Collective excitations of Bose Einstein condensates

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Abstract: In this work we compare the collective monopole excitation energies for Bose-Einstein condensates of atoms in spherically symmetric traps, described by either the Gross-Pitaevskii equation or the Modified Gross-Pitaevskii equation. The excitation energies are computed from the ground state via energy weighted sum rules, and the results are compared to time-evolving pulsating condensates. We finally compare the excitation energies for systems obeying both equations and demonstrate that the results obtained through the Modified Gross-Pitaevskii are clearly different than the results obtained through the Gross-Pitaevskii equation in the strong interaction regime.

I. INTRODUCTION

A Bose-Einstein condensate (BEC) is a state of matter in which a large fraction of a diluted gas of bosons at very cold temperatures (ideally, $T = 0$) is occupying simultaneously the lowest single particle quantum state. This phenomenon, first described by Bose and Einstein between 1924 and 1925, was first observed in 1995, which sparked a great interest in both experimental and theoretical studies of Bose gases[1].

Most of such experiments are done by cooling magnetically or optically trapped atoms down to extremely low temperatures, of the order of nanokelvin. These situations are described through the Gross-Pitaevskii (GP) equation, which deals with very diluted Bose gases, that is, when the average distance between particles is much larger than the range of interatomic interactions. In such circumstances, the physics of the problem is dominated by low energy two-body collisions, which are very well described in terms of the s-wave scattering length a_s.

In order to characterize the *diluteness* of a system we use the gas parameter $\chi(\vec{r}) = n(\vec{r})a_s^3$, where $n(\vec{r})$ is the local density of the system. The GP equation has been observed to do an excellent job for low values of the average gas parameter, $\bar{\chi} \leq 10^{-3}$. Recent experiments, however, have shown values of the gas parameter that well exceed this number. In these contexts, it seems natural to expand the energy contribution of the two-body interaction in the GP equation to the next term in the local density expansion of the energy density, obtaining the so called Modified Gross-Pitaevskii equation [2, 3].

Concerns about the validity of this equation have, however, arisen, mainly questioning if similar results could be obtained by rescaling the scattering length instead of adding further orders to the GP equation.

The objective of this work is, then, to study and compare the results for these two equations for trapped BECs. In particular, we will compute the energy of the collective excitations of such condensates under monopole excitations. This excitation energy will be estimated through sum rules. In addition, the validity of the sum rules will also be established by comparing their values with the pulsating frequency of a monople excited BEC.

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II. THEORETICAL BACKGROUND

A. Gross-Pitaevskii equation

Let us consider a condensate of N atoms in a spherically symmetric trap, which takes the form of $V_{\text{trap}} = \frac{1}{2}m\omega^2 r^2$, in equilibrium, at $T = 0$ K. We will study this system in the framework of the *local density approximation* (LDA), considering that the system will behave as a diluted hard spheres with diameter equal to the scattering length a_s. Taking the low density expansion of the energy density up to second order we obtain

$$\frac{E}{V} = \frac{2\pi n^2 a_s^2 \hbar^2}{m}\left[1 + \frac{128}{15}\left(\frac{na_s^3}{\pi}\right)^{1/2} + \cdots\right], \quad (1)$$

where m is the mass of the atoms. Within the LDA framework, the energy functional associated with the GP equation can be obtained from Eq. (1) by keeping the first term in the expansion, obtaining the following energy functional:

$$e_{GP}[\psi] = \int d^3r \left[\frac{1}{2}|\nabla\psi(r)|^2 + \frac{1}{2}r^2|\psi(r)|^2 + 2\pi a_s N|\psi(r)|^4\right]. \quad (2)$$

To write this equation we have used the units that naturaly arise from the trap potential , i.e. harmonic oscillator (HO) units, and use dimensionless parameters. The energy and length units related to the harmonic oscillator potential are, respectively [3] $e_{HO} = \hbar\omega$ and $a_{HO} = \sqrt{\frac{\hbar}{m\omega}}$. HO units will be used throughout this work.

