Andrea Richaud

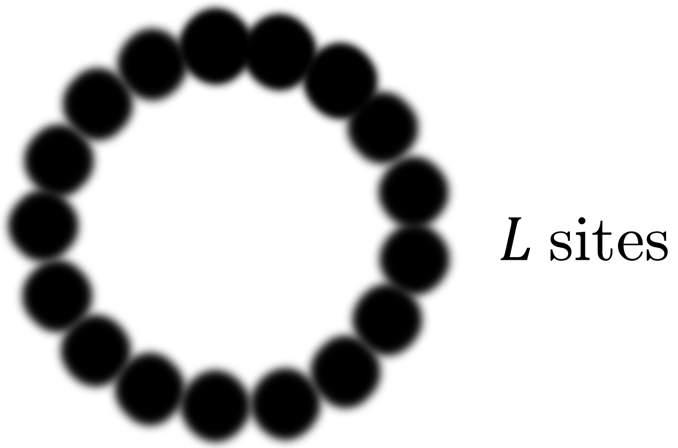
Formation of supermixed states in ultracold boson mixtures loaded in ring lattices

Benasque, May 15th, 2019

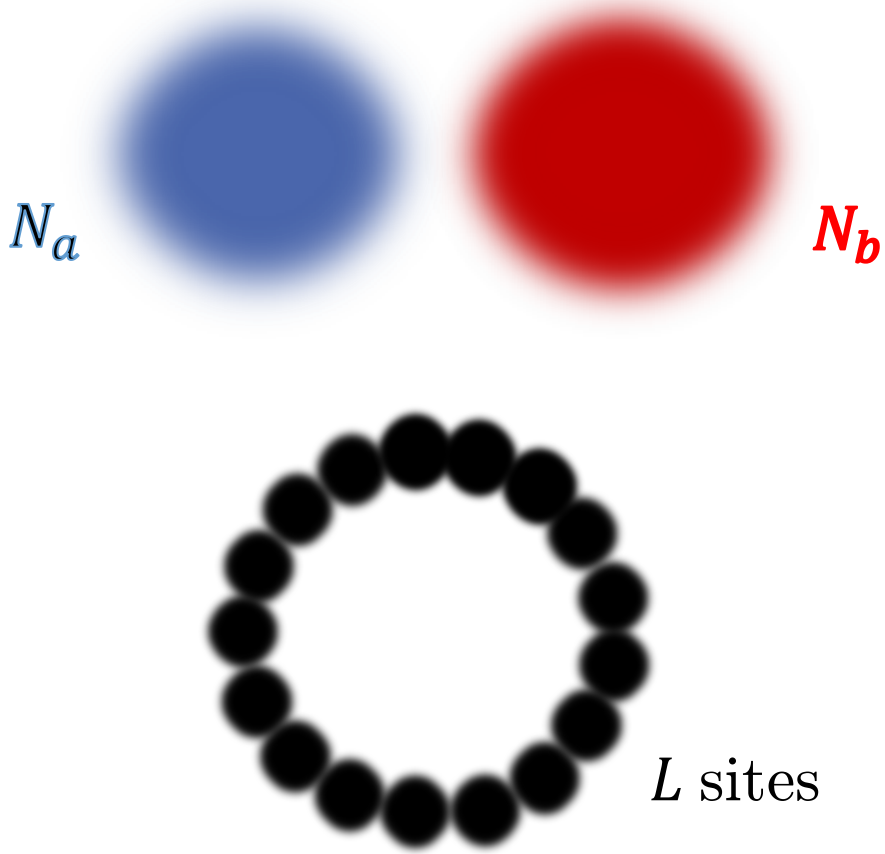
Ingredients

Bose-Bose mixture

Ring optical lattice



Target



Finding the **ground state** according to the strength of the **inter-species attraction**.

The model

$$H = -T_a \sum_{j=1}^{L} \left(a_{j+1}^\dagger a_j + a_j^\dagger a_{j+1}\right) + \frac{\boxed{U_a}}{2} \sum_{j=1}^{L} n_j(n_j - 1) \longrightarrow \text{Repulsive}$$

$$-T_b \sum_{j=1}^{L} \left(b_{j+1}^\dagger b_j + b_j^\dagger b_{j+1}\right) + \frac{\boxed{U_b}}{2} \sum_{j=1}^{L} m_j(m_j - 1) \longrightarrow \text{Repulsive}$$

$$\boxed{+W} \sum_{j=1}^{L} n_j m_j, \longrightarrow \text{Attractive}$$

Conserved quantities: $N_a = \sum_i^L n_i$ $\quad N_b = \sum_i^L m_i$

The Continuous Variable Picture

Ground state of Hamiltonian H → **Minimum** of effective potential $\mathcal{V}$

$$\mathcal{V} = -2N_aT_a\sum_{j=1}^{L}\sqrt{x_jx_{j+1}} - 2N_bT_b\sum_{j=1}^{L}\sqrt{y_jy_{j+1}}$$

$$+\frac{U_aN_a^2}{2}\sum_{j=1}^{L}x_j(x_j-\epsilon_a) + \frac{U_bN_b^2}{2}\sum_{j=1}^{L}y_j(y_j-\epsilon_b)$$

$$+WN_aN_b\sum_{j=1}^{L}x_jy_j$$

Where $x_i, y_i \in [0,1]$ are normalized boson populations.

$$x_i = \frac{n_i}{N_a}; \quad y_i = \frac{m_i}{N_b}$$

A technique already successfully used in e.g.:

- F. Lingua and V. Penna, PRE 95, 062142 (2017);
- R. W. Spekkens and J. E. Sipe, PRA 59, 3868 (1999);

The Continuous Variable Picture

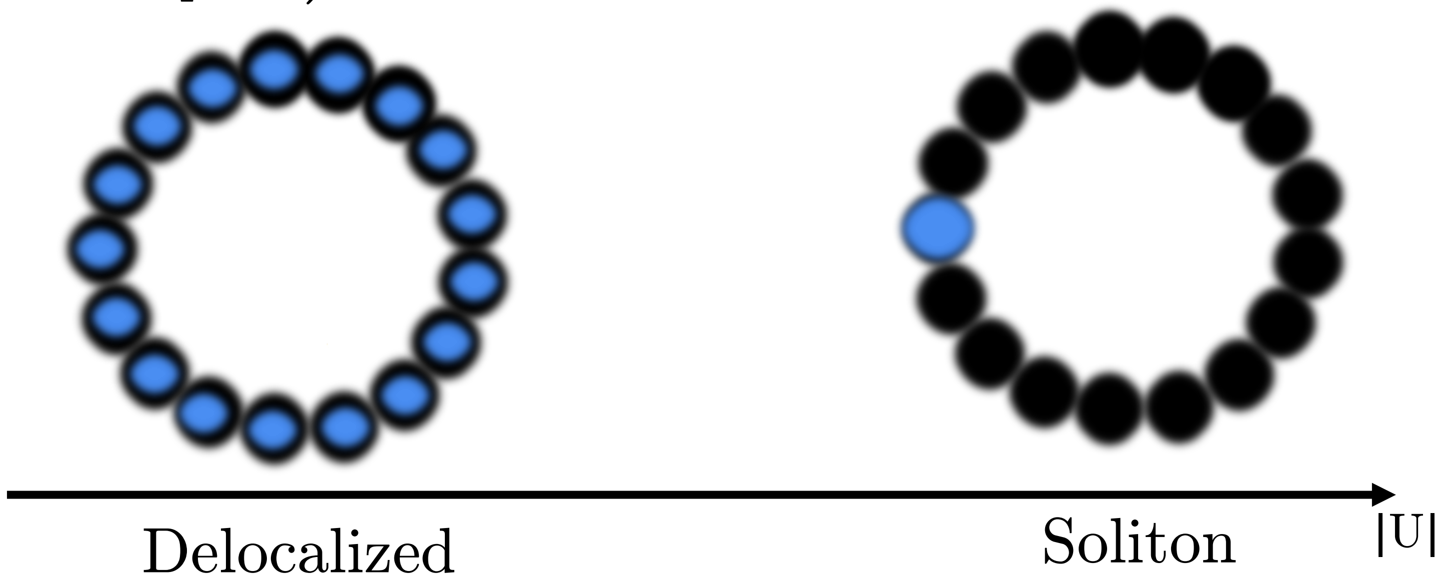
Ground state of Hamiltonian H → **Minimum** of effective potential $\mathcal{V}$

$$\mathcal{V} = -2N_a T_a \sum_{j=1}^{L} \sqrt{x_j x_{j+1}}$$

$$+\frac{\boxed{U_a} N_a^2}{2} \sum_{j=1}^{L} x_j (x_j - \epsilon_a)$$

Attractive

Technique used in N. Oelkers and J. Links, PRB 75, 115119 (2007) to find the ground state properties of the **attractive one-dimensional Bose-Hubbard model (single species)**.



