

# Some Remarks on the Fragmentation of Bose Condensates

R. W. Spekkens and J. E. Sipe  
*Department of Physics, University of Toronto, Toronto,  
 Ontario, Canada M5S 1A7*  
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We show how fragmentation of a Bose-Einstein condensate can occur given repulsive inter-particle interactions and a non-uniform external potential.

## I. INTRODUCTION

It is customary to approximate the  $N$ -body ground state of a system of spinless bosons by the Hartree-Fock state

$$|N, \phi_0\rangle = \frac{\left(\int d^3\mathbf{r}\phi_0(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r})\right)^N}{\sqrt{N!}}|\text{vac}\rangle,$$

where  $\phi_0(\mathbf{r})$  is a normalized single particle wavefunction [1]. This describes an accumulation of  $N$  particles in the wavefunction  $\phi_0(\mathbf{r})$ . One can, however, also consider states of the form

$$|N_1, \phi_1; N_2, \phi_2\rangle = \frac{\left(\int d^3\mathbf{r}\phi_1(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r})\right)^{N_1}}{\sqrt{N_1!}} \frac{\left(\int d^3\mathbf{r}\phi_2(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r})\right)^{N_2}}{\sqrt{N_2!}}|\text{vac}\rangle, \quad (1)$$

where  $\phi_1(\mathbf{r})$  and  $\phi_2(\mathbf{r})$  are normalized and orthogonal single-particle wavefunctions, and where  $N_1 + N_2 = N$ . Such a state describes an accumulation of  $N_1$  particles in the wavefunction  $\phi_1(\mathbf{r})$ , and  $N_2$  particles in  $\phi_2(\mathbf{r})$ . We distinguish states of the form  $|N, \phi_0\rangle$  from those of the form  $|N_1, \phi_1; N_2, \phi_2\rangle$  by designating the first as ‘single condensates’ and the second as ‘dual condensates’. It is evident that one can also introduce states describing the accumulation of particles in an arbitrary number of orthogonal single-particle wavefunctions. Such states can be referred to collectively as ‘fragmented condensates’ [2]. In this paper, we show how a non-uniform trap potential can encourage fragmentation. In particular, we demonstrate that in a double minimum potential a dual condensate can have an expectation value of the energy smaller than that of a single condensate, and therefore can constitute a better approximation to the fully interacting ground state and a better starting point for treatments beyond Hartree-Fock.

This result may be surprising to some and obvious to others. Specifically, it seems remarkable in light of Nozières’ argument against fragmentation of condensates [2]. On the other hand, it seems natural to describe bosons in well-separated traps by a product of single condensate states for each trap; for two traps, such a product state would be a dual condensate wherein each of  $\phi_1(\mathbf{r})$  and  $\phi_2(\mathbf{r})$  is centered in only one of the traps. Indeed, this has been assumed implicitly in the literature when discussing the interference of condensates [3]. Our analysis justifies this intuition and specifies the circumstances under which Nozières’ argument is inapplicable.

## II. DESIDERATA FOR FRAGMENTATION

We consider a two-particle interaction that is local and completely repulsive:  $V(\mathbf{r}, \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}')$ , The interaction strength is given by  $g = 4\pi a_{sc}\hbar^2/m$ , where  $a_{sc}$  is the s-wave scattering length, assumed to be positive, and where  $m$  is the mass of the particle. For simplicity we restrict ourselves to wavefunctions  $\phi_0(\mathbf{r})$ ,  $\phi_1(\mathbf{r})$ , and  $\phi_2(\mathbf{r})$  that are real. Consider the expectation value of the energy for a single condensate  $|N, \phi_0\rangle$ ,

$$E_s = N\epsilon(\phi_0) + \frac{1}{2}gN(N-1)\int\phi_0^4(\mathbf{r})d^3\mathbf{r}, \quad (2)$$