The Gross-Pitaevskii equation is obtained by imposing the functional in Eq. (2) to be stationary with respect

to variations of ψ^*:

$$\left[-\frac{1}{2}\nabla^2 + \frac{1}{2}r^2 + 4\pi a_s N|\varphi|^2\right]\varphi = \mu\varphi. \tag{3}$$

Here μ is the chemical potential (as justified by Koopman's theorem), which takes into account the conservation of the number of particles. If we do the same reasoning taking into account the second term of the expansion in Eq. (1) we obtain the so called Modified Gross Pitaevskii equation (MGP):

$$\left[-\frac{1}{2}\nabla^2 + \frac{1}{2}r^2 + 4\pi a_s N|\varphi|^2 + 5\pi^{1/2}a_s^{5/2}N^{3/2}\frac{128}{15}|\varphi|^3\right]\varphi = \mu\varphi. \tag{4}$$

B. Virial Theorem

In quantum mechanics we can get the results of the virial theorem by performing an scaling of the system [4]. In particular, we will use the one body wave function $\varphi(r)$, which will be rescaled as $\tilde{\varphi}(\vec{r}') = \lambda^{3/2}\varphi(\lambda\vec{r})$, in order to maintain the norm. Now, the virial theorem can be written as

$$\left.\frac{de(\tilde{\varphi},\lambda)}{d\lambda}\right|_{\lambda=1} = 0, \tag{5}$$

where $e(\tilde{\varphi},\lambda)$ is the energy per particle of such an scaled system. In order to use this identity, we will need to define different contributions to the total energy. For the GP equation these are:

$$t_{\text{kin}} = \int d^3r \frac{1}{2}|\vec{\nabla}\varphi(r)|^2,$$
$$e_{\text{HO}} = \frac{1}{2}\int d^3r|\varphi(r)|^2r^2,$$
$$e_{\text{int}} = 2\pi a_s \int d^3r|\varphi(r)|^4.$$

If we apply the scaling introduced formerly, we can see that the contributions to the energy scale differently, and the total energy can be written as

$$e(\tilde{\varphi},\lambda) = \lambda^2 t_{\text{kin}}(\varphi) + \frac{1}{\lambda^2}e_{\text{HO}}(\varphi) + \lambda^3 e_{\text{int}}(\varphi). \tag{6}$$

Which, by means of Eq. (5), gives us the relation

$$2t_{\text{kin}} - 2e_{\text{HO}} + 3e_{\text{int}} = 0. \tag{7}$$

Let us now proceed similarly with the MGP energy functional in order to obtain a similar expression for systems under the MGP equation. In this case, we will incorporate one further term:

$$e_{\text{int},2} = \frac{256}{15}a_s^{5/2}N^{3/2}\int d^3r|\varphi(r)|^5. \tag{8}$$

With that new term, the scaled energy will be

$$e(\tilde{\varphi},\lambda)_{\text{MGP}} = \lambda^2 t_{\text{kin}}(\varphi) + \frac{1}{\lambda^2}e_{\text{HO}}(\varphi) + \lambda^3 e_{\text{int},1}(\varphi) + \lambda^{9/2}e_{\text{int},2}(\varphi). \tag{9}$$

Finally, we obtain the corresponding MGP virial theorem:

$$2t_{\text{kin}} - 2e_{\text{HO}} + 3e_{\text{int},1} + \frac{9}{2}e_{\text{int},2} = 0. \tag{10}$$

