GROUND STATE FRAGMENTATION OF REPULSIVE BOSE-EINSTEIN CONDENSATES IN DOUBLE-TRAP POTENTIALS

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The Hamiltonian

We consider a system of N identical bosons in an external potential $\hat{V}(\vec{r})$
$\Longrightarrow h(\vec{r}) = \hat{T} + \hat{V}(\vec{r})$ unperturbed one-particle Hamiltonian
$\Longrightarrow$ Bosons interact via a δ-function potential: $W(\vec{r}_1 - \vec{r}_2) = \lambda_0\,\delta(\vec{r}_1 - \vec{r}_2)$
$\lambda_0 = \frac{4\pi a_{sc}}{m}$, a_{sc} - is the s-wave scattering length.
Here, repulsive interaction only $\lambda_0 > 0$.

$$H = \int d\vec{r}\Psi^\dagger h\,\Psi + \frac{\lambda_0}{2}\int d\vec{r}\,\Psi^\dagger\,\Psi^\dagger\,\Psi\,\Psi$$

Fragmentation

The general mathematical formulation of the condensation phenomenon for an ideal gas in equilibrium has been given by Penrose and Onsager [1] in 1956. The generalized one-particle reduced density matrix of N-particle system:

$$\rho^N(\vec{r}\,',\vec{r}) = N\int \Psi^{N\dagger}(\vec{r}\,',\vec{r}_2,\cdots,\vec{r}_N)\Psi^N(\vec{r},\vec{r}_2,\cdots,\vec{r}_N)\,d\vec{r}_2\,d\vec{r}_3\cdots d\vec{r}_N$$

where Ψ^N is a normalized N-body wave function. One can write:

$$\rho^N(\vec{r}\,',\vec{r}) = \textstyle\sum_i\, n_i\,\varphi_i^*(\vec{r}\,')\varphi_i(\vec{r})$$

Eigenvalues of ρ^N -*occupation numbers*, eigenvectors -*natural orbitals*
Condensation MACROscopic occupation of one natural orbital [1]

Fragmentation MACROscopic occupation of several natural orbitals [2]

Gross-Pitaevskii Mean-Field

Usual assumption: All bosons reside in a single spatial orbital φ

$$\Psi^N_{GP}(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N) = \varphi(\vec{r}_1)\varphi(\vec{r}_2)\cdots\varphi(\vec{r}_N)$$

$$E_{GP} = N\int \varphi^* h\,\varphi\,d\vec{r} + \frac{\lambda_0\,N(N-1)}{2}\int |\varphi|^4\,d\vec{r}$$

The well-known Gross-Pitaevskii (GP) mean-field equation [3] is obtained by minimizing this energy:

$$\{\,h(\vec{r}) + \lambda_0(N-1)|\varphi(\vec{r})|^2\}\,\varphi(\vec{r}) = \mu_{GP}\,\varphi(\vec{r})$$

The reduced one-particle density operator and the corresponding spatial density are given by

$\rho_{GP}(\vec{r}\,',\vec{r}) = \varphi^*(\vec{r}\,')\varphi(\vec{r})$ and $\rho_{GP}(\vec{r}) = |\varphi(\vec{r})|^2$ respectively.

Main conclusion: By definition, this equation cannot describe fragmentation because all bosons reside in a single orbital.

Best Mean-Field Description

Main assumption: Bosons may reside in several different spatial orbitals ϕ_i

$$\Psi^N_{BMF} = \hat{\mathcal{S}}\phi_1(\vec{r}_1)\cdots\phi_1(\vec{r}_{n_1})\phi_2(\vec{r}_{n_1+1})\cdots\phi_2(\vec{r}_{n_1+n_2})\phi_3(\vec{r}_{n_1+n_2+1})\cdots\phi_3(\vec{r}_N)$$

where $\hat{\mathcal{S}}$ is the symmetrizing operator and $N \equiv n_1 + n_2 + n_3$.

$$\begin{aligned}E_{BMF} &= n_1h_{11} + \lambda_0\frac{n_1(n_1-1)}{2}\int|\phi_1|^4d\vec{r} + 2\lambda_0n_1n_2\int|\phi_1|^2|\phi_2|^2d\vec{r}\\ &+ n_2h_{22} + \lambda_0\frac{n_2(n_2-1)}{2}\int|\phi_2|^4d\vec{r} + 2\lambda_0n_1n_3\int|\phi_1|^2|\phi_3|^2d\vec{r}\\ &+ n_3h_{33} + \lambda_0\frac{n_3(n_3-1)}{2}\int|\phi_3|^4d\vec{r} + 2\lambda_0n_2n_3\int|\phi_2|^2|\phi_3|^2d\vec{r}\end{aligned}$$

