we choose λ as a controllable anharmonic parameter and $|\lambda| \ll 1.0$. The quartic term (λ) considered here corroborates with the experimental situation. In experiment [28], dramatic change in the appearance of repulsive ⁸⁷Rb quantum gas was studied in a fast rotation regime. We are also interested in repulsive ⁸⁷Rb quantum gas but in non-rotating condensate and calculate the zerotemperature ground state properties of the condensate confined in such an anharmonic trap. By slowly tuning λ from harmonic to anharmonic, we study the crucial dependency of these properties on the strength of anharmonicity (λ).

Earlier theoretical calculations to describe the basic features of BEC are based on the mean-field theory, which produces the well-known Gross-Pitaevskii (GP) equation. In the mean-field approximation, the interatomic interaction is characterized by a contact interaction of strength proportional to s-wave scattering length (a_{sc}). This equation describes the general gross properties of BEC, which are well understood [32]. However, the scattering length description in the mean-field approach does not represent the true atom-atom interaction which was also pointed and well documented [33-35]. Another important drawback of the mean-field approach is that the contact pseudo potential form of atom-atom interaction does not consider inter-atomic correlations [36]. Although the condensate is dilute, the interaction between particles plays an important role. So, an exact treatment of full many-body formalism is desirable, which uses realistic atom-atom interactions. We employ a method, called the potential harmonic expansion method (PHEM), to solve the linear schrödinger equation for a large number of bosons (A) under certain approximations [37-39]. In PHEM, we assume that three and higher-body

correlations are negligible, but retain all two-body correlations. This choice is justified as a first approximation since the experimental condensate is very dilute, and we go beyond the mean-field approximation by including all two-body correlations. Our calculation is facilitated by using the potential harmonic (PH) basis and the realistic van der Waals interaction as it correctly describes the many-body system to give the realistic picture. We observe that the effective potential in the hyperradial space, in which the condensate is confined, is shifted upward and becomes steeper at larger distances from the centre of the cloud when the condensate is trapped by quadratic plus quartic potential. We also observe that the steepness of the effective potential increases more on increasing the strength of the anharmonic coefficient (λ). In this perturbed well, we aim to calculate the trapping potential energy, the interaction energy, the kinetic energy along with the total ground state energy of the condensate. Calculated ground state properties of trapped BEC are also modified accordingly, which are clearly described here. By slowly varying λ , we study the significant changes of these observables. A large number of theoretical studies exist on trapping of the BEC with quadratic plus quartic type potential, but the study of zero temperature energies in this type of deformed well has not been undertaken so far. Another important observation is the calculation of the average root mean square (rms) radius (r_{av}) of the individual atoms from the centre of the mass of the system [38]. The r_{av} gives the idea of the average size of the condensate in an anharmonic trap well. For a fixed number of trapped bosons, if the strength of λ is increased, it causes a decrease in the size of the condensate. It is in harmony with the experimental observation, which is clearly demonstrated here. It is nicely shown here that the kinetic energy of particles and the interaction energy among particles both increase on enhancing the strength of λ , which propel the system towards more stability. The notable effect of stability of the condensate by changing the distortion parameter (λ) is a very interesting observation here. The role of interatomic interaction of the condensate and its dependency on anharmonicity is also revealed in the present study as the height of the barrier, and the shape of the well depends significantly on λ . In keeping with our focus on experiments [28,29] we hope that our theoretical calculations are quite relevant, and it will help to achieve properties of BEC in deformed trap experiments.

The paper is organized as follows. In the next section, we present the many-body calculation with correlated harmonic potential basis used to solve the Schrödinger equation for a large number of trapped bosons. Section 3 discusses our numerical results and section 4 concludes the summary of our work. Throughout our calculations, we adopt harmonic oscillator unit (*o.u.*) where $\hbar\omega$ is the oscillator energy unit and $(\hbar/2\pi mv)^{1/2}$ is the oscillator length unit.

2. Methodology

The many-body method we adopt here has been used successfully to study BEC and is well documented [21-24,30,31,37-42]. Here, we describe the methodology briefly for the interested readers. Details of the technique and explanation of the adopted notations and terminology can be found in the mentioned references.