Semiclassical limit

$$\mathcal{V} = \cancel{-2N_aT_a\sum_{j=1}^{L}\sqrt{x_jx_{j+1}}} - \cancel{2N_bT_b\sum_{j=1}^{L}\sqrt{y_jy_{j+1}}}$$

$$+\frac{U_aN_a^2}{2}\sum_{j=1}^{L}x_j(x_j-\epsilon_a)+\frac{U_bN_b^2}{2}\sum_{j=1}^{L}y_j(y_j-\epsilon_b)$$

$$+WN_aN_b\sum_{j=1}^{L}x_jy_j$$

Where $x_i, y_i \in [0,1]$ are normalized boson populations.

$$x_i = \frac{n_i}{N_a}; \quad y_i = \frac{m_i}{N_b}$$

If the boson populations are **large enough**, for **fixed** L, one can focus on leading terms.

This is a possible way of performing the **thermodynamic limt**, according to the schemes described in:

- N. Oelkers and J. Links, PRB 75, 115119 (2007);
- P. Buonsante, V. Penna, and A. Vezzani, PRA 84, 061601 (2011).

Semiclassical limit

$$\mathcal{V} = \cancel{-2N_aT_a\sum_{j=1}^{L}\sqrt{x_jx_{j+1}}} \cancel{-2N_bT_b\sum_{j=1}^{L}\sqrt{y_jy_{j+1}}}$$

$$+\frac{U_aN_a^2}{2}\sum_{j=1}^{L}x_j(x_j-\epsilon_a)+\frac{U_bN_b^2}{2}\sum_{j=1}^{L}y_j(y_j-\epsilon_b)$$

$$+WN_aN_b\sum_{j=1}^{L}x_jy_j$$

$$V \approx \frac{\mathcal{V}}{U_aN_a^2} = \frac{1}{2}\sum_{j=1}^{L}x_j^2+\frac{\beta^2}{2}\sum_{j=1}^{L}y_j^2+\alpha\beta\sum_{j=1}^{L}x_jy_j$$

$$\boxed{\alpha = \frac{W}{\sqrt{U_aU_b}}, \qquad \beta = \frac{N_b}{N_a}\sqrt{\frac{U_b}{U_a}}}$$

Where $x_i, y_i \in [0,1]$ are normalized boson populations.

$$x_i = \frac{n_i}{N_a}; \quad y_i = \frac{m_i}{N_b}$$

Effective model

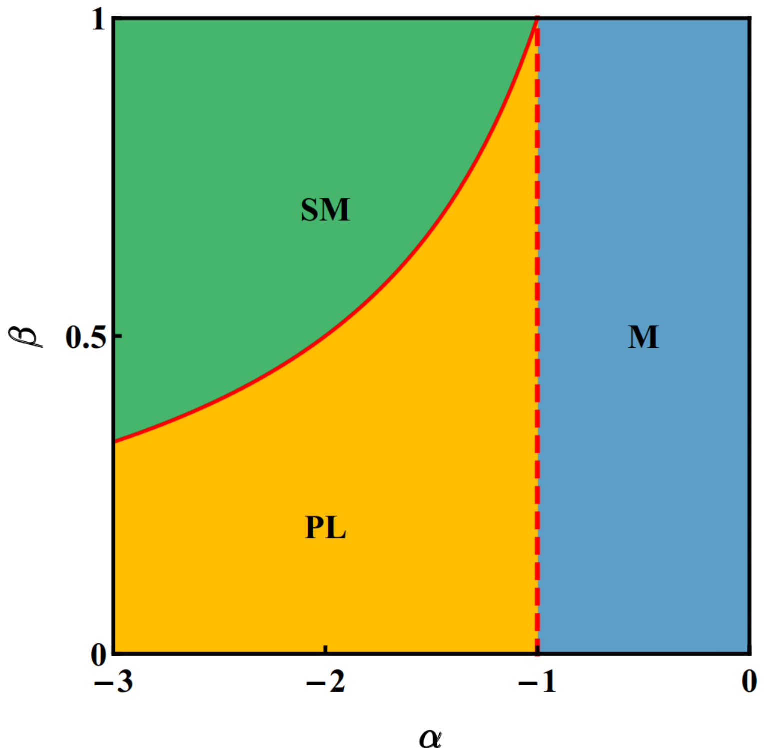
$$V \approx \frac{\mathcal{V}}{U_a N_a^2} = \frac{1}{2}\sum_{j=1}^{L} x_j^2 + \frac{\beta^2}{2}\sum_{j=1}^{L} y_j^2 + \alpha\beta\sum_{j=1}^{L} x_j y_j$$

$$\boxed{\alpha = \frac{W}{\sqrt{U_a U_b}}, \qquad \beta = \frac{N_b}{N_a}\sqrt{\frac{U_b}{U_a}}}$$

$$\frac{\textbf{Inter}\text{species attraction}}{\textbf{Intra}\text{species repulsions}}$$

Degree of asimmetry between the 2 atomic species

Phase diagram



$$\alpha = \frac{W}{\sqrt{U_a U_b}}, \qquad \beta = \frac{N_b}{N_a}\sqrt{\frac{U_b}{U_a}}$$

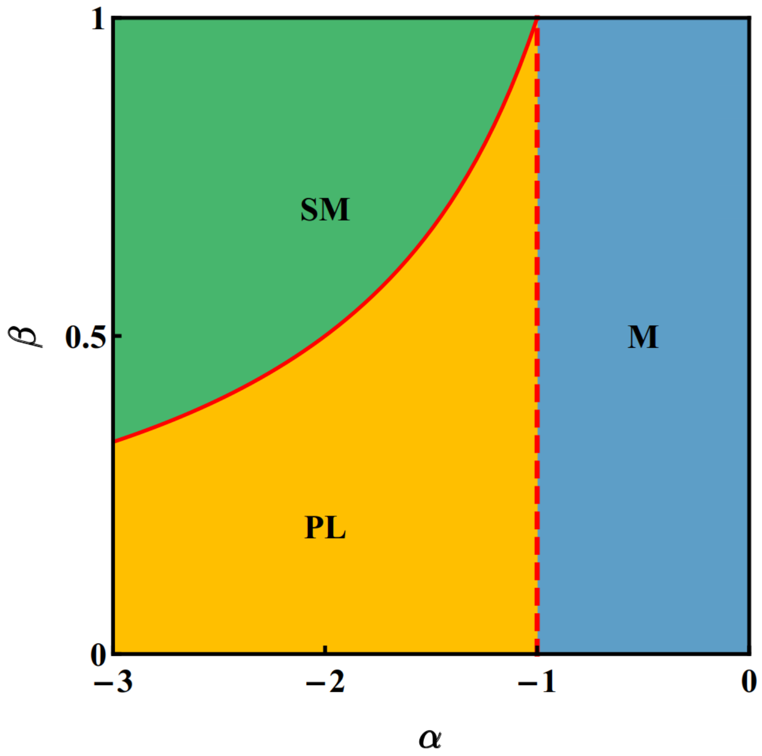
$$V \approx \frac{\mathcal{V}}{U_a N_a^2} = \frac{1}{2}\sum_{j=1}^{L} x_j^2 + \frac{\beta^2}{2}\sum_{j=1}^{L} y_j^2 + \alpha\beta\sum_{j=1}^{L} x_j y_j$$

Search for the constrained minimum of V in the parameters' space (α, β)

$$\Downarrow$$

Same phase diagram, no matter the specific value of L (sites)

Phase diagram



$$\alpha = \frac{W}{\sqrt{U_a U_b}}, \qquad \beta = \frac{N_b}{N_a}\sqrt{\frac{U_b}{U_a}}$$