By minimizing this energy with respect to the orbitals under the constraints that they are orthogonal and normalized, i.e., $<\phi_i|\phi_j>=\delta_{ij}$, we get the following three coupled Best Mean-Field (BMF) equations [4] for the optimal orbitals:

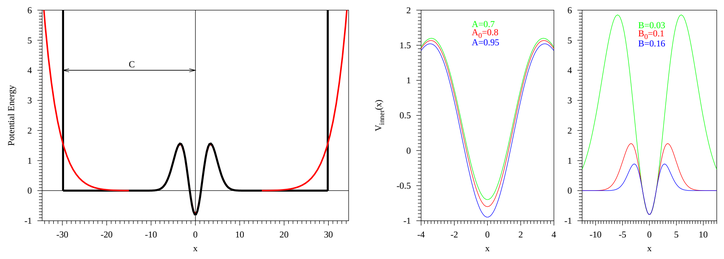
$$\begin{aligned}\{\,h(\vec{r}) + \lambda_0(n_1-1)|\phi_1(\vec{r})|^2 + 2\lambda_0n_2|\phi_2(\vec{r})|^2 + 2\lambda_0n_3|\phi_3(\vec{r})|^2\}\,\phi_1(\vec{r}) &= \\ = \mu_{11}\,\phi_1(\vec{r}) + \mu_{12}\,\phi_2(\vec{r}) + \mu_{13}\,\phi_3(\vec{r})\\ \{\,h(\vec{r}) + \lambda_0(n_2-1)|\phi_2(\vec{r})|^2 + 2\lambda_0n_1|\phi_1(\vec{r})|^2 + 2\lambda_0n_3|\phi_3(\vec{r})|^2\}\,\phi_2(\vec{r}) &= \\ = \mu_{21}\,\phi_1(\vec{r}) + \mu_{22}\,\phi_2(\vec{r}) + \mu_{23}\,\phi_3(\vec{r})\\ \{\,h(\vec{r}) + \lambda_0(n_3-1)|\phi_3(\vec{r})|^2 + 2\lambda_0n_1|\phi_1(\vec{r})|^2 + 2\lambda_0n_2|\phi_2(\vec{r})|^2\}\,\phi_3(\vec{r}) &= \\ = \mu_{31}\,\phi_1(\vec{r}) + \mu_{32}\,\phi_2(\vec{r}) + \mu_{33}\,\phi_3(\vec{r})\end{aligned}$$

Main features of this approach should be mentioned:

- This mean-field includes GP as a special case: when the occupation of two of the three orbitals vanish, i.e. $n_2 = n_3 = 0$, the system of BMF equations is reduced to the single GP equation and the respective energy coincides with the GP one.
- By construction, this method can describe fragmentation for a finite number of fragments. The reduced one-particle density operator can be written as $\rho_{BMF}(\vec{r}\,',\vec{r}) = \sum_i^3\, n_i\,\phi_i^*(\vec{r}\,')\phi_i(\vec{r})$ and the corresponding spatial density becomes $\rho_{BMF}(\vec{r}) = n_1|\phi_1(\vec{r})|^2 + n_2|\phi_2(\vec{r})|^2 + n_3|\phi_3(\vec{r})|^2$.
- Occupation number n_i are variational parameters, minimizing the full energy.

In order to find an optimal value of the energy, BMF equations are solved for all possible occupation numbers, and the respective energies are evaluated and compared.
As we mentioned before, the results obtained for the specific occupation numbers $n_2 = n_3 = 0$ are identical to the standart GP ones. Therefore, within this computational scheme we automatically clarify the question on the favorability of fragmentation.

