Amplitude modulated phase in Bose-Einstein condensate: the role of non-local interactions

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We consider a Gross-Pitaevskii model of BEC with non-local interactions of range of the order of the s-wave scattering length. With this model, we study the density modulated phase in 1D and 2D, which are solutions of this modified model along with the usual uniform density state. We find an exact free energy functional for our model and show that the 1D density modulated state can have lower energy than the uniform density state. Although, the density modulated state can be made to be energetically favourable, we show also that, this state is inherently dynamically unstable due to the coupling of instabilities to the spatial order.

INTRODUCTION

The Bose-Einstein condensate (BEC) is a superfluid macroscopic quantum phase of matter. It has tremendous importance in applications across a wide range of physics. To mention a few, BEC has applications in the field of Quantum Information[1], Quantum Metrology[2], Atomic Lasers[3, 4], Atom Holography[5], Interferometry[6], Slow Light[7], Atom Clocks[8] and Analogue Gravity[9]. Normally, the considered uniform ground state of this inherently unstable gas phase at nano-kelvin temperatures is given by the complex order parameter $\psi = e^{i\theta}$. This ground state is the chemical potential. In such a system, one considers two-body s-wave scattering to be the means of interaction between bosons and the s-wave scattering length $a$ to be much smaller than the average inter-particle separation $n^{-1/3}$. This ground state is dynamically stable to small amplitude fluctuations of the form $\theta(r, t) = \sum_i |u_i| \langle br e^{-i\omega t} + v_i^* e^{i\omega t} \rangle$, provided $\int |u_i|^2 \neq \int |v_i|^2$. These small amplitude excitations are important in determining the thermodynamics of this short lived ground state of BEC.

Because of the superfluid character of the BEC for the velocities below the velocity of sound in it, a modulated density phase is of particular interest. A modulated density phase, if exists, can have a non-zero group velocity. If this group velocity is below the critical velocity of the Landau criterion of superfluidity one can get the superflow of an ordered phase which is the yet unachieved supersolid phase. Supersolid is a state of matter with a crystalline order flowing without dissipation. Penrose and Onsager (PO) [10] have shown the impossibility of having such a phase (considering superfluid helium). Since then, many have contended this result and tried to circumvent the PO observations by postulating the presence of a lattice of vacancies in the solid and considering a super-flow of these vacancies [11, 12]. This is a situation where there are not always particles sitting at each lattice site as has been modelled by PO. There are some recent interesting proposals based on dynamical creation of super-solid in optical lattice [13] and using Rydberg-excited BEC [14].

Significant early work in this direction, involving a condensate, has been done by Pomeau and Rica (PR). They considered a Gross-Pitaevskii model with non-local interactions (in the form of a non-local differential equation). In their analytical treatment, they considered a density modulation on top of a uniform density state and argued on the basis of lowering of the roton minimum that, such a state can be a ground state of the condensate [15, 16]. By numerical simulations, PR have been able to capture a hexagonal lattice structure with sharp peaks in 2D and bcc/hcp in 3D as zero-temperature phase of BEC. Josserand and PR extended these works to a considerable extent in predicting the mechanical properties of such a phase [17]. The most important insight offered by PR, in these works, is the possibility of lowering the roton energy gap by increasing the density of the condensate and getting a subcritical (first order) transition to a coexisting superfluid and crystalline order.

In the present paper we are going to show analytically that, a pure density modulated phase (not a density modulated over a uniform density phase) can be identified as a state of lower free energy than the uniform density ground state of BEC in the presence of weak, repulsive, non-local interaction. By weak interactions we mean that, we are considering only two-body s-wave scattering (conventionally called zero energy scattering) as the means of cross-talks between bosons. The only constraint that be relaxed is the $\delta$-correlated interaction between bosons as is considered in the local format of a Gross-Pitaevskii (GP) equation. We take into account that, the s-wave scattering length being tunable by Feshbach Resonance [18], the condition $a_a << n^{-3}$ can be relaxed. Important to note again that, in the above mentioned works of PR non-locality of the interactions is the most important ingredient.

We add the minimal correction to the local GP equation capturing the non-locality of interactions and find out the corresponding exact free energy functional to this modified GP equation. We solve this modified GP equation to show density modulated states and identify these
states to be a lower energy state than the uniform density state using the free energy functional for the modified dynamics. However, it explicitly comes out that such an amplitude modulated state is generically dynamically unstable. The reason of the dynamical instability is the very existence of the spatial order. In this paper, we would first explain the model considering the non-local s-wave scattering, then we would show results in 1D and 2D followed by a linear stability analysis of the 1D solution to show the generic instability. We conclude the paper with a discussion.