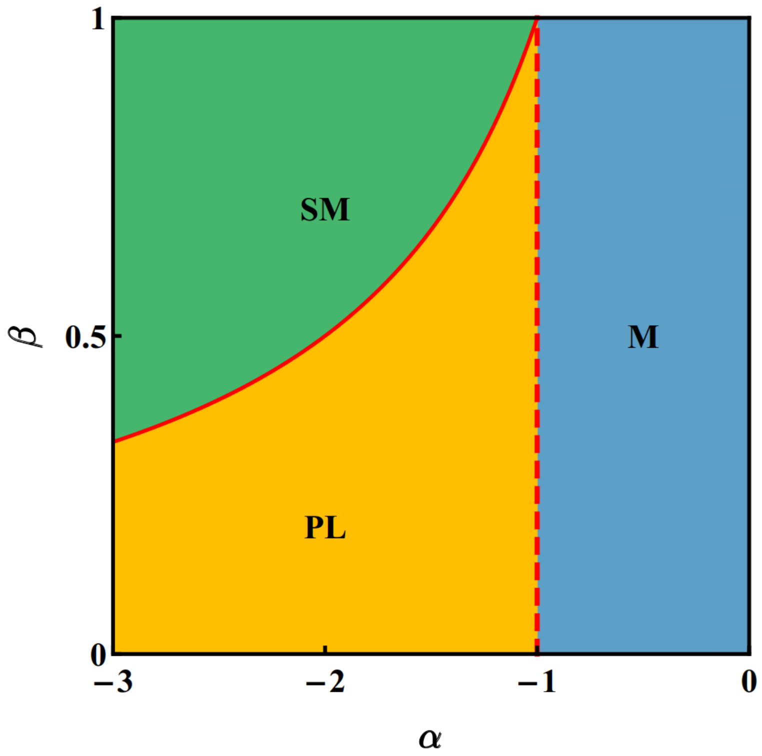
Search for the **constrained minimum of V** in the parameters' space (α, β):

$$V_* := V(\vec{x}_*, \vec{y}_*) := \min_{(\vec{x},\vec{y})\in\mathcal{R}} V(\vec{x}, \vec{y})$$

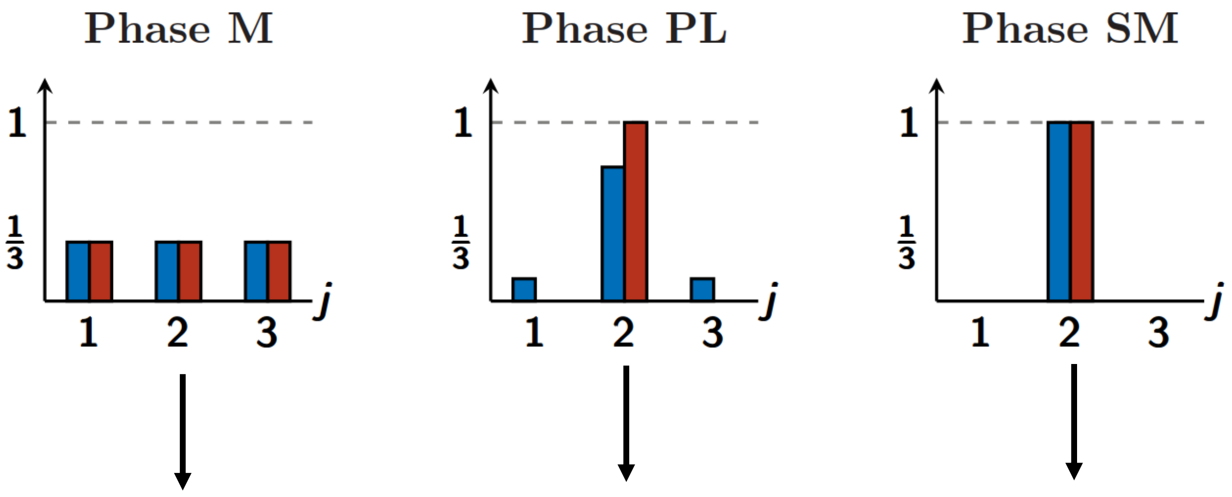
From a mathematical standpoint, it is not an easy task, as V_* may fall on the **boundary** of its domain $\mathcal{R}$.

Exhaustive **exploration of the polytope-like domain** $\mathcal{R}$, [→ V. Penna and A. Richaud, Sci Rep 8, 10242 (2018)]

Example: L=3



$$\alpha = \frac{W}{\sqrt{U_a U_b}}, \qquad \beta = \frac{N_b}{N_a}\sqrt{\frac{U_b}{U_a}}$$