where  $\epsilon(\phi) = \int\phi(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right]\phi(\mathbf{r})d^3\mathbf{r}$  is the single particle energy associated with  $\phi(\mathbf{r})$ , and  $U(\mathbf{r})$  is the trap potential. For the dual condensate  $|N_1, \phi_1; N_2, \phi_2\rangle$ ,

$$E_d = N_1\epsilon(\phi_1) + N_2\epsilon(\phi_2) + \frac{1}{2}gN_1(N_1-1)\int\phi_1^4(\mathbf{r})d^3r + \frac{1}{2}gN_2(N_2-1)\int\phi_2^4(\mathbf{r})d^3r + 2gN_1N_2\int\phi_1^2(\mathbf{r})\phi_2^2(\mathbf{r})d^3r. \quad (3)$$

If we assume that the particle densities are similar throughout the single and dual condensates,  $N_1\phi_1^2(\mathbf{r}) + N_2\phi_2^2(\mathbf{r}) \simeq N\phi_0^2(\mathbf{r})$ , then the pieces of the interaction energies that scale as  $N^2$  are

$$\begin{aligned} E_s^{\text{quad}} &= \frac{1}{2}gN^2 \int \phi_0^4(\mathbf{r})d^3\mathbf{r} \\ E_d^{\text{quad}} &= \frac{1}{2}gN_1^2 \int \phi_1^4(\mathbf{r})d^3\mathbf{r} + \frac{1}{2}gN_2^2 \int \phi_2^4(\mathbf{r})d^3\mathbf{r} + 2gN_1N_2 \int \phi_1^2(\mathbf{r})\phi_2^2(\mathbf{r})d^3\mathbf{r} \\ &\simeq \frac{1}{2}gN^2 \int \phi_0^4(\mathbf{r})d^3\mathbf{r} + gN_1N_2 \int \phi_1^2(\mathbf{r})\phi_2^2(\mathbf{r})d^3\mathbf{r} \end{aligned} \quad (4)$$

We can think of this in the following way: while the Hartree contributions to the interaction energy of the single and dual condensates are essentially equal, the interaction energy of the dual condensate also includes an exchange term, proportional to  $N_1N_2$ , arising from symmetrization.

This extra exchange energy was identified by Nozières [2] and is the basis of his argument against fragmentation of the condensate, since in the limit of a macroscopic number of particles,  $E_d^{\text{quad}}$  exceeds  $E_s^{\text{quad}}$  by a macroscopic energy. However, this argument assumes that the wavefunctions have a similar spatial extent  $\phi_1^2(\mathbf{r}) \simeq \phi_2^2(\mathbf{r}) \simeq \phi_0^2(\mathbf{r})$ . If instead one considers a dual condensate wherein  $\phi_1$  and  $\phi_2$  have little density overlap, then the exchange term may be small compared to other terms in (4) that are linear in  $N$ , and we must consider the relative weights of all the terms.

The energies  $E_d^{\text{quad}}$  and  $E_s^{\text{quad}}$  overestimate the interaction energy since they incorporate a particle's interaction with itself. Thus, to obtain the proper interaction energy, we must add to  $E_s^{\text{quad}}$  a term linear in  $N$

$$E_s^{\text{lin}} = -\frac{1}{2}gN \int \phi_0^4(\mathbf{r})d^3\mathbf{r}. \quad (5)$$

Similarly, we must add to  $E_d^{\text{quad}}$  the linear term

$$E_d^{\text{lin}} = -\frac{1}{2}gN_1 \int \phi_1^4(\mathbf{r})d^3\mathbf{r} - \frac{1}{2}gN_2 \int \phi_2^4(\mathbf{r})d^3\mathbf{r}. \quad (6)$$

If  $\phi_1$  and  $\phi_2$  are more localized than  $\phi_0$ , then  $\int \phi_{1,2}^4(\mathbf{r})d^3\mathbf{r} > \int \phi_0^4(\mathbf{r})d^3\mathbf{r}$ . It follows that  $E_d^{\text{lin}} - E_s^{\text{lin}} < -\frac{1}{2}gN \int \phi_0^4(\mathbf{r})d^3\mathbf{r}$ . Thus, the linear piece of the interaction energy favors the dual condensate.

