Molecular fraction calculation for an atomic-molecular Bose-Einstein condensate model

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Hamiltonian

The model consists of three interacting bosonic degrees of freedom:

$$H = U_{aa}N_a^2 + U_{bb}N_b^2 + U_{cc}N_c^2 + U_{ab}N_aN_b + U_{ac}N_aN_c + U_{bc}N_bN_c \\ + \mu_aN_a + \mu_bN_b + \mu_cN_c + \Omega(a^\dagger b^\dagger c + c^\dagger ba).$$

It commutes with the total atom number $N = N_a + N_b + 2N_c$ and the atomic imbalance $J = N_a - N_b$. We introduce

$$k = J/N,\ k \in [-1, 1]$$

as the fractional atomic imbalance. The classical analogue is the non-linear pendulum

$$H = \lambda p_\phi^2 + 2(\alpha - \lambda)p_\phi + \lambda - 2\alpha + \beta \\ + \sqrt{2(1 - p_\phi)(p_\phi + c_+)(p_\phi + c_-)}\cos\left(\frac{4\phi}{N}\right)$$

with

$$\lambda = \frac{\sqrt{2N}}{\Omega}\left(\frac{U_{aa}}{4} + \frac{U_{bb}}{4} + \frac{U_{cc}}{4} + \frac{U_{ab}}{4} - \frac{U_{ac}}{4} - \frac{U_{bc}}{4}\right)$$

$$\alpha = \frac{\sqrt{2N}}{\Omega}\left(\frac{1+k}{2}U_{aa} + \frac{1-k}{2}U_{bb} + \frac{1}{2}U_{ab} - \frac{1+k}{4}U_{ac} - \frac{1-k}{4}U_{bc} + \frac{1}{2N}(\mu_a + \mu_b - \mu_c)\right)$$

$$\beta = \frac{\sqrt{2N}}{\Omega}\left((1+k)^2 U_{aa} + (1-k)^2 U_{bb} + (1-k^2)U_{ab} + \frac{2}{N}((1+k)\mu_a + (1-k)\mu_b)\right)$$

$$c_\pm = 1 \pm 2k.$$

Order parameter - the molecular fraction

Define the order parameter

$$\mathcal{O} = 2\frac{\langle N_c \rangle}{N} = \frac{2}{N}\frac{\partial E_0}{\partial \mu_c}$$

which measures the average molecular fraction:

$$\begin{aligned} \mathcal{O} &= 0 & \text{atomic} \quad &\text{phase,} \\ 0 < \mathcal{O} &< 1 & \text{mixed} \quad &\text{phase,} \\ \mathcal{O} &= 1 & \text{molecular} \quad &\text{phase.} \end{aligned}$$

The order parameter relates to the momentum of the classical system through

$$\mathcal{O} \mapsto \frac{1}{2}(1 - p_\phi).$$

It is not associated with symmetry breaking.

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Classical fixed points

The dynamical evolution is governed by Hamilton's equations:

$$\frac{dp_\phi}{dt} = \frac{\partial H}{\partial \phi} = -\frac{4}{N}\sqrt{2(1-p_\phi)(p_\phi+c_+)(p_\phi+c_-)}\sin\left(\frac{4\phi}{N}\right),$$

$$-\frac{d\phi}{dt} = \frac{\partial H}{\partial p_\phi} = 2\lambda p_\phi + 2\alpha - 2\lambda + \frac{(1-p_\phi)(2p_\phi+2)-(p_\phi+c_+)(p_\phi+c_-)}{\sqrt{2(1-p_\phi)(p_\phi+c_+)(p_\phi+c_-)}}\cos\left(\frac{4\phi}{N}\right).$$

The fixed points of the system are determined by the condition

$$\frac{\partial H}{\partial \phi} = \frac{\partial H}{\partial p_\phi} = 0.$$

Phase boundaries of the parameter space are identified according to fixed point bifurcations.