736 Repulsive Bose-Einstein Condensate

We consider A = (N+1) identical bosons, each of mass *m* interacting via two-body potential $V(\vec{r}_{ij}) = V(\vec{r}_i) - V(\vec{r}_j)$ and confined in an external trap modeled as a harmonic potential with a quartic term. The relative motion (after removal of the center of mass motion) is described in the many-body Schrödinger picture as

$$\left[-\frac{\hbar^{2}}{m}\sum_{i=1}^{m}\nabla_{\zeta_{i}}^{2}+\sum_{i=1}^{m}\left(\frac{1}{2}m\omega^{2}\zeta_{i}^{2}+\lambda\zeta_{i}^{4}\right)+V_{int}(\zeta_{1},..,\zeta_{N})-E\right]\psi(\vec{\zeta_{1}},..,\vec{\zeta_{N}})=0.....(1)$$

Where $\{\vec{\zeta}_1, \vec{\zeta}_2, \dots, \vec{\zeta}_N\}$ is the set of N Jacobi coordinates [39]. The second term represents the trapping potential and V_{int} is the sum of all pair-wise interactions. Hyperspherical harmonics expansion method (HHEM) [43,44] is an *ab initio* many-body tool to solve the many-body Schrödinger equation. The hyperspherical variables are constituted by the 'hyperradius' (r) and (3N-1) 'hyperangles'. Hyperangles are consisting of 2N spherical polar angles of $\{\vec{\zeta}_1, \vec{\zeta}_2, ..., \vec{\zeta}_N\}$ and (N-1) hyperangles $\{\phi_2, \phi_3, ..., \phi_N\}$ (with associated quantum numbers $\{n_2, n_3, \dots, n_N\}$) giving relative length of N Jacobi vectors [39,43,44]. However, due to the large degeneracy of the HH basis, HHEM is practically applicable for three particles only [43]. Thus for (N+1) bosonic systems, we adopt a subset of the full HH basis for the expansion of many-body wave function. This technique is known as the potential harmonic expansion method (PHEM). The basic assumption is in the decomposition of the total (global) hyperradius in two parts. We choose $\vec{\zeta}_N = \vec{r}_{ij}$ the interacting (ij) pair, and for remaining (N-1) Jacobi coordinates, we define the hyperradius $\rho_{ij} = \left[\sum_{i=1}^{N-1} \zeta_i^2\right]^{1/2}$. In this expansion, we ignore higher-body correlations and include the function $\eta(r_{ij})$ [31,41], which takes the effect of two-body correlation (through a function of (r_{ij})). In a typical BEC experiment, the condensate is kept at a very low temperature and in very dilute conditions. Hence only binary collision at almost zero kinetic energy is relevant. The inclusion of two-body correlations in the wave function puts the many-body calculations one step ahead of the mean-field theory. The full wave function (ψ) is decomposed into Faddeev components (ψ_{ij}) as [39]

Note that, ψ_{ij} , which corresponds to (*ij*) interacting pair, is a function of the pair separation \vec{r}_{ij} and global hyperradius *r*. We expand ψ_{ij} in a subset of the full HH basis, called potential harmonic (PH) basis [37,39,41]. When ψ_{ij} is expanded on the appropriate PH basis [21,22,31,41],

 $\mathcal{P}_{2K+l}^{lm}(\Omega_N^{ij})$ is a PH basis function and Ω_N^{ij} is the set of all hyperangles for the choice $\vec{\zeta}_N = \vec{r}_{ij}$. Here we introduce $\eta(r_{ij})$ a short-range correlation function in each Faddeev component which properly simulates the short separation behavior of an interacting pair and enhances the convergence rate of the expansion basis [41]. The function $\eta(r_{ij})$ is calculated from zero energy solutions of *ij* pair relative motion [41]. The need for such a correlation function is perfectly justified from the experimental context, as discussed earlier. Substituting Eq. (3) in the many-body equation and taking projection on a particular PH basis, a set of the coupled differential equation (CDE) in *r* is obtained

[37,39,41]. We solve it by hyperspherical adiabatic approximation (HAA) [45]. In HAA, one assumes that the hyperradial motion is slow compared to the hyperangular motion. CDE is solved by diagonalizing the potential matrix together with the diagonal hypercentrifugal repulsion and the anharmonic trapping potential for each value of *r*. The lowest eigenvalue gives the lowest eigenpotential as a parametric function of hyperradius *r*. This eigenpotential ($\omega_0(r)$) is chosen as the effective potential in which the entire condensate moves as a single entity. The energy and wave function of the condensate is obtained by solving the adiabatically separated hyperradial equation [22].