Admittedly, it will cost more single particle energy to place particles in localized wavefunctions like  $\phi_1$  and  $\phi_2$  than in  $\phi_0$ , so the single particle energy favors the single condensate. Thus we see that there is a competition between the interaction energy benefit that may arise from separating the bosons, and the single particle energy cost of establishing this separation. The role of the trap potential in fragmentation is now clear: for a non-uniform potential, one can construct wavefunctions that are confined to the valleys of the potential and which have little density overlap without a large cost of single particle energy. A non-uniform potential therefore encourages spatial fragmentation.

### III. FRAGMENTATION IN A DOUBLE WELL POTENTIAL

We now turn to a simple model of the condensate in a potential well that is symmetric along each Cartesian axis, but which along one axis ( $x$ ) exhibits a double minimum. We wish to consider which of the single or dual condensate is energetically favored as a function of the strength of the central barrier of the potential. As is customary, one minimizes the energy of the single condensate with respect to variations in  $\phi_0$  to obtain a non-linear Schrödinger equation (NLSE) for  $\phi_0$ . Due to the symmetry of the potential, we expect that the energetically favored dual condensate will have the particles distributed equally between wavefunctions that are mirror images of one another across  $x = 0$ , that is,  $\phi_1(-x, y, z) = \phi_2(x, y, z)$  and  $N_1 = N_2 = N/2$ . Assuming a dual condensate of this form, we can minimize its energy with respect to variations in  $\phi_1$  and  $\phi_2$  to obtain two coupled NLSEs for  $\phi_1$  and  $\phi_2$ .

Let us first consider the case of an infinitely strong barrier; all wavefunctions will then have zero amplitude at the center of the barrier. The single condensate that minimizes the expectation value of the energy has a degeneracy associated with the different possible symmetries of the wavefunction across the barrier. Let us denote the symmetric solution of the single condensate NLSE as  $\phi_s$  and the antisymmetric solution as  $\phi_a$ . We can then construct two wavefunctions  $\phi_l = 2^{-1/2}(\phi_s + \phi_a)$  and  $\phi_r = 2^{-1/2}(\phi_s - \phi_a)$  that are confined respectively to the left ( $x < 0$ ) and right ( $x > 0$ ) of the barrier, and which have the same single particle energy as  $\phi_s$ .

In the single condensate  $|N, \phi_s\rangle$ , the magnitude of the interaction energy is  $\frac{1}{2}gN(N-1) \int \phi_s^2(\mathbf{r})d^3\mathbf{r}$ . This can be understood as follows: there are  $N$  particles interacting with  $N-1$  others with an interaction strength of  $g \int \phi_s^2(\mathbf{r})d^3\mathbf{r}$ ,

and the factor of  $1/2$  is due to over-counting. Now consider the particular dual condensate that is of the form  $|N/2, \phi_l; N/2, \phi_r\rangle$ , noting that this state is *not* necessarily the solution of the dual condensate variational problem. The interaction energy of this state originates solely from the interaction of particles with others in the same wavefunction, since the density overlap of the two wavefunctions,  $\int \phi_l^2(\mathbf{r})\phi_r^2(\mathbf{r})d^3\mathbf{r}$ , is zero. Particles in this dual condensate interact twice as intensely with one another than in the single condensate since  $\int \phi_l^4(\mathbf{r})d^3\mathbf{r} = \int \phi_r^4(\mathbf{r})d^3\mathbf{r} = 2 \int \phi_s^4(\mathbf{r})d^3\mathbf{r}$ . However, each of the  $N$  particles sees only  $N/2 - 1$  others rather than  $N - 1$  others. Including the over-counting factor of  $1/2$ , the total interaction energy of this dual condensate is  $\frac{1}{2}gN(N - 2) \int \phi_s^4(\mathbf{r})d^3\mathbf{r}$ . This interaction energy is clearly less than that of the single condensate. Since the single particle energies are the same for the two states, it follows that the dual condensate  $|N/2, \phi_l; N/2, \phi_r\rangle$  is energetically favored overall. Further, the dual condensate that is obtained from solving the variational problem may have an energy that is lower still.