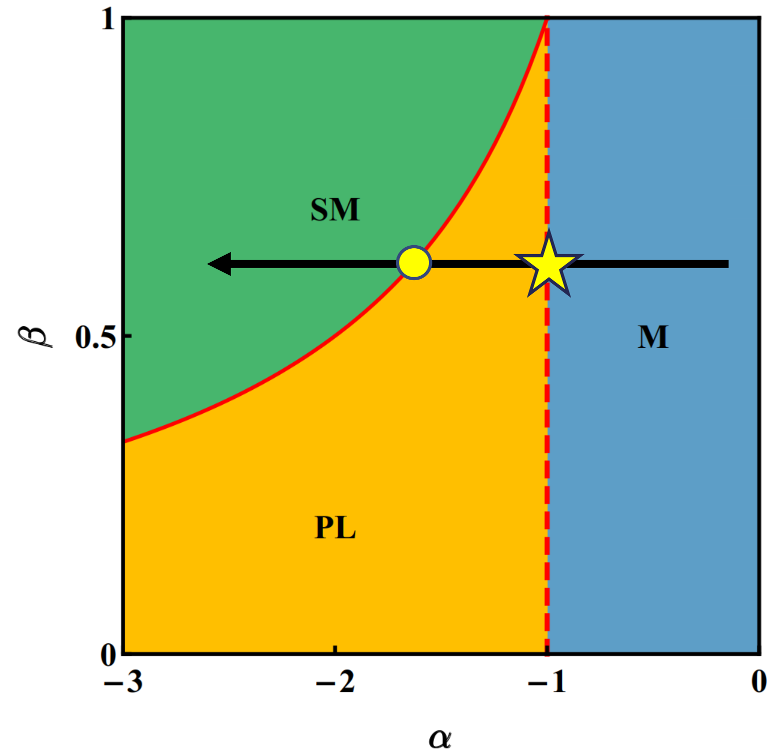


M=Mixed

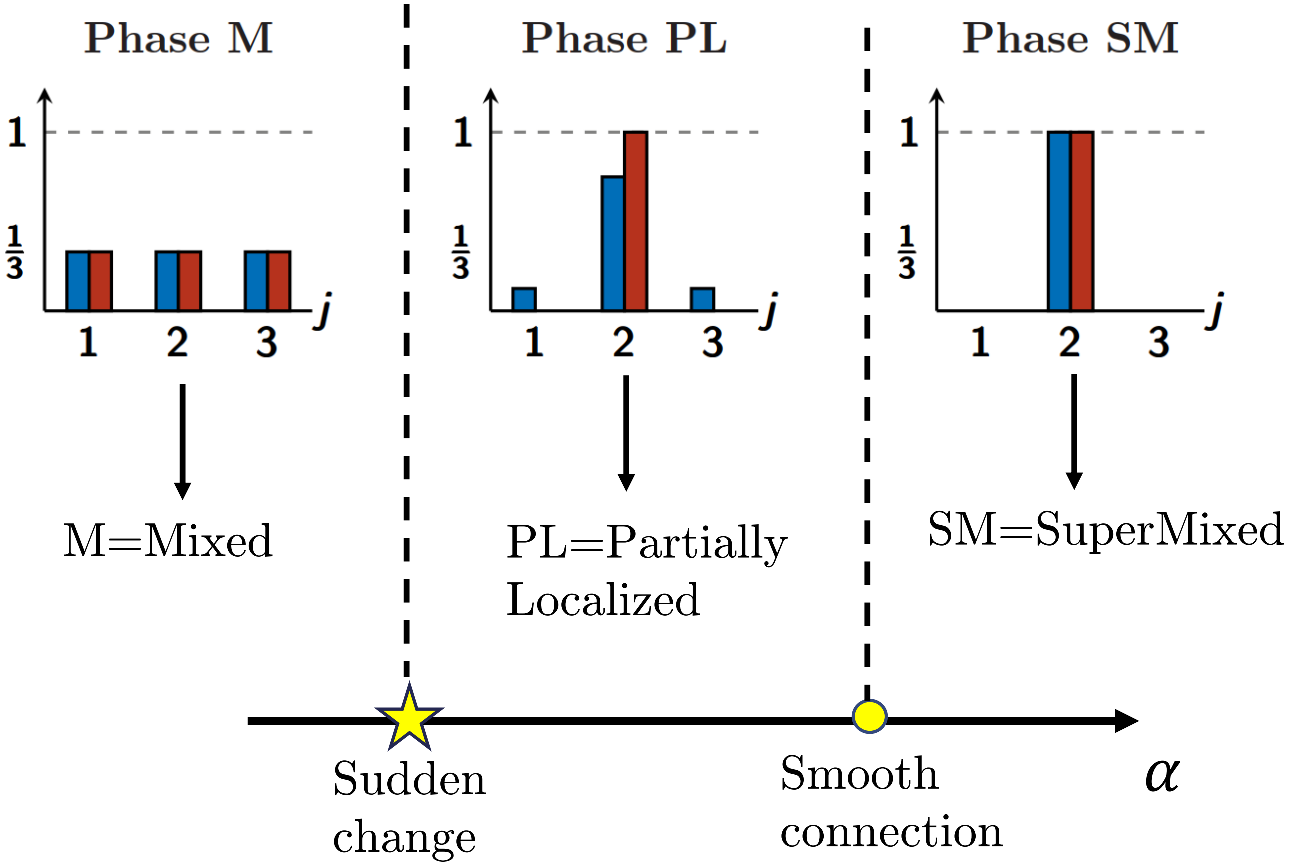
PL=Partially Localized

SM=SuperMixed

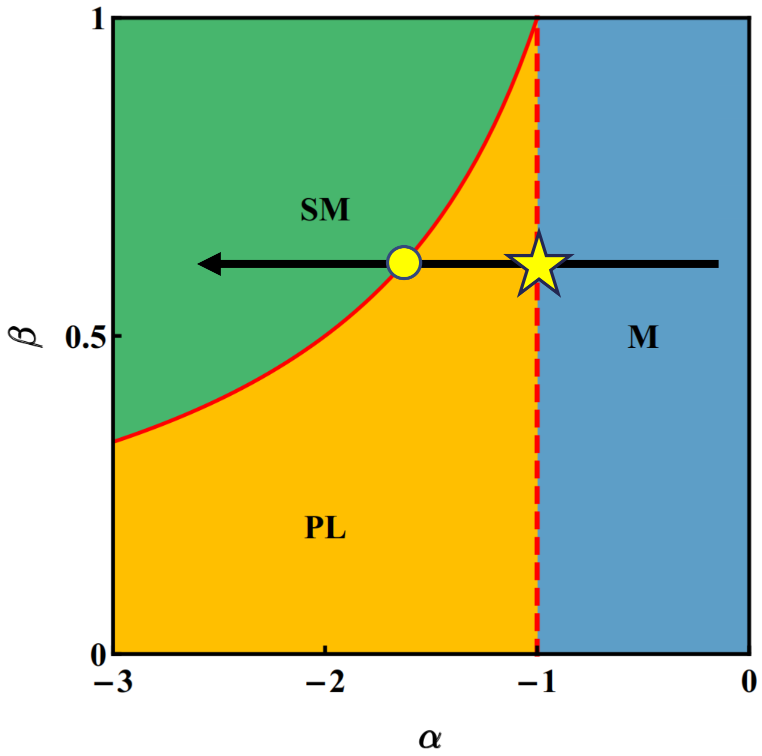
Two different kinds of transitions



$$\alpha = \frac{W}{\sqrt{U_a U_b}}, \qquad \beta = \frac{N_b}{N_a}\sqrt{\frac{U_b}{U_a}}$$



Two different kinds of non-analiticities of V_*



$$\alpha = \frac{W}{\sqrt{U_a U_b}}, \qquad \beta = \frac{M}{N}\sqrt{\frac{U_b}{U_a}}$$

$$V \approx \frac{\mathcal{V}}{U_a N_a^2} = \frac{1}{2}\sum_{j=1}^{L} x_j^2 + \frac{\beta^2}{2}\sum_{j=1}^{L} y_j^2 + \alpha\beta\sum_{j=1}^{L} x_j y_j$$

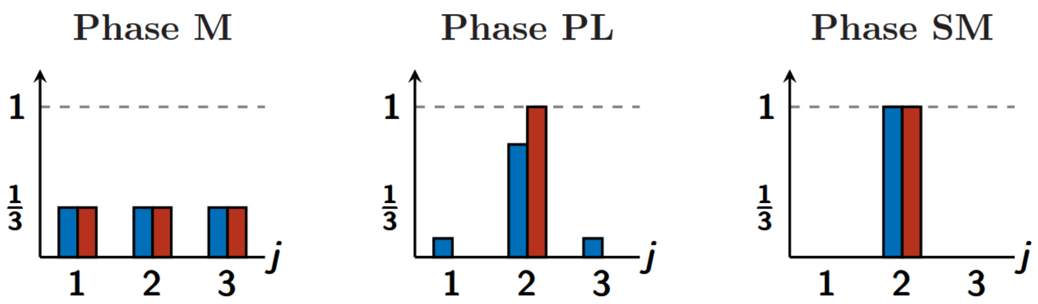
$$\boxed{V_*} := V(\vec{x}_*, \vec{y}_*) := \min_{(\vec{x},\vec{y})\in\mathcal{R}} V(\vec{x},\vec{y})$$

Continuous everywhere
on the (α, β) plane

$\frac{\partial V_*}{\partial \alpha}$
discontinuous

$\frac{\partial^2 V_*}{\partial \alpha^2}$
discontinuous

How to characterize the 3 phases?



$$S_{mix} = -\frac{1}{2}\sum_{j=1}^{L}\left(x_j \log\frac{x_j}{x_j+y_j} + y_j \log\frac{y_j}{x_j+y_j}\right)$$

→ Entropy of mixing → Degree of mixing

$$S_{loc} = -\sum_{j=1}^{L}\frac{x_j+y_j}{2}\log\frac{x_j+y_j}{2}.$$

→ Entropy of location → Degree of localization

Where $x_i, y_i \in [0,1]$ are normalized boson populations.

$$x_i = \frac{n_i}{N_a}; \quad y_i = \frac{m_i}{N_b}$$

Entropies to quantify the degrees of mixing and localization

$$S_{mix} = -\frac{1}{2}\sum_{j=1}^{L}\left(x_j \log\frac{x_j}{x_j+y_j} + y_j \log\frac{y_j}{x_j+y_j}\right)$$ → Entropy of mixing → Degree of mixing

$$S_{loc} = -\sum_{j=1}^{L}\frac{x_j+y_j}{2}\log\frac{x_j+y_j}{2}.$$ → Entropy of location → Degree of localization

Used to in Physical Chemistry to quantify the miscibility of classical fluids.

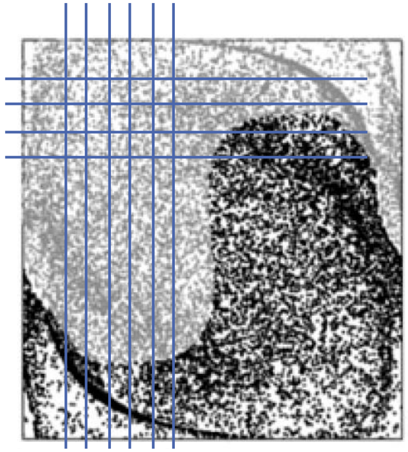


Image taken by M. Camesasca et al, *Quantifying Fluid Mixing with the Shannon Entropy*, Macromolecular theory and simulation 15, 8 (2006).

Where $x_i, y_i \in [0,1]$ are chemical species concentrations.