**THE MODEL**

We consider here a mean field model in keeping with the spirit of local GP dynamics for an interacting inhomogeneous condensate. We use the conventional local GP model with a correction term capturing the non-locality of interactions as

\[ i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar^2}{2m} \nabla^2 \psi + g|\psi|^2 \psi + \frac{a^2 g}{6} \psi \nabla^2 |\psi|^2, \]  

(1)

where the last term arises due to the consideration of the non-local s-wave scattering. In the above equation, \( m \) is the mass of a boson, \( g = 4\pi \hbar^2 a/m \) is the strength of inter-particle interactions (s-wave scattering), and \( a \) is the s-wave scattering length. This model was introduced by us in the context of analogue gravity showing a possibility of rapid variation of healing length \( \xi \) by a variation of the s-wave scattering length \( a \) as the scattering length comes closer to the average separation between particles. Similar model has been used by a number of people to show the effect of weak non-local interactions under various circumstances.

The idea behind deriving this modified GP model is in the following. If, in the interaction term in the GP equation \( \psi(r) \int dr' \psi^*(r') V(r - r') \psi(r') \), one does not consider the interaction range for s-wave scattering as \( a << n^{-1/3} \), then, one cannot make a \( \delta \)-function approximation for the range of interactions \( V(r - r') \). One has to Taylor expand \( \psi(r') \) about \( r \) and the resulting gradient part of the correction vanishes on integration due to the spherical symmetry of the interactions. The next term comes out to be the one taken here. Note that, We consider here a flat, repulsive effective potential of a range the same as the s-wave scattering length \( a \) as is done in the standard GP procedure. The consideration of the range of interaction the same as s-wave scattering length is a good approximation for s-wave scattering. The only constraint relaxed is \( a << n^{-\frac{1}{3}} \) which is doable because Feshbach resonance can make \( a \) vary between \( -\infty \) to \( \infty \) and has already been demonstrated in a BEC. Equation (1) is a particularly nice model in the sense that, it is a the simplest local dynamics capturing effects of non-local interactions. The higher order correction term containing odd order derivatives are ruled out by symmetry when one sticks to the s-wave scattering and the even order ones are neglected considering \( \psi \) does not vary that rapidly over space. However, one must retain the minimal correction involving the second order spatial derivative, as has been done here, because, the kinetic term already involves a similar derivative.

Now, the first thing to note is that, due to the presence of the extra non-linear term in Eq.1, not only the uniform density globally oscillating state \( \psi_0 = \sqrt{n}e^{-i\mu t/\hbar} \) is a solution, it can also have a spatially oscillating solution where the non-linear terms would cancel out each other under particular conditions. In the above mentioned uniform solution, \( \mu = gn \) is the chemical potential where \( n = |\psi_0|^2 \) is the density of the condensate. It is not difficult to check that Eq.1 can be derived by variation of a free energy functional of the form

\[ F = \int d^3r \left( \frac{\hbar^2}{2m} |\nabla \psi|^2 + \frac{g}{2} |\psi|^4 + \frac{a^2 g}{6} (|\psi|^2 \nabla |\psi|^2) + \frac{\psi^* |\psi|^2 \nabla^2 \psi^*}{2} + \frac{\psi^* |\psi|^2 \nabla^2 \psi}{2} \right) \]  

(2)

where the integrand is the free energy density. This is a generalization of the energy functional from which the conventional local GP equation results and the last three terms of the functional are the ones responsible for the addition of the correction term to the local GP dynamics. Being able to write this exact free energy functional for the modified GP dynamics clearly opens up the opportunity to actually look at the relative free energy of different solutions and in what follows, we would be doing that.

**AMPLITUDE MODULATED PHASE**

For the sake of simplicity, let us first work in 1D. Consider a solution of Eq.(1) of the standard form \( \psi(r, t) = \psi'(r, t)e^{i\omega t} \) where \( \omega \) is the global oscillation frequency which gets identified as the chemical potential \( \mu \) of the system in the case of a uniform ground state and would be of the same order for the modulated density states as we will see in the following. The uniform density GP ground state solution \( \psi_0 = \sqrt{n}e^{-i\mu t/\hbar} \) is still a solution of Eq.(1) with the same free energy \( F = \frac{2N^2}{2V} \) where the
total number of particles \( N = n \int d\mathbf{r} = nV \) and \( V \) is the volume. We would refer to this particular uniform density solution as the ground state frequently in what follows. There could be other single particle states as the solution of Eq.1 as \( \psi(\mathbf{r}, t) = \sqrt{n} e^{i(\mathbf{kx} - \omega t)} \). These are the solutions of the local GP equation as well where there is a kinetic energy cost which makes them higher energy states compared to the ground state at the same density. These are moving solutions with phase velocity \( v = \hbar k/m \). The ground state is the \( k \to 0 \) limit of these single particle states. Interestingly, in what follows we will see another uniform state at a \( k \to 0 \) limit which would be quite different from this ground state.