Here $\chi_{K0}(r)$ is the *K*-th component of the column vector corresponding to the eigenvalue $\omega_0(r)$, and the third term is a correction to the lowest order HAA approximation [45]. The *K*-sum is truncated to a maximum value K_{max} [37,38], subject to the desired convergence in energy. The $\zeta_0(r)$ is the condensate wave function in the hyperradial space and the lowest state in the effective potential, $\omega_0(r)$, corresponding to the ground state of the condensate. The wave function and energy of the system are obtained by solving Eq. (4) numerically.

3. Results

3.1. Choice of the inter-atomic potential

From a theoretical point of view, particle separation is one of the appealing features of the alkali vapor cloud, which is typical of order 10^2 nm [46]. These separations are large compared with the scattering length (a_{sc}) , which characterizes the strength of interactions. For alkali atoms, a_{sc} is of the order of $100a_0$ [46], where a_0 is the Bohr radius. So, it can be assumed that the dominant effects of interaction are due to two-body encounters, which are supported by the extreme diluteness of alkali atom vapors. It is, therefore, possible to calculate properties of the gas reliably from knowledge of two-body scattering at low energies [46]. This two-body interaction is very crucial in studies of properties of BEC as it affects the important measurable quantities like the temperature dependence of the condensate, energy and density distribution, other static, dynamic and thermodynamic properties [40,41,46,47]. Since the inclusion of realistic interatomic interaction makes the many-body Schrödinger equation extremely complicated, the usual practice is to take contact δ interaction in the mean-field theory, which results in the GP equation. But the δ type of interaction is not sufficient for repulsive BEC, when it is trapped by quadratic plus quartic type potential. Due to the anharmonicity created by quartic term, the many-body effective potential becomes less flat than harmonic trapping, and bosons are induced to come closer. At this point, the realistic atom-atom interaction must be considered. The δ function interaction is not a physical one since it diverges at $r_{ii} = 0$ and the Hamiltonian becomes unbound from below [33-35]. This is manifested in our effective many-body potential, and there are no acceptable, stable solutions for any A for this type of singularity at $r_{ij} = 0$. It is again remarkable that for polarised alkali atoms, scattering lengths are

typically about two orders of magnitude greater than the size of an atom ($\sim a_0$) [46]. It is established that van der Waals interaction can give rise to such large scattering lengths as it is caused by the electric dipole-dipole interaction between atoms [40,46,47]. The r^{-6} contribution to this potential is the leading term in the expansion of the long-range part of the two-body interaction in inverse powers of r. From the physical point of view of repulsive BEC, interatomic interaction will not allow the interacting particles to come too close to each other. Focusing on these features, we also model the interatomic interaction by realistic long-range potential, the van der Waals potential with a hardcore radius (r_c) $V(r_{ij}) = \infty$ for $r_{ij} \leq r_c$ and $V(r_{ij}) = C_6/r_{ij}^6$ when $r_{ij} > r_c$. The value of C_6 is known for a specific atom, and the value r_c is adjusted to get the desired value of scattering length a_{sc} [42]. For Rb atoms, $C_6 = 6.4898 \times 10^{-11} o.u$, in the limit of $C_6 \rightarrow 0$, the potential becomes a hardcore potential, and r_c coincides with the s-wave scattering length. However, with a $1/r^6$ tail, we have to solve the two-body schrödinger equation with zero energy to get the value of r_c , which corresponds to the experimental scattering length (a_{sc}) . With a tiny change in r_c , a_{sc} may even change sign [46]. Thus, the choice of r_c is very crucial, and one may belong to a wrong region with an improper choice of r_c . For our study with repulsive BEC, we consider ⁸⁷Rb atom, and we find that $r_c = 1.121 \times 10^{-3} o.u.$ can produce scattering length $(a_{sc}) = 0.00433 \text{ o.u.}$ with a trap frequency v = 77.78 Hz. These parameters correspond to the JILA trap experiment [44]. In actual experiments, the number of atoms is generally quite small; it ranges from even just a few to a few thousand atoms in the external trap.