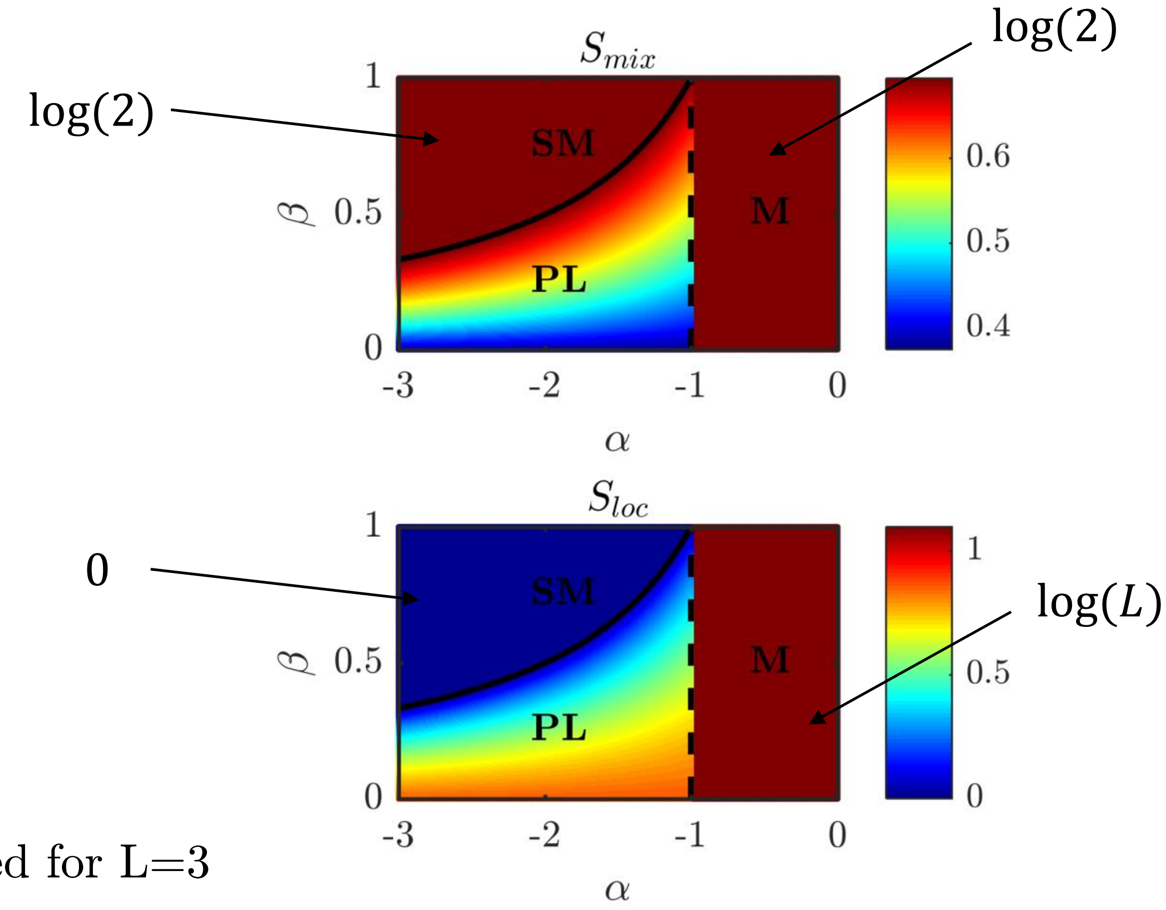
$$x_i = \frac{n_i}{N_a}; \quad y_i = \frac{m_i}{N_b}$$

Entropies to quantify the degrees of mixing and localization

$$S_{mix} = -\frac{1}{2}\sum_{j=1}^{L}\left(x_j \log\frac{x_j}{x_j+y_j} + y_j \log\frac{y_j}{x_j+y_j}\right)$$

$$S_{loc} = -\sum_{j=1}^{L}\frac{x_j+y_j}{2}\log\frac{x_j+y_j}{2}.$$

The combined use of these indicators allows one to recognize the phase.



Plots obtained for L=3

Finite-size effects

$$\mathcal{V} = -2N_aT_a\cancel{\sum_{j=1}^{L}\sqrt{x_jx_{j+1}}} - 2N_bT_b\cancel{\sum_{j=1}^{L}\sqrt{y_jy_{j+1}}}$$

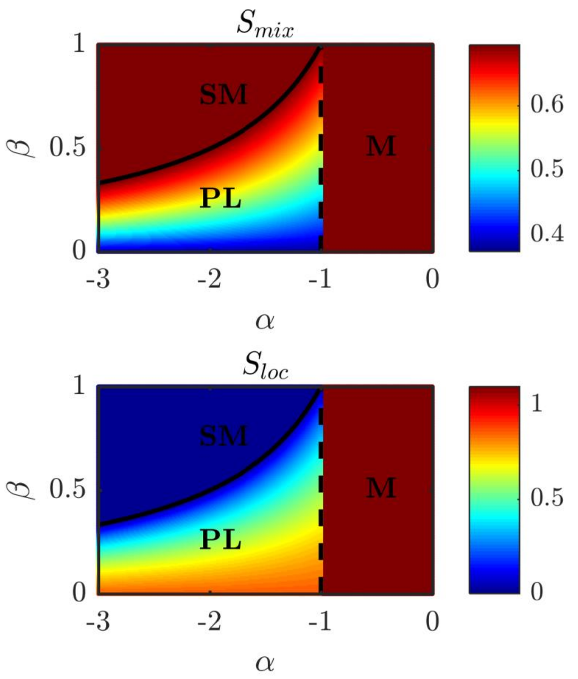
$$+\frac{U_aN_a^2}{2}\sum_{j=1}^{L}x_j(x_j-\epsilon_a)+\frac{U_bN_b^2}{2}\sum_{j=1}^{L}y_j(y_j-\epsilon_b)$$

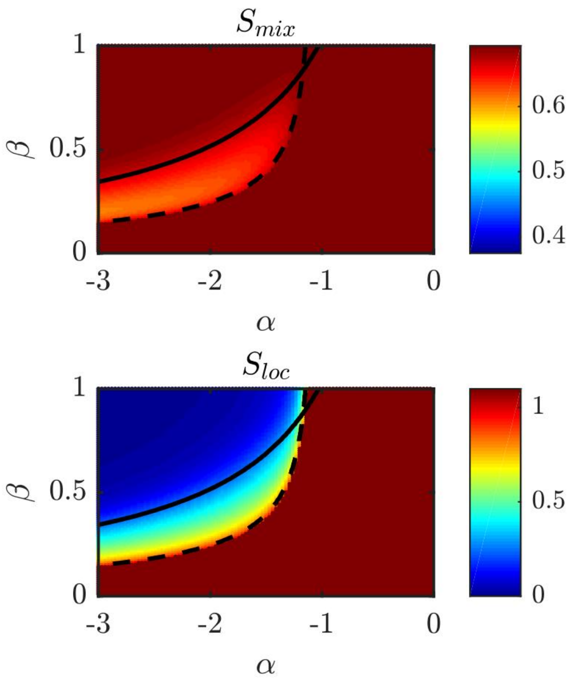
$$+WN_aN_b\sum_{j=1}^{L}x_jy_j$$

$$V \approx \frac{\mathcal{V}}{U_aN_a^2} = \frac{1}{2}\sum_{j=1}^{L}x_j^2 + \frac{\beta^2}{2}\sum_{j=1}^{L}y_j^2 + \alpha\beta\sum_{j=1}^{L}x_jy_j$$

Keeping L fixed, we reduce the boson populations N_a and N_b in such a way to take into account the tunnelling processes.