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Bifurcation diagram: $k \neq 0$

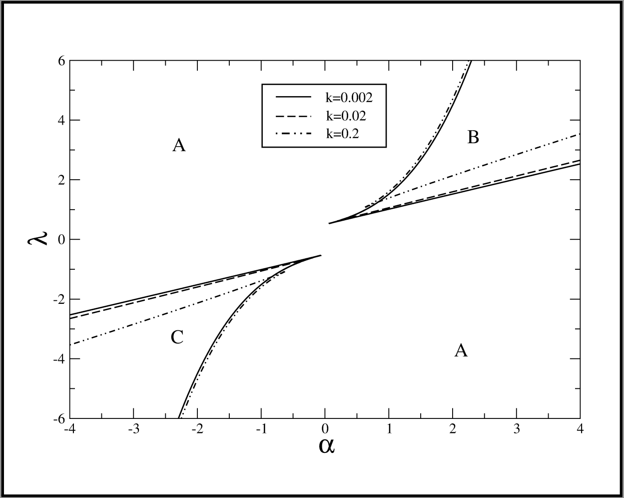

Figure : Regions A, B, C determined by bifurcation analysis.

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Bifurcation diagram: $k = 0$

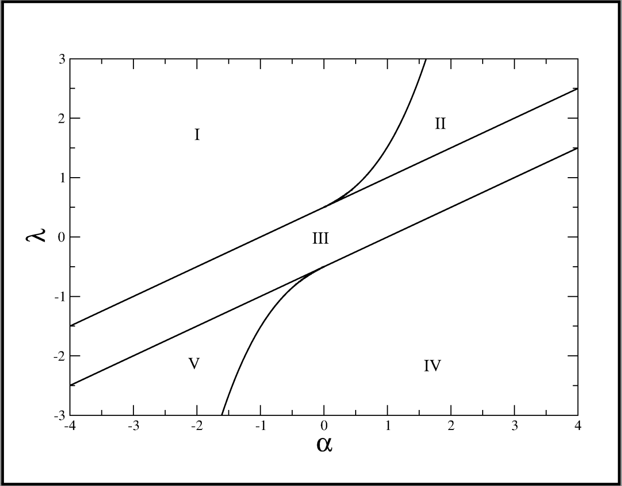

Figure : Regions I, II, III, IV, V determined by bifurcation analysis.

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Molecular fraction: $\lambda = \mu_a = \mu_b = 0$ - numerical

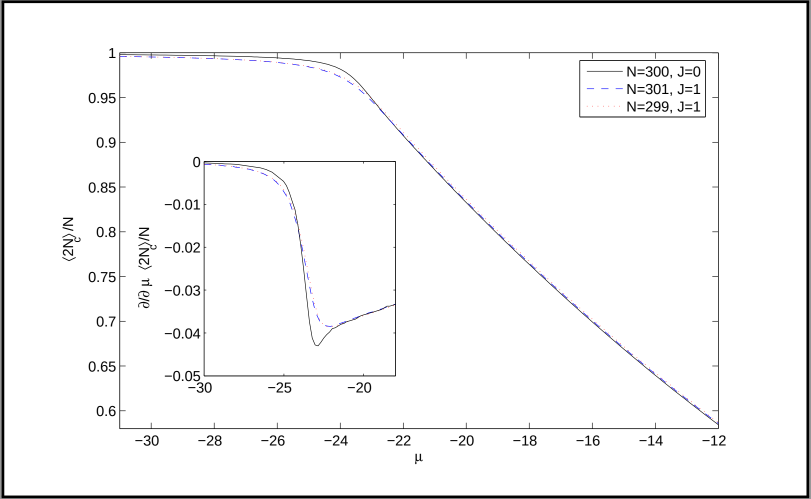

Figure : Order parameter. Inset shows the first derivative.