3.2. Properties of BEC

As stated earlier, our choice of trapping potential models the optical trap used in many experiments where the height of the potential well is gradually controlled by controlling the laser intensity along the axial direction in the optical trap [28,29]. In the experiment, the dynamical response of the condensate confined in harmonic-plus-Gaussian laser trap is investigated in a controlled manner, probing the rich physics of dramatic condensate properties. In our study, we consider the collective motion of the condensate in the effective many-body potential ($\omega_0(r)$) in the hyperradial space. We calculate several ground state properties: the trapped energy ($\langle V_{trap} \rangle = \langle \sum_{i=1}^{A} 1/2 m \omega^2 r_i^2 + \lambda r_i^2 \rangle$), the interaction energy ($\langle V_{int} \rangle = \langle \sum_{i,j < i}^{A} V_{ij} \rangle$), Kinetic energy ($\langle T \rangle$), the ground state energy (E_0) of bosons confined in both harmonic (λ =0) and anharmonic (λ ≠0) trapping potential. We know that repulsive BEC is always stable for any number of bosons. Our many-body effective eigenpotential ($\omega_0(r)$) is shown in Fig. 1 for 100 number of bosons trapped by harmonic and anharmonic external potentials.



Fig. 1. Plot of effective potential $\omega_0(r)$ in *o.u.* of ⁸⁷Rb BEC against r (*o.u.*) for 100 number of bosons, confined in a pure harmonic trap (λ =0.0) and for anharmonic trap (λ =0.0001, 0.0004).

For $\lambda=0$, $\omega_0(r)$ is roughly harmonic but shifted upward due to the repulsive interatomic interaction. As the condensate is very dilute, the effect of trapping is dominating. Now for $\lambda=0.0001 \ o.u.$, the effective potential is upwardly shifted, and the shift is significant. This effect is more notable on increasing λ very slightly. It also becomes tighter as the quartic term grows much faster than the quadratic term for large distances from the center of the atomic cloud. This causes stronger binding, and naturally, ground state energy will increase. We observe that the stability of the condensate increases on switching from harmonic to anharmonic even for a very small value of anharmonicity $(0 < \lambda \le 10^{-4})$. To be more quantitative, we study the average size of the condensate (r_{av}) , which is defined as the root mean square distance of individual atoms from the center of the mass and is given by

where \vec{X} is the center of mass coordinate. The last step in Eq. (5) follows from the definition of the hyperradius, r [44]. Table 1 presents the obtained value of total ground state energy per particle (E_0/A) and r_{av} for a selective number of bosons (A) for both harmonic and anharmonic traps. With the increase of A for repulsive condensate in the harmonic trap, the region of the hyperspace available for the motion of atoms increases. This will increase the size of the condensate. But on switching to an anharmonic one for the same A, as the effective potential becomes tighter for more growth of quartic term. As a result the system contracts. So r_{av} decreases on increasing λ for a fixed number of bosons as expected. The decreasing nature of the size of the condensate clearly shows the greater stability of the condensate.

740 Repulsive Bose-Einstein Condensate

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A	Distortion (λ) (<i>o.u.</i>)	$E_0/A(o.u.)$	$r_{av}(o.u.)$
100	0.0	1.65227	1.34394
	0.00001	1.66337	1.33582
	0.0001	1.75663	1.24316
	0.001	2.31140	1.05721
500	0.0	2.06813	1.51624
	0.00001	2.08414	1.44474
	0.0001	2.62748	1.25730
	0.001	4.85185	0.96655

Table 1. Calculated total ground state energy per particle (E_0/A) and an average size of the condensate (r_{av}) for ⁸⁷*Rb* atoms with scattering length = 0.00433 o.u., for harmonic and different anharmonic (λ) external trap.



Fig. 2. Plot of trapping potential energy per particle in *o.u.* of ⁸⁷Rb condensate as a function of the anharmonic parameter (λ) (*o.u.*) for different indicated values of particles (*A*).

Next, we calculate the expectation value of trapping potential energy (V_{trap}) of the condensate confined in the anharmonic trap, and we tune the anharmonic parameter (λ) from very close to harmonic to anharmonic. The trapping potential (V_{trap}) increases steadily as *r* increases in the same manner for all *A* in a harmonic trap. In an anharmonic one, it increases more rapidly with quartic term depending on the value λ . The expectation value of V_{trap} per particle is plotted in Fig. 2, for A=100, 200, 500 number of bosons. As the minimum of the effective potential gets shifted for higher *r* value on increasing *A* for harmonic trapping, $\langle V_{trap} \rangle/A$ enhances. For fixed *A*, if we tune λ from a very small value (but keeping $\lambda \ll 1.0$) $\langle V_{trap} \rangle/A$ increases prominently in quadratic plus quartic confinement. The rate of increase is more significant for a larger number of particles through the scattering length is quite small. This also gives a clear picture of increasing stability in the anharmonic trap.