C. Strong and weak interacting limits

One of the first things we can consider is which are the limits when studying the dependency of a system on the interaction. First of all we must decide what parameter better describes the strength of the interaction.
By looking at Eq. (2), we can see that the interacting energy, depends only on the product a_sN.
We can see, however, that this does not hold for the MGP equation. If we separate both expansion terms as two different energy contributions (e_{int_1} and e_{int_2}, respectively), we can see how e_{int_1} will scale with Na_s but e_{int_2} will have an extra contribution from a_s, which does not allow us to freely change N and a_s while maintaining their product constant when studying the MGP equation.
With that being said, the first limit is quite obvious, and takes place when there is no interaction. Then, both equations will be equivalent to the single particle harmonic oscillator equation, and the virial theorem will be

$$t_{\text{kin}} = e_{\text{HO}}, \tag{11}$$

for both equations.
The second limit applies when the interactions became very strong and the interaction terms dominate on the overall energy. It can bee seen that, as the interaction increases the kinetic energy contribution becomes less and less important. Then, for large interactions, we can neglect the kinetic term and use only the HO and interacting ones. This is known as the Thomas-Fermi approximation.

D. Sum Rules

In order to study the differences between the GP and MGP solutions for large interactions, we will study the collective excitation energies under a monopole excitation. It would appear necessary, then, to find a way to compute such excited states. Fortunately, there are procedures to compute such excited energies from the ground state [5].
We begin by introducing the dynamic structure function, which is defined as

$$S_F(E) = \frac{1}{N}\sum_j^N |\langle j|F|0\rangle|^2\delta(E-(E_j-E_0)), \tag{12}$$

where F is the excitation operator and $|j\rangle$ and E_j are the hamiltonian eigenstates and eigenvalues, respectively. Alternatively, the dynamic structure function can be characterized by its energy sum rules:

$$M_n(F) = \int_0^\infty E^n S_F(E) dE. \tag{13}$$

Therefore, if the response of the system to a certain excitation operator is concentrated in a narrow range of energies, we will be able to describe $S_F(E)$ with only a few moments.
The most interesting thing, however, is that we can compute these moments without explicitly knowing neither $S_F(E)$ nor the excited state, but we can compute it through expected values of a given operator on the ground state. Then, we can also see that using the previous equations we will be able to estimate the excitation energy as

$$\bar{E}_m = \sqrt{\frac{M_n}{M_{n-2}}}. \tag{14}$$

Our objective will be to compute this energy from the ground state of the BEC given by either the GP or the MGP equation.
We will now see what form take some of these energy sum-rules for the excitation we will focus mainly on monopole excitations, $F = r^2$. First, it can be shown that M_1 is simply computed as [6]

$$M_1 = \frac{1}{2}\langle 0|r^2|0\rangle = \frac{1}{2}\int d^3 r r^2 \rho(r) = e_{\text{HO}}, \tag{15}$$

so it will be equal to the harmonic trap energy contribution, E_{HO}.
M_{-1} can be computed through a perturbational method. In this case, we will add a certain excitation term to the Hamiltonian, $F(\alpha) = \alpha r^2$, and compute the energy associated to the new ground state, $E_0(\alpha)$. Then, the sum rule can be computed as [6]:

$$M_{-1} = -\frac{1}{2}\frac{\partial^2 E_0(\alpha)}{\partial \alpha^2}\bigg|_{\alpha=0}. \tag{16}$$

Finally, we also compute M_3 through a scaling approach equal to that used for the virial theorem. If we consider the energy of an scaled system as $E(\lambda)$, the sum rule will read as [6]

$$M_3 = \frac{1}{2}\frac{d^2 E(\lambda)}{d\lambda^2}\bigg|_{\lambda=1}. \tag{17}$$