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Bethe ansatz solution

$$E = AM(M-1) + BM + C - \Omega \sum_{j=1}^{M} v_j,$$

where for $J \geq 0$

$$\frac{\Omega(J+1-v_j^2) + Bv_j}{v_j(\Omega + Av_j)} = \sum_{k \neq j}^{M} \frac{2}{v_k - v_j}, \qquad j = 1, 2, ..., M,$$

$M = (N-J)/2$, $L = (N+J)/2$, and

$$A = U_{aa} + U_{bb} + U_{cc} + U_{ab} - U_{ac} - U_{bc},$$

$$B = (1+2L-2M)U_{aa} + U_{bb} + (1-2M)U_{cc} + (1+L-M)U_{ab} + (2M-L-1)U_{ac} + (M-1)U_{bc} + \mu_a + \mu_b - \mu_c,$$

$$C = (L-M)^2 U_{aa} + M(L-M)U_{ac} + M^2 U_{cc} + (L-M)\mu_a + M\mu_c.$$

Rubeni, Foerster, Mattei, Roditi, Nucl. Phys. B 856 (2012) 698 - 715

Ground-state roots: $\lambda = \mu_a = \mu_b = 0$

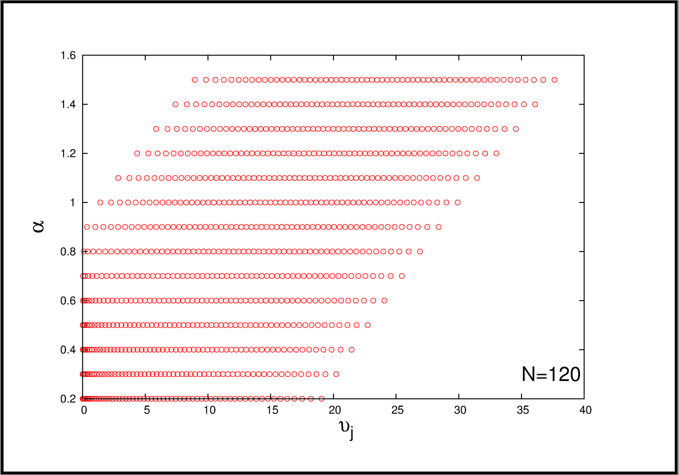

Figure : Ground-state root distribution for $\lambda = 0$, $N = 120$.

Large-N limit

Ground-state root density:

$$\rho(v) = \sqrt{(\mathfrak{b} - v)(v - \mathfrak{a})} \left(\frac{1}{2\pi M} + \frac{J+1}{2\pi M \sqrt{\mathfrak{a}\mathfrak{b}} v} \right)$$

$$1 = \int_{\mathfrak{a}}^{\mathfrak{b}} dv \, \rho(v)$$

Ground-state energy:

$$E_0 = \quad = \mu \left(\frac{N+1}{2} + \frac{(J+1)^2}{2\mathfrak{a}\mathfrak{b}} \right) - \frac{(J+1)\mu}{2\alpha\sqrt{2N}\sqrt{\mathfrak{a}\mathfrak{b}}} \left(\mathfrak{a}\mathfrak{b} - \frac{(J+1)^2}{\mathfrak{a}\mathfrak{b}} \right)$$

Bethe ansatz equation:

$$\frac{J+1}{v} - v - \frac{\mu_c}{\Omega} = 2M \lim_{\varepsilon \to 0} \int_{\mathfrak{a}}^{v-\varepsilon} dw \, \frac{\rho(w)}{w - v} + 2M \lim_{\varepsilon \to 0} \int_{v+\varepsilon}^{\mathfrak{b}} dw \, \frac{\rho(w)}{w - v}$$

Links and Marquette, work in preparation

leads to

$$(\mathfrak{ab})^2 + 2(1-\alpha^2)N\mathfrak{ab} - 4(J+1)\alpha\sqrt{2N}\sqrt{\mathfrak{ab}} - 3(J+1)^2 = 0.$$