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

The effective potential $\omega_0(r)$ in PHEM has a large contribution from the trapping potential. If the number of the particle is increased in harmonically trapped bosons, the interparticle separation is reduced. This increases the strength of interaction energy (V_{int}) as the number of pair-wise bonds increases. But in an anharmonic trap, $\omega_0(r)$ becomes less flat near its minimum, and it shifted upward (Fig. 1) due to the quartic term of the potential. More particles squeeze inward the metastable region (MSR) in the tight trap of the condensate, which takes care of increasing mutual repulsion. So, V_{int} again increases with the increase of the value of λ for a fixed number of bosons (A). This effect is justified in Fig. 3, where $\langle V_{int} \rangle / A$ is plotted against λ , for small distortion and a selected number of particles in the condensate. Although the anharmonic strength is very small, the energy shift is large due to the magnified effect from the atom-atom interaction. So the effect of anharmonicity is quite significant even when λ is quite small and $\langle V_{int} \rangle / A$ gradually increases with λ for fixed A. For large A the effect is more prominent. It nicely presents that on increasing λ , the condensate gets better stability and less tunneling. We also observe an interesting dependency of the kinetic energy of particles on anharmonicity. To study the addiction of expectation value of the kinetic energy per particle ($\langle T \rangle / A$) on λ , it is plotted as a function of λ for A = 100, 200, 500 in Fig. 4.



Fig. 4. Plot of kinetic energy per particle in *o.u.* of ⁸⁷Rb condensate as a function of the anharmonic parameter (λ) (*o.u.*) for different indicated values of particles (*A*).

As stated earlier, for harmonically trapped bosons with repulsive interaction, the accumulation of more particles within the trap causes a decrease of the region of the hyperspace available for the motion of atoms. As a consequent result, kinetic energy per particle will decrease, which is nicely notable in Fig. 4. But when the condensate is confined in a quadratic plus quartic trapping potential, its average size shrinks with the increase of anharmonic parameter λ . This causes more mutual repulsion of atoms and an increase of $\langle T \rangle / A$ as a function of λ . This effect is also quite large due to the magnified effect of an anharmonic term and gets enhanced for larger A as expected.

4. Conclusion

We have paid main attention to the study of ground-state properties and stability of the condensate when the effective trap height is tuned from very close to harmonic to weak quartic anharmonic well. In the actual experimental setup, BEC is observed with a finite extent trap. It necessarily involves anharmonic terms near periphery. In modern experiments [28,29] quartic confinement is created with a Gaussian laser directed along the axial direction. By adjusting the amplitude of the Gaussian laser trap potential, quadratic-plus-quartic potential ($V_{trap}(r) = 1/2 m\omega^2 r^2 + \lambda r^4$) is created in the experiment. In our study, we slowly tune the coefficient of the quartic term (λ) to observe the properties of BEC for repulsive interatomic interactions of ⁸⁷Rb condensate of JILA experiment [48]. The use of correlated PH basis and the van der Waals interaction correctly gives the realistic picture. The laser blue-shifted ($\lambda > 0$) properties of BEC caused by an anharmonic distortion are revealed and found to be more dramatic in the presence of interatomic interaction. In this confinement, the many-particle effective potential becomes steeper in the outer region, forcing atoms inwards. On the other hand, if the number of

bosons is increased in the same trap, atoms are forced to come closer towards the origin. Both effects are in the same direction, which takes care of the increase of atom-atom mutual repulsion within the trap. This is divulged by the growth of kinetic energy with an increase of λ . The total ground state energy, trap energy and interaction energy values are also modified. The enhancing effect due to the increase of the number of bosons is noted. The reducing effect of the size of the condensate is also significant in increasing the λ . The considered anharmonic trap can also be approximated as a parabolic potential with a Gaussian envelope. Naturally, the quantitative estimate of the properties of BEC and their instability is also applicable for another type of shallow trap. Complying with experiments, our theoretical study of ground-state properties of BEC in anharmonic confinement is very significant.

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