Proposed Double-Trap Potential



Our proposed 1D double-trap potentials effectively may be obtained as a superposition of two potentials (inner and outer). We model the inner potential as:

$$V_{inner}(x) = \omega(\frac{x^2}{2} - A)e^{(-Bx^2)}$$

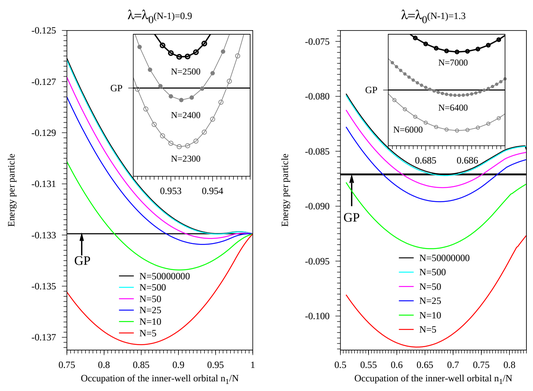
where A and B are parameters of the inner trap (see Right figure), $A_0 = 0.8$, $B_0 = 0.1$ are reference parameters.
As an outer trap embedding the inner one we used:

- Infinite square well with half-width equal C obtained by placing the infinite walls at $[-C:+C]$ (see black curve in the Left figure)
- Smooth power potential $V_{outer}(x) = (0.035x)^{10}$ (red curve in the Left figure).

Default outer trap is a square well with walls at $C_0 = 9.5\pi$.
Kinetic energy: $\hat{T} = -\frac{\omega}{2}\frac{\partial^2}{\partial x^2}$ implying that coordinate x and all the parameters A, B, C of the double-trap potential are dimensionless while all energies and λ_0 are now in units of the frequency ω.

Optimal Energies

Keeping the quantity $\lambda = \lambda_0(N-1)$ fixed, BMF equations have been solved numerically for the systems of different numbers of bosons, and different fractional occupation numbers n_1, n_2, n_3. Due to symmetry of our double-trap potential, instead of searching for the minimum of a functional $E(n_1,n_2,n_3)$ of two independent variables $(n_3 \equiv N - n_1 - n_2)$, we can do the search using $n_2 = n_3$.



Main Observation:

For $\lambda = 0.9$ and $N \leq 2400$, $\lambda = 1.3$ and $N \leq 6400$ the optimal BMF solution energetically more favorable then GP one. Therefore, for these systems the

Ground State is three-fold FRAGMENTED!

The combined potential $(V_{inner} + V_{outer})$ has three well-separated wells. Therefore, if fragmentation takes place, bosons will be accumulated in each of these three wells. More precisely, the reduced one-particle density of the system of N identical bosons in this double-trap potential would have three *macroscopic* (with respect to N) eigenvalues. The condition that all three wells are well separated from each other implies that the respective eigenvectors (natural orbital) will be predominantly localized in each of these wells.

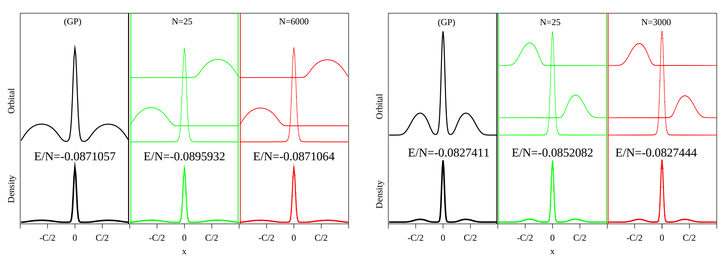
Optimal Orbitals and Occupation numbers

Double-trap potential with *infinite walls*, $\lambda = 1.3$:

- For $N = 6000$: $n_1/N \approx 68.58\%$ for the orbital localized in the central well and $n_2/N \approx n_3/N = 17.71\%$ for the orbitals localized in the outer wells
- For $N = 25$: $n_1/N \approx 67.5\%$ and $n_2/N \approx n_3/N = 16.25\%$.

Double-trap potential with a *smooth power outer trap*, $\lambda = 1.3$:

- For $N = 3000$: $n_1/N \approx 72.2\%$ for the orbital localized in the central well and $n_2/N \approx n_3/N = 13.9\%$ for the orbitals localized in the outer wells
- For $N = 25$: $n_1/N \approx 71.0\%$ and $n_2/N \approx n_3/N = 14.5\%$.