Finite-size effects

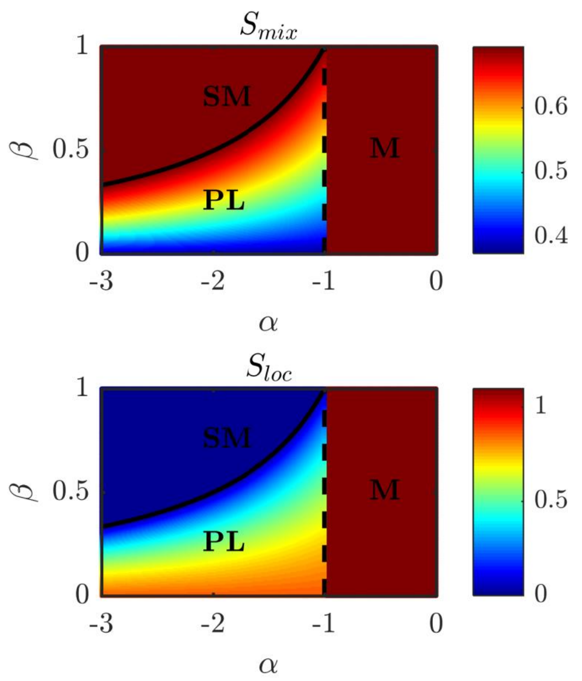


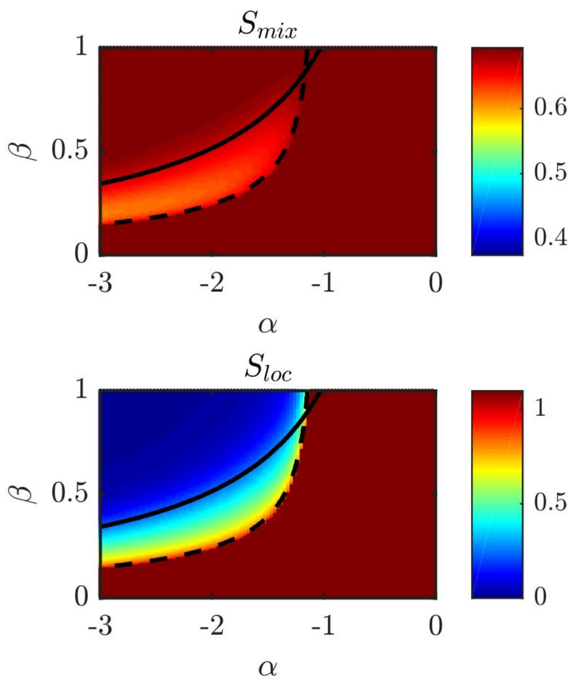


$\frac{T}{UN} \to 0$ (Thermodynamic limit)	$\frac{T}{UN} = 0.03$ (Finite size)

Plots obtained for L=3

Finite-size effects

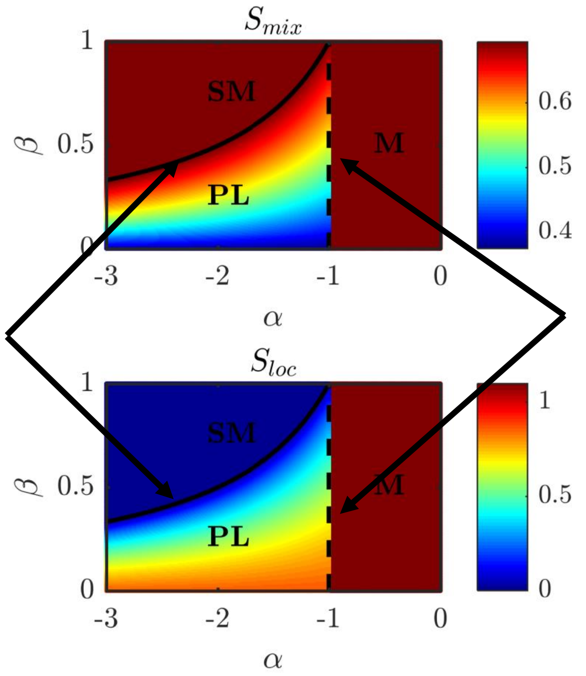




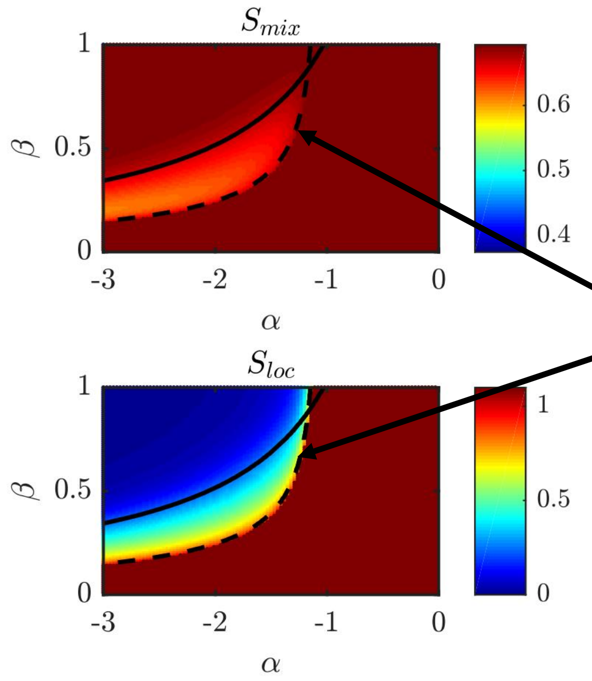
Walking away from the thermodynamic limit, the ideal phase diagram gets **smoothed** and **deformed**. But still, three qualitatively different regions can be recognized.

Finite-size effects

$\beta = -\frac{1}{\alpha}$



$\alpha = -1$



New borders given by the collapse of Bogolyubov frequencies (see later).

Agreement between CVP and BH

BH:

$$H = -T_a \sum_{j=1}^{L} \left(a_{j+1}^\dagger a_j + a_j^\dagger a_{j+1} \right) + \frac{U_a}{2} \sum_{j=1}^{L} n_j (n_j - 1)$$
$$-T_b \sum_{j=1}^{L} \left(b_{j+1}^\dagger b_j + b_j^\dagger b_{j+1} \right) + \frac{U_b}{2} \sum_{j=1}^{L} m_j (m_j - 1)$$
$$+W \sum_{j=1}^{L} n_j \, m_j,$$

CVP:

$$\mathcal{V} = -2N_a T_a \sum_{j=1}^{L} \sqrt{x_j x_{j+1}} - 2N_b T_b \sum_{j=1}^{L} \sqrt{y_j y_{j+1}}$$
$$+\frac{U_a N_a^2}{2} \sum_{j=1}^{L} x_j (x_j - \epsilon_a) + \frac{U_b N_b^2}{2} \sum_{j=1}^{L} y_j (y_j - \epsilon_b)$$
$$+W N_a N_b \sum_{j=1}^{L} x_j y_j$$

Quantum analysis: entropies

We import the concept of S_{mix} and S_{loc} into the quantum framework:

$$\tilde{S}_{mix} := \sum_{\vec{n},\vec{m}}^{Q} \boxed{|c(\vec{n},\vec{m})|^2} \boxed{S_{mix}(\vec{n},\vec{m}),}$$

$$\tilde{S}_{loc} := \sum_{\vec{n},\vec{m}}^{Q} \boxed{|c(\vec{n},\vec{m})|^2} \boxed{S_{loc}(\vec{n},\vec{m})}$$

$$\vec{x} = \frac{\vec{n}}{N_a}$$

$$\vec{y} = \frac{\vec{m}}{N_b}$$

$$\boxed{S_{mix} = -\frac{1}{2}\sum_{j=1}^{L}\left(x_j \log \frac{x_j}{x_j+y_j} + y_j \log \frac{y_j}{x_j+y_j}\right)}$$

$$\boxed{S_{loc} = -\sum_{j=1}^{L} \frac{x_j+y_j}{2} \log \frac{x_j+y_j}{2}.}$$

Entropy of mixing and Entropy of location of a single Fock state.

Coefficients coming from exact diagonalization of the BH Hamiltonian:

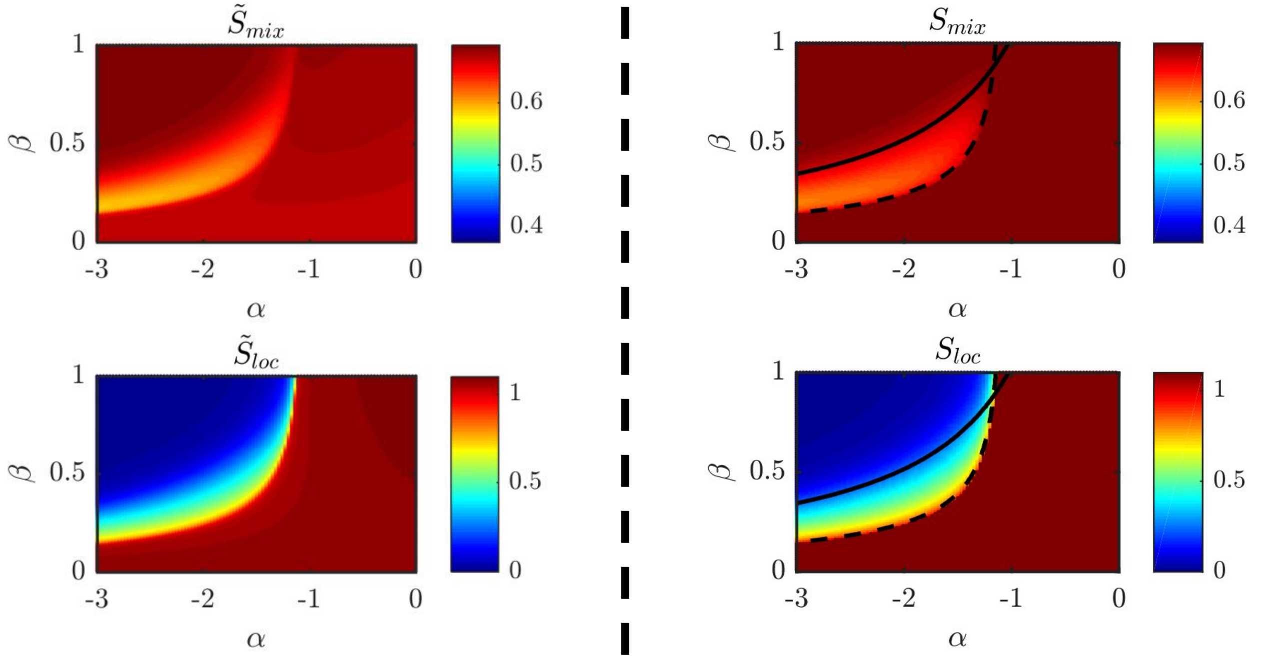
$$c(\vec{n},\vec{m}) = \langle \vec{n},\vec{m}|\psi_0\rangle$$

Quantum analysis: entropies

We import the concept of S_{mix} and S_{loc} into the quantum framework:

$$\tilde{S}_{mix} := \sum_{\vec{n},\vec{m}}^{Q} |c(\vec{n},\vec{m})|^2 S_{mix}(\vec{n},\vec{m}),$$

$$\tilde{S}_{loc} := \sum_{\vec{n},\vec{m}}^{Q} |c(\vec{n},\vec{m})|^2 S_{loc}(\vec{n},\vec{m})$$

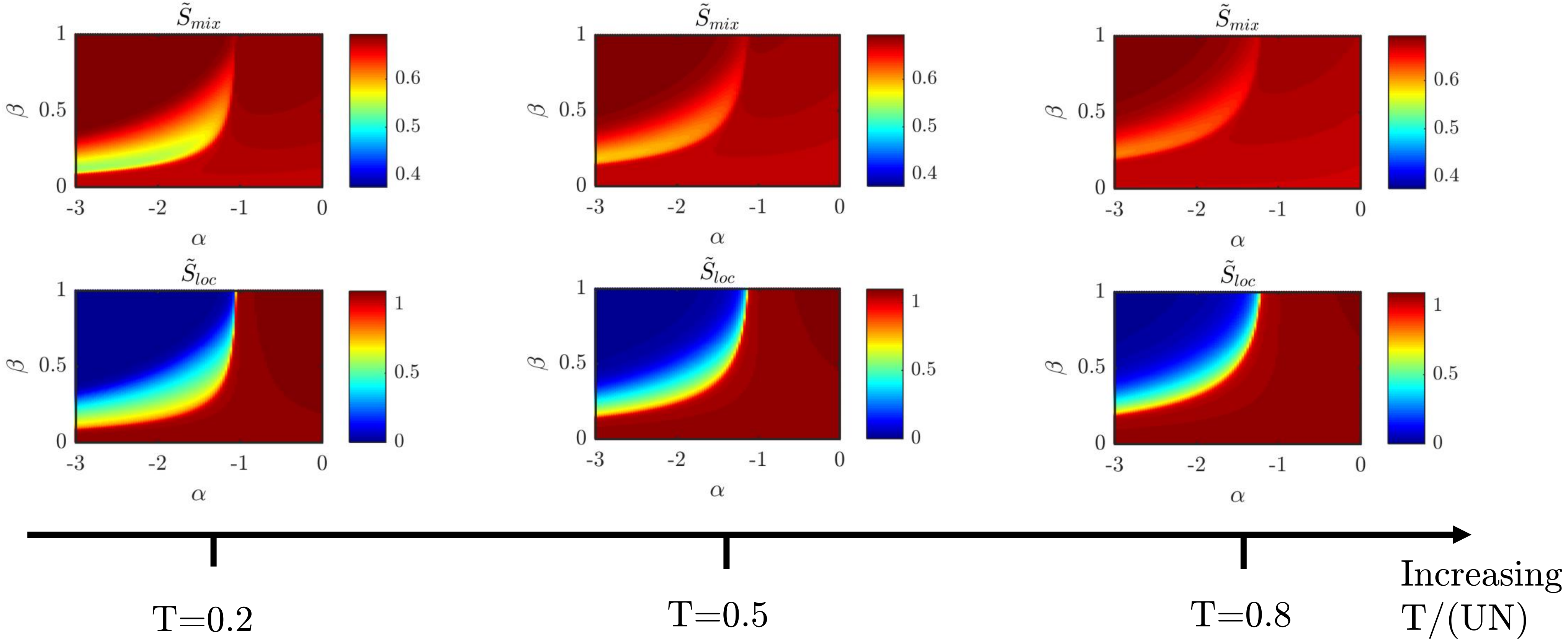


Fully Quantum

CVP

Quantum analysis: entropies

We import the concept of S_{mix} and S_{loc} into the quantum framework:

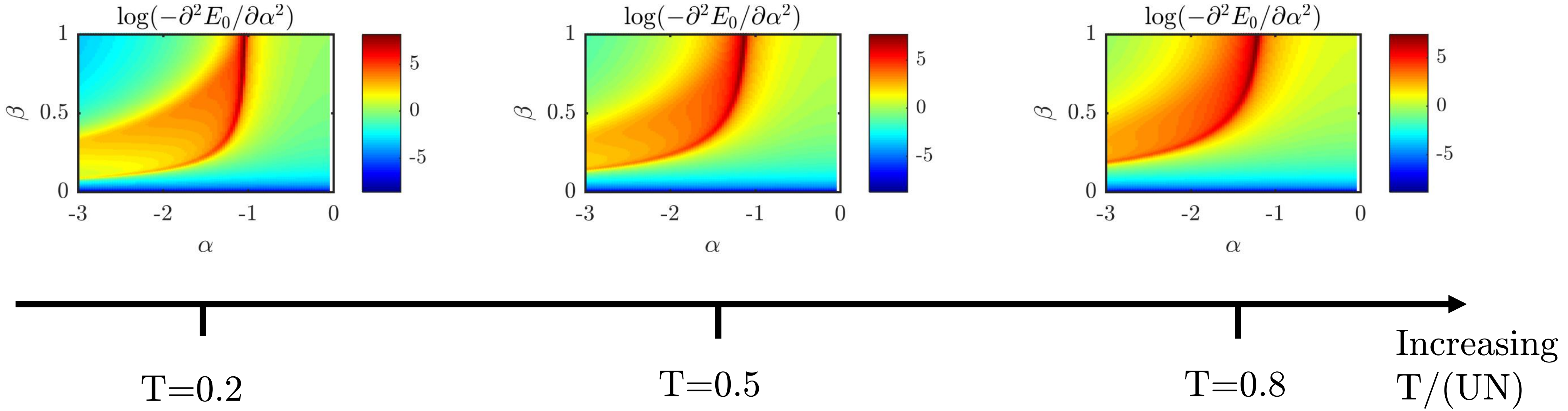


Quantum analysis: E_0

Based on the exact numerical diagonalization of the Bose-Hubbard Hamiltonian.

Second derivative of the ground state energy E_0 as a function of the control parameter α.