This allows to obtain upper and lower bound values for $\bar{E}_m$. By taking Eq. (17) into account, we can see that, for the GP equation, we obtain:

$$M_3 = e_{HO}\left(5 - \frac{t_{\text{kin}}}{e_{\text{HO}}}\right). \tag{18}$$

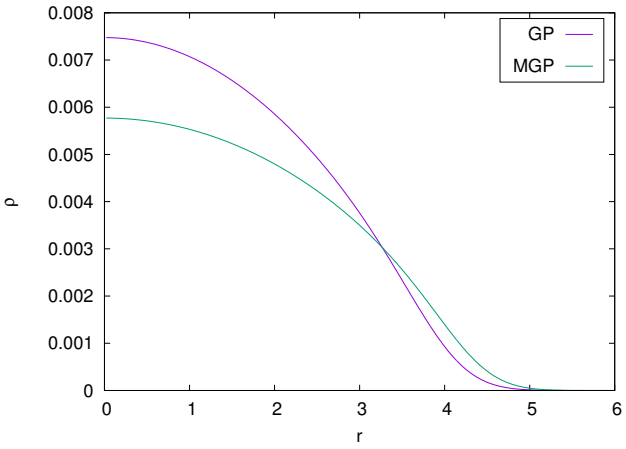

FIG. 1: Comparison of the density profiles $\rho(r)$ for systems under the GP and MGP equations, for $a_s = 0.1$, $N = 1000$, which corresponds to $\chi \sim 10^{-2}$, beyond the range of validity of the GP equation.

Then, by knowing that $M_1 = e_{HO}$, we can compute the excitation energy as

$$\bar{E}_m = \sqrt{\frac{M_3}{M_1}} = \left(5 - \frac{t_{\text{kin}}}{e_{\text{HO}}}\right)^{1/2}. \tag{19}$$

That expression is useful because it let us set both upper and lower bounds on the value of $\bar{E}_m$. When there is no interaction, we will get the results of Eq. (11) back and $\bar{E}_m = 2$. If the interactions are large, we will enter the domain of validity of the Thomas-Fermi approximation and $E_{\text{kin}} \sim 0$, so $\bar{E}_m = \sqrt{5}$. That tells us a very interesting result, however large the interactions are, the excitation energy cannot be greater than $\sqrt{5}$ (in HO units, of course) in the framework of the GP equation.

Let us now compute a parallel result for the MGP equation. Using the same development we obtain

$$M_3 = e_{HO}\left(5 - \frac{t_{\text{kin}}}{e_{\text{HO}}} + \frac{27}{8}\frac{e_{\text{int},2}}{e_{\text{HO}}}\right). \tag{20}$$

In that case we recover the lower bound $\bar{E}_m = 2$ back, but clearly overpass the upper bound in the MGP case. This is a very characteristic difference between the result for the MGP and the result for the GP equation which can allow for an experimental verification.

III. RESULTS

To check the results presented in the previous section, numerical simulations were used. To begin with, we obtain the ground state from the GP and MGP equations. First, we will solve the equation for a spherically symmetric system, so our wave function will be written as

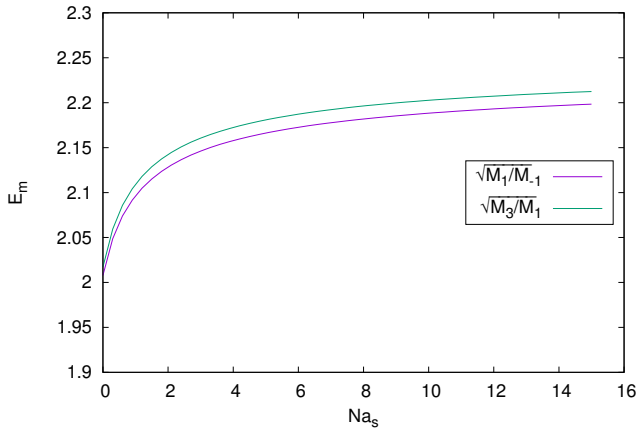

FIG. 2: $\bar{E}_m$ for a monopole excitation as a function of Na_s for a system obeying the GP equation, computed via both $\sqrt{M_3/M_1}$ and $\sqrt{M_1/M_{-1}}$.