\[
F_n = \frac{|A|^2 \hbar^2 k^2 \sigma L}{2m} + \frac{g(|A|^2)^2 \sigma L}{4} \pm \left( \frac{g(|A|^2)^2 \sigma}{8k} - \frac{|A|^2 \hbar^2 k \sigma}{4m} \right) \sin 2kL. \tag{4}
\]

If we take \( \epsilon = \frac{\sin(2kL)}{2kL} \) then we can write \(|A|^2 = \frac{2m}{\hbar^2} \) and get the expression for free energy density as

\[
f_n = F_n \frac{V}{\hbar^2 k^2 n} + \frac{g n^2}{2} (1 \mp \epsilon), \tag{5}
\]

which gives the change in free energy density with respect to the ground state energy density \( \frac{g n^2}{2} \) as

\[
\Delta f_n = \frac{\hbar^2 k^2 n}{2m} \mp \frac{g n^2}{2} \epsilon. \tag{6}
\]

In the above expression, the minus sign corresponds to the cos solution which would be energetically favourable at large densities. Now, as \( g = \frac{4\pi \hbar^2 a}{m} \) or, equivalently, \( g = \frac{2\sqrt{3} \pi k^2}{mk} \), we can write eq.(6) equivalently as

\[
\Delta f_n = \frac{\hbar^2}{m} \left( \frac{k^2 n}{2} + \sqrt{6} \pi n^2 \epsilon \right). \tag{7}
\]

Fixing \( a = 2 \times 10^{-4} \text{cm} \) (so, \( k = \left( \frac{3}{2} \right) \sqrt{\frac{3}{2}} \times 10^4 \text{cm}^{-1} \) and \( L = 10^{-2} \text{cm} \), we get \( \epsilon = 0.3886 \times 10^{-5} \) and varying the density \( n \), we get the plot in Fig.1. Note that Fig.(1) is the plot of \( \Delta f_n \) for the modulated cosine phase. From eqn.(6) , it is clear that \( \Delta f_n \) for the modulate sine phase will always be positive. However, making \( kL \to kL + \pi \) will turn the sine phase into the cosine phase and vice versa. Fig.1 indicates that the free energy of the modulated cosine phase is greater than the free energy of the uniform density state till some value of density and then it becomes less than that of the uniform density state. This crossover happens around \( n = \frac{3}{\sqrt{2}} \) i.e. \( n = \left( \frac{4}{7} \right) k^4 L \). Further, fixing the density \( n = 10^{14} \text{cm}^{-3} \) and \( L = 10^{-2} \text{cm} \), and varying \( k \), we get the plot in Fig.2. Note now that after a certain value of \( k \), the free energy of the modulate sine phase becomes less than the free energy of the uniform density phase and the free energy of the cosine phase becomes greater than the free energy of the uniform density phase as \( k \) increases.

![Fig. 1](image)

**Fig. 1:** Figure shows the variation of \( \Delta f_n \), keeping \( k \) and the length of the condensate(L) to be constant, for the modulated cosine phase. \( k = \left( \frac{3}{2} \right) \sqrt{\frac{3}{2}} \times 10^4 \text{cm}^{-1} \) and \( L = 10^{-2} \text{cm} \).

These figures clearly show that there are wide regions over which the free energy density of the ordered phase is less than that of the uniform ground state. As is obvious from the expression of \( F_n \), such a state would obviously have a group velocity \( (\partial F_n/\partial k) \) which will diverge at large \( k \) and at \( k \to 0 \) as well. So, a possible supersolid candidate state should lie at intermediate small \( k \) values i.e. for relatively large s-wave scattering lengths.

Note that, the state with a finite \( k \) and \( L \) having \( \sin 2kL = 0 \) would have the free energy density \( f_n = \frac{\hbar^2 k^2}{2m} n + \frac{\alpha n^2}{2} \) which is always more than the free energy
of the so-called uniform density ground state. For the free energy to be comparable or less than that of the uniform density ground state, the $k$ should be such that $\sin 2kL \neq 0$ at the boundary and such a situation in principle can be achieved by using Feshbach resonance. For such a modulated density phase moving through a uniform density ground state the co-existence of the states would be necessary and Feshbach resonance can come handy even in such situations at least in principle as well. If the boundary condition is such that, the ordered phase does not vanish at the boundary, then, there will obviously be a healing region at the hard boundaries for which there will be an energy cost. If the energy gain in the ordered phase is sufficiently large to make up for this energy cost, the ordered phase can be energetically favourable over the uniform phase. Our plot of free energy in Fig.1 shows that it can be considerably lowered below the uniform ground state energy and, therefore, the cost of healing can be afforded.