For small barrier strengths we expect the single condensate to be energetically favored. This is because a dual condensate that has little density overlap of  $\phi_1$  and  $\phi_2$  will necessarily have a greater single particle energy than the single condensate. Alternatively, if the single particle energies are comparable, the wavefunctions  $\phi_1$  and  $\phi_2$  will necessarily have a large density overlap. It is conceivable that if the interaction strength were strong enough, it could become energetically favorable for the condensate to fragment even in the absence of any trap potential. However, if the scattering length,  $a_{sc}$  is much less than the average width of the ground state of the trap, it can be verified that a single condensate is preferred at small barrier strengths.

To determine precisely the barrier strength at which the dual condensate becomes energetically preferred over the single condensate, one must solve the variational problems for both types of condensate and compare the energies obtained.

#### IV. THE EXPERIMENTAL SIGNATURE OF FRAGMENTATION

The most conspicuous difference between spatially fragmented and non-fragmented condensates is the extent of spatial coherence, or long range order, in the system. Specifically, let us imagine a double well potential with a large central barrier and ask how one could distinguish a single condensate  $|N, \phi_s\rangle$  where  $\phi_s$  is a doubly peaked symmetric wavefunction, from a dual condensate  $|N/2, \phi_l; N/2, \phi_r\rangle$  where  $\phi_l$  and  $\phi_r$  are mirror images of one another centered on the left and right sides of the barrier respectively. The answer to this question can be found in the recent literature [4]; essentially, the difference is revealed through interference experiments.

A single run of such an experiment proceeds as follows: after the condensate is formed, the trap potential is removed instantaneously and the particles are allowed to expand freely until the wavefunctions from either side of the barrier have overlapped, at which time the positions of the particles are measured. Assuming the particles do not interact much during the expansion, the wavefunctions for each particle will evolve independently. If one models the particle detection in a manner analogous to the standard theory of photon detection, as is proposed in [5], then both the single and dual condensates will generate an interference pattern. The single condensate exhibits interference since each particle interferes with itself just as it would in a double slit experiment. In the dual condensate, the probability density for each particle is essentially uniform before the first detection, but as is described in [5], the first detection modifies the state such that the probability densities for the second and subsequent detections are no longer uniform, and an interference pattern emerges.

The difference between the single and dual condensates can only be seen by a comparison of how the spatial phase of the interference pattern varies from one experimental run to the next. For the single condensate, the spatial phase is the same in every run, while for the dual condensate, it varies randomly.

In the experiment of Andrews *et al.* [6] a cloud of sodium atoms was cooled to below the phase-space density threshold for Bose-Einstein condensation in a double well potential. Upon releasing and detecting these atoms, an interference pattern was observed. Whether the spatial phase of interference patterns from different experimental runs are fixed relative to one another or not has not yet been determined due to mechanical instabilities in the apparatus. Although it was not our intention in this paper to provide a detailed model of this experiment, it is clear that the considerations outlined herein will be relevant to any such model.

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[1] Another common approach is to associate with the condensate a coherent state over Hartree-Fock states,  $|\alpha, \phi_0\rangle = \exp(\alpha \int d^3\mathbf{r} \phi_0(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r})) |\text{vac}\rangle$ , where  $\alpha$  is a complex parameter with modulus squared equal to  $N$ . It is unclear how one could describe the effects discussed herein using such an approach.

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