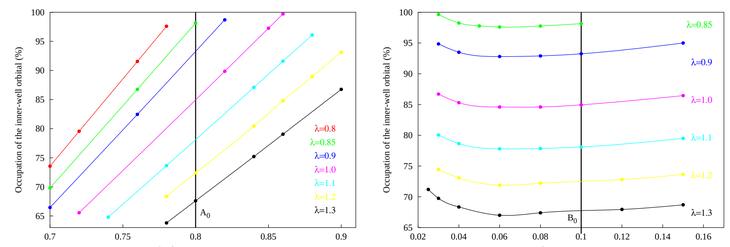


The optimal BMF orbitals $\phi_1(x)$, $\phi_2(x)$, $\phi_3(x)$ and respective density per particle $\rho_{BMF} = (n_1|\phi_1|^2 + n_2|\phi_2|^2 + n_3|\phi_3|^2)/N$ of the three-fold fragmented ground state for the double-trap potentials with infinite walls (Left figure) and with a smooth power outer trap (Right figure). The energy per particle is indicated. For convenience, the base-line of the orbitals $\phi_2(x)$ and $\phi_3(x)$ has been moved upwards artificially from zero. All orbitals and densities are dimensionless and plotted as function of the dimensionless coordinate x, $C = C_0 = 9.5\pi$.

Manipulation of Fragmentation

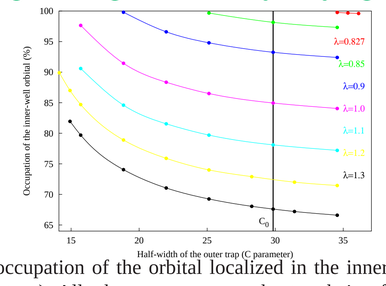
By "manipulation of the fragmentation" we mean the possibility to choose the shape of the trap potential as well as the number of bosons (and possibly also their scattering length) in such a way that all fragments acquire the desired occupation numbers.

Manipulating the fragmentation by varying the inner trap



Shown is the relative occupation of the orbital localized in the inner well.
Left figure: Dependence on the parameter A. $(B = B_0,\, C = C_0)$
Right figure: Dependence on the parameter B. $(A = A_0,\, C = C_0)$

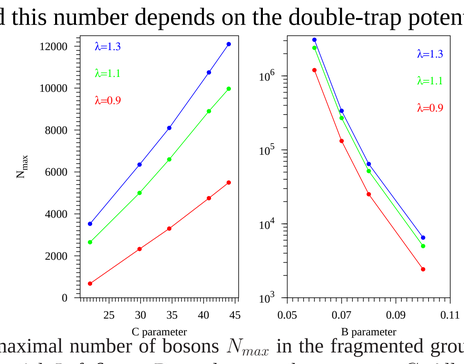
Manipulating the fragmentation by varying the outer trap



Shown is the relative occupation of the orbital localized in the inner well as a function of C (half-width of the outer trap). All other parameters are kept at their reference values A_0 and B_0.

Critical parameters of fragmentation

From the above figure it is clear that the fragmentation starts to take place when λ exceeds some threshold. Another limitation comes from the fact that when λ becomes so large that the chemical potential is larger than the barrier height, particles can flow freely out of the inner trap and the fragmentation disappears. Consequently, there is a maximal number N_{max} of bosons in a fragmented ground state and this number depends on the double-trap potential.



Manipulating the maximal number of bosons N_{max} in the fragmented ground state by varying the double-trap potential. Left figure: Dependence on the parameter C. All other parameters are kept at their reference values A_0 and B_0. Right figure: Dependence on the parameter B (note the logarithmic scale). All other parameters are kept at their reference values A_0 and C_0.

Summary

We have investigated the fragmentation phenomenon in the ground state of a repulsive condensate immersed into the double-trap potential.

- We demonstrate that fragmentation can be successfully characterized by the Best Mean-Field approach.
- For many choices of the potentials, the macroscopic occupation of the three orbitals may become energetically more favorable than accumulating all the particles in a single orbital.
- The fragmentation of the ground state is found to occur when the number of bosons exceeds some critical value which depends on the scattering length and on the shape of the inner trap potential.
- If fragmentation is observed for a large number of bosons, then it exists also for any smaller number of bosons (of course $N > 1$) when λ is kept fixed. When λ is kept fixed, there exists, however, a maximal number of bosons for which the ground state is fragmented.
- The interplay between the inner and outer trap potentials provides a sensitive tool to manipulate fragmentation of repulsive condensates.
  Varying the number of bosons in the condensate and the scattering length are also instrumental in this respect.
- The results obtained for three-well potentials can naturally be extended to an array of multiple wells.
- Finite particle number is needed to observe fragmentation in the ground state.

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