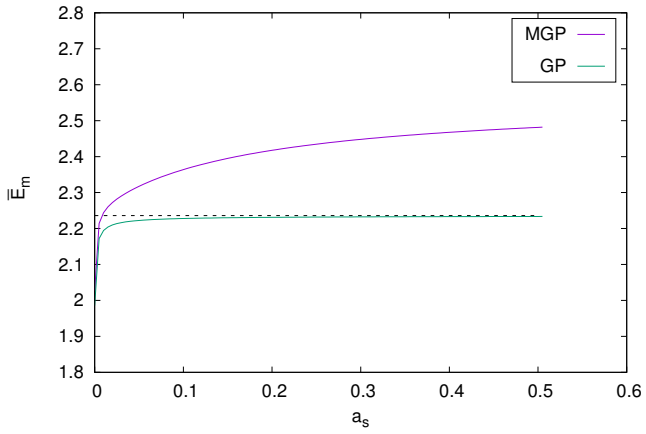

FIG. 3: $\bar{E}_m$ for a monopole excitation in function of a_s for systems with $N = 1000$ obeying the MGP and the GP equation, respectively. $\bar{E}_m$ is computed through $\sqrt{M_3/M_1}$. The values of a_s greater than 0.01 correspond to $\chi > 10^{-3}$.

$\varphi(r) = \frac{R(r)}{r}Y_{00}$, so we will only need to compute the radial part $R(r)$. If we assume our ground state non degenerate, we can use imaginary time methods, with time increments such that the linear approach is reliable:

$$R(r, t + \Delta t) = R(r, t) - \Delta t\, \mu(r) R(r, t), \qquad (21)$$

where the chemical potential $\mu(r)$ is computed from either the GP or the MGP equations. This method, however, does not guarantee that the norm $\langle R(r)|R(r)\rangle = 1$ is conserved, so this will have to bee imposed in every iteration. After a large number of iterations, we will get an stable solution for $R(r)$, with μ independent of r. The results for the wave function of the GP and MGP equations can be seen in Fig. (1).

Once the ground state wave function is computed we may start tackling the computation of the sum rules. Computing M_1 is straightforward, as the wave function is necessarily real (given the method used to obtain it) we will only need to multiply the squared wave function times the operator, $\frac{1}{2}r^2$ and integrate the result.

To compute M_{-1} we will need to perform perturbations to the system. To do so, we will compute the ground state energy for a system with an excitation of the form αr^2. Since there is already one contribution of the form of r^2 in both the GP and MGP equations, we will only need to add the perturbation parameter as a constant to such contribution. This is done for five values of α and then a 5-point finite differences method is used to compute the second derivative.

On the other hand, the computation of M_3 only requires to combine the different energy contributions to the virial theorem.

A. Results for $\bar{E}_m$

First of all, given that we have two different ways to compute $\bar{E}_m = \sqrt{M_3/M_1}$ and $= \sqrt{M_1/M_{-1}}$, we want to explore the compatibility of the results.

We can see in Fig. 2 that while the energies computed using the two methods are slightly different, both methods render what we expected from Eq. (19): the energy starts at $\bar{E}_m = 2$ and increases up to values close to $\bar{E}_m \sim \sqrt{5}$. This is usually attributed to the fact that there could be more than one excited state available for the considered perturbation.

So now that we have seen how should $\bar{E}_m$ behave for the GP , let us compare the results of $\bar{E}_m$ for the GP and MGP equations. Now, however, as discussed in section II.C, Na_s is not a suitable choice for the interaction parameter, as the extra interaction term in the MGP will have an extra a_s term, so we will use a_s as a parameter.

As we can see, the MGP renders greater excitation energies than the GP equation. what is more interesting, while the results for the GP equation are clearly bounded by $\bar{E}_m = \sqrt{5}$, the results for the MGP exceed the upper bound, thus marking a clear difference in the behaviour of the system under the GP or the MGP equations. We can see also common points: as expected both energies are equal to 2 when there is no interaction.