For $J = O(N^0)$

$$\alpha > 1 \quad \Rightarrow \quad \mathfrak{ab} \sim 2(\alpha^2 - 1)N,$$

$$\alpha = 1 \quad \Rightarrow \quad \mathfrak{ab} \sim 2^{5/3}(J+1)^{2/3}N^{1/3},$$

$$\alpha < 1 \quad \Rightarrow \quad \mathfrak{ab} \sim (J+1)^2 \left(\frac{2\sqrt{2}\alpha + \sqrt{2\alpha^2+6}}{2(1-\alpha^2)}\right)^2 N^{-1}.$$

This yields

$$\alpha \geq 1 \quad \Rightarrow \quad \mathcal{O} = 1,$$

$$\alpha \leq 1 \quad \Rightarrow \quad \mathcal{O} = 1 + f^2 + \alpha\left(2f + \frac{3}{\sqrt{2}\alpha}f^2\right)\frac{df}{d\alpha}$$

where

$$f = \frac{2(1-\alpha^2)}{2\sqrt{2}\alpha + \sqrt{2\alpha^2+6}}.$$

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Molecular fraction: $\lambda = \mu_a = \mu_b = 0$ - numerical

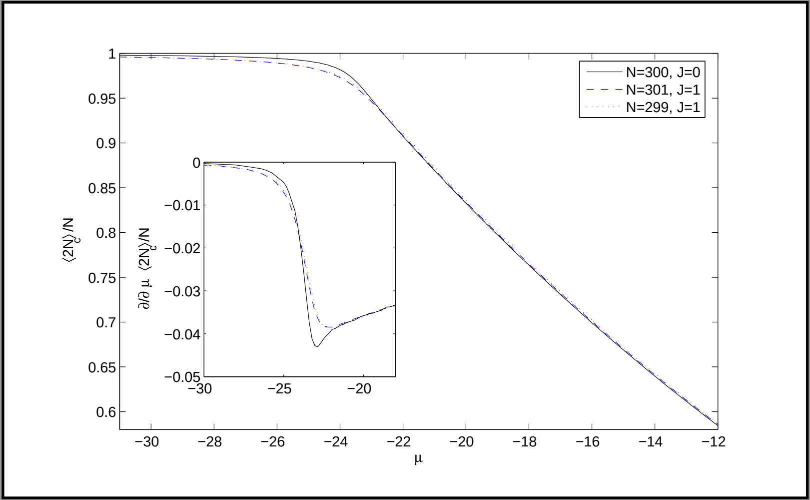

Figure : Order parameter. Inset shows the first derivative.

Links and Marquette, work in preparation

Molecular fraction: $\lambda = \mu_a = \mu_b = 0$ - analytic curve for all finite J in the $N \to \infty$ limit

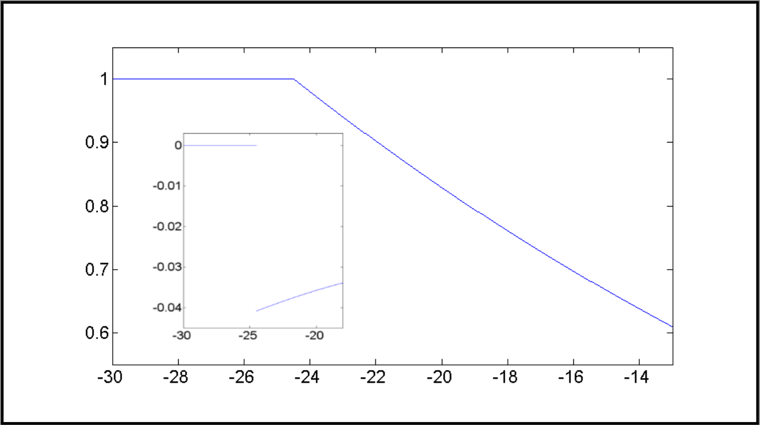

Figure : Order parameter. Inset shows the first derivative.

Future work

Extend the analysis to cover the entire parameter space.