It is not difficult to see that, in 2D, the system would admit modulated density states of the form $(\cos kx + i \cos ky)$. Such a state would have the same wave number as that in 1D states mentioned above. The free energy of such a state will be twice as much as the energy of its 1D form under the same conditions. The stability of such a 2D phase can also be inferred to follow the same qualitative conditions as its 1D form which we will show in the following. Such a state can be considered as a vacancy lattice as is shown in Fig.3. A vacancy lattice state is of interest in the context of supersolids where one tries to get around the PO condition of having a particle at each lattice point.

To look at the stability of these states, let us consider the specific case $\psi(x, t) = A \cos k x e^{-i \omega t/\hbar}$ and perturb it by the small amplitude modes $\vartheta(x,t) = \sum_i [u_i(x)e^{-i \omega_i t} + v_i^*(x)e^{i \omega_i t}]e^{-i \omega t/\hbar}$. Taking the ansatz

$$u_i(x) = u_i e^{i q x} \text{ and } v_i(x) = v_i e^{i q x},$$

the ensuing linear equations in the small amplitudes $u_i$ and $v_i$ would be of the form

$$\left( \frac{\hbar^2 q^2}{2m} + \frac{3g|A|^2 \cos^2 k x}{4} + \frac{g|A|^2}{2} - \mu - \hbar \omega_i + \Phi \right) u_i + \frac{3g|A|^2 \cos^2 k x}{4} + \frac{g|A|^2}{2} - \mu + \hbar \omega_i + \Phi^* \right) (u_i / v_i) = 0, \quad (8)$$

where

$$\Phi = - \left( \frac{a g^2}{2} \right) \left( i |A|^2 k q \sin 2k x + |A|^2 q^2 \cos^2 k x \right). \quad (9)$$

Because of the presence of the imaginary term in the expression of $\Phi$, $\omega_i$ is always complex and this is a generic instability of the ordered phase arising out of the coupling of the instability with the amplitude modulated state in

![Cosine phase – Sine phase —](image)

**FIG. 2:** Figure shows the variation of $\Delta f_n$ with the variation of $k$ at constant density (n) and length of the condensate (L) for both the modulated sine as well as the cosine phase. $n = 10^{14} \text{ cm}^{-3}$ and $L = 10^{-2} \text{ cm}$

![Density variation](image)

**FIG. 3:** Figure shows the variation of density of the two dimensional density modulated state, viz., $\cos kx + i \cos ky$. The grey scale denotes the density variation and X-axis and Y-axis denote position. $k$ is set to be equal to 1.
amplitude modulated phase in the presence of non-local interactions being proportional to the scattering length, the uniform density ground state cannot be obtained as a $k \to 0$ limit of the amplitude modulated phase. This is a different uniform density state with a huge energy cost.

**DISCUSSIONS**

In the present paper, we have done an analysis of non-local interactions induced density modulated solutions in a 1D free Bose-Einstein condensate with an exact free energy functional. We have considered the long-range $s$-wave scattering of particles. On the basis of that, we have incorporated an extra local term on the conventional local GP equation. This has been got by truncating a Taylor expansion of the order parameter for relatively small higher order derivatives which, in effect, restricts us considering very small length scales. We have seen that the density modulated state comes with a characteristic length scale of the order of the $s$-wave scattering length $a$ and that is well within the acceptable limit.

We have shown that the amplitude modulated state can have a lower free energy than the uniform density single particle ground state and this fact depends on the boundary conditions. The modulated density ground state, which happens to be a superposition of the single particle states is not a momentum eigenstate and can have a group velocity diverging at large $k$. So, to consider such a state as a supersolid one has to work with long range interactions. This density modulated state is generically unstable because of a coupling of the small amplitude excitations with the spatial order. A stable state can only be considered at zero temperatures. There exists at least 1 2D version of such a state which can also be considered as a lattice of vacancies. This state would also be unstable at finite temperatures. Our simple analysis on the basis of an exact free energy functional for the dynamical model we have considered is indicating the role of the long-range interactions in getting density modulated states in a BEC. It shows that such a state is a zero temperature entity as was envisaged by PR.

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