B. Comparison of $\bar{E}_m$ with a pulsating BEC.

While we have been able to accurately compute and compare the values of $\bar{E}_m$, we still have to see how well they represent the excitation energy, since they have been computed through only two sum rules. To this end, we will first compute the ground state wave function of a perturbed system, with a monopole excitation βr^2. Then,

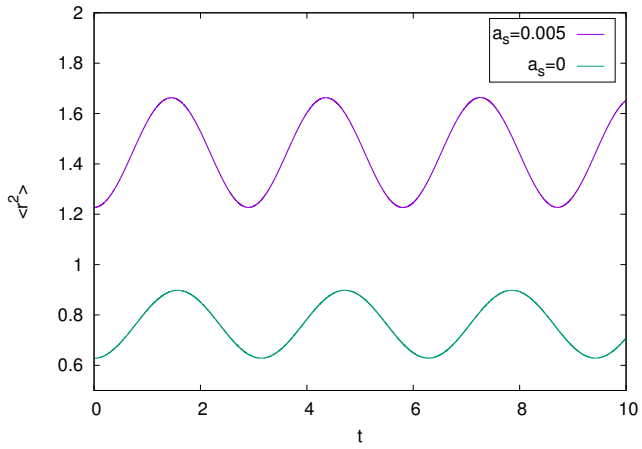

FIG. 4: $< r^2 > (t)$ for a system with $N = 1000$, following the MGP equation. We can see how for weaker interactions the frequency is smaller.

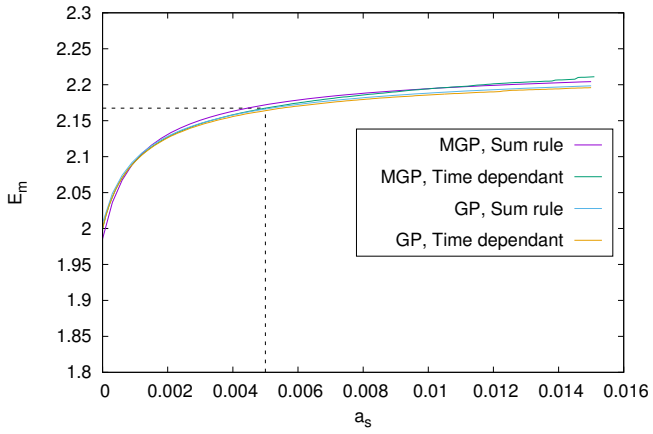

FIG. 5: Comparison of $\bar{E}_m$, obtained through sum rules and the time dependant method (extracting the frequency form pulsating BEC such as found in Fig. 4) for systems with $N = 1000$ obeying the MGP and GP equation respectively. The value for a_s from Fig. 4 is marked.

we will make this wave function evolve with the Hamiltonian of the non perturbed system. The condensate pulsates with a given frequency, which, by means of $E = \hbar\omega$ should coincide with $\bar{E}_m$.

As we can see, the system does indeed pulsate, since $\langle r^2 \rangle(t)$ follows a periodical form. This, however, only holds for weak and medium interaction values. When the interactions are very strong the solutions become unstable and no frequency can be extracted from the evolution of the system.

Let us now see how does the pulsating frequency compare to $\bar{E}_m$. In Fig. 5 we can see that the values computed through either the sum rule or frequency method are in agreement, . In this figure we can also see that the values for the MGP and GP equations are very similar, this is due to the low interaction values.

IV. CONCLUSIONS

- First of all, we have been able to see that, in the framework of mean field theories for BEC given by the GP and MGP equations, sum rules from the dynamic structure function are useful tools to extract information about the dynamics of system, at least for condensates under monopole excitations.
- We have also seen that, within the sum rules formalism, the results obtained for the MGP are clearly different to those from the GP equation, due to the fact that the system under the MGP equation exceeds the upper bound of $\bar{E}_m$ for systems under the GP equation at the regime of strong interactions. That clearly indicates the impossibility to obtain the MGP results by scaling the scattering length in the GP equation and should allow us to discriminate between the two equations by comparing with experimental results.

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