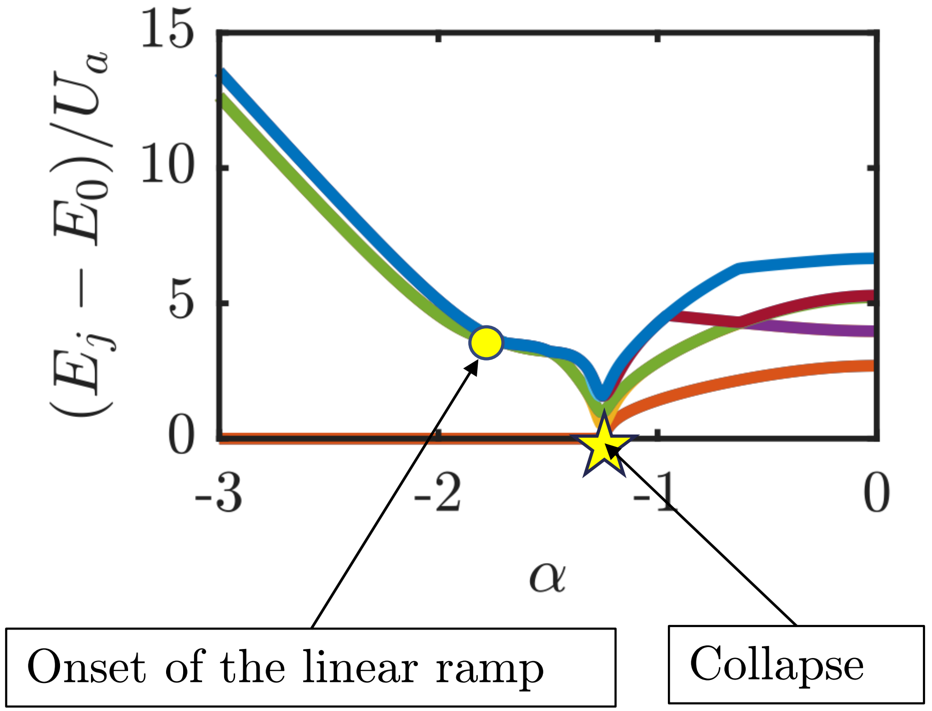
$$E_0 = \langle \psi_0 | H | \psi_0 \rangle$$

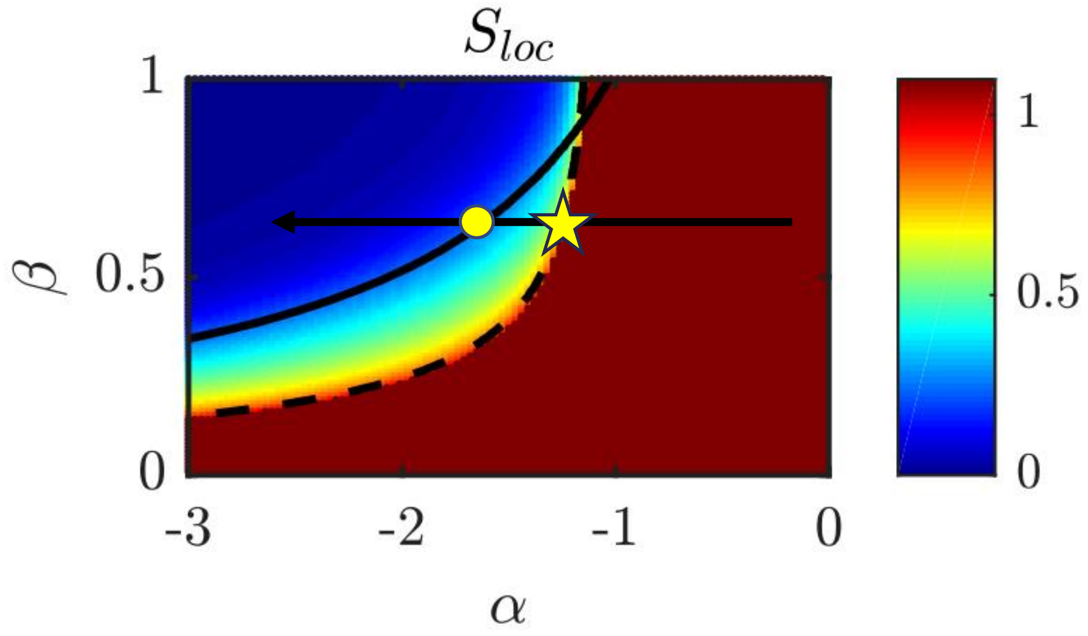


Quantum analysis: Energy levels

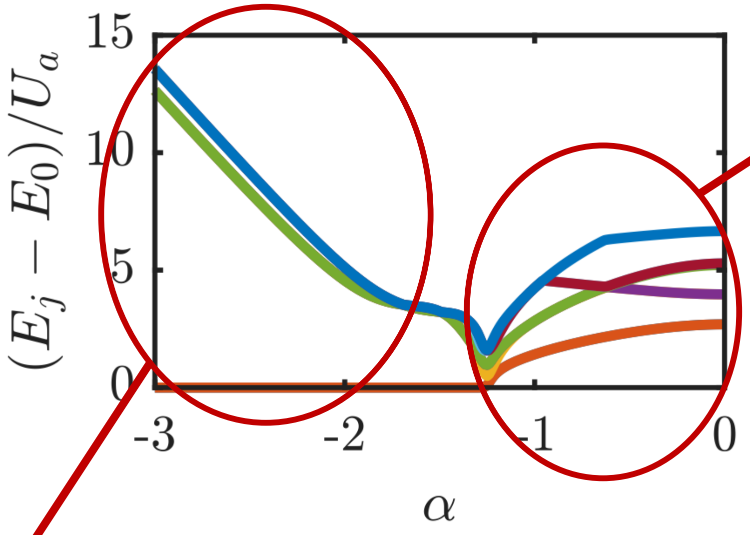
$$E_i = \langle \psi_i | H | \psi_i \rangle$$

Computed by means of exact numerical diagonalization





Quantum analysis: Energy levels



Functional dependence well captured by the **momentum-based** Bogolyubov approximation scheme:
V. Penna, A. Richaud
PRA 96 (5), 053631

$$\omega_k = \frac{1}{\hbar}\sqrt{2T(1-c_k)[2T(1-c_k)+2u+2w]},$$

$$\Omega_k = \frac{1}{\hbar}\sqrt{2T(1-c_k)[2T(1-c_k)+2u-2w]}.$$

Functional dependence well captured by the **sites-based** Bogolyubov approximation scheme:

$$H_D = n_2(T_a - U_a N_a - N_b W) + n_3(-T_a - U_a N_a - N_b W)$$

$$+m_2(T_b - U_b N_b - N_a W) + m_3(-T_b - U_b N_b - N_a W),$$

Quantum analysis: Energy levels

$$H_D = n_2(T_a - U_aN_a - N_bW) + n_3(-T_a - U_aN_a - N_bW)$$

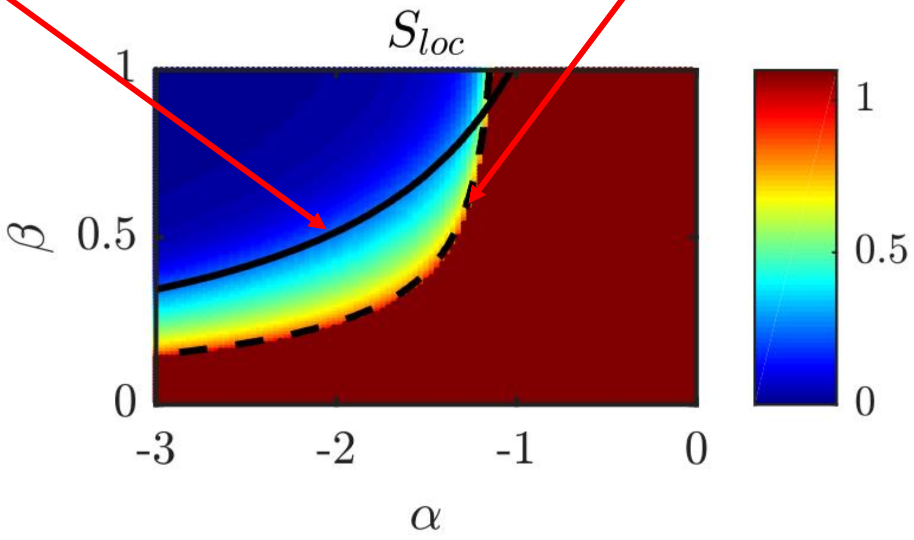
$$+m_2(T_b - U_bN_b - N_aW) + m_3(-T_b - U_bN_b - N_aW),$$

$$\omega_k = \frac{1}{\hbar}\sqrt{2T(1-c_k)[2T(1-c_k)+2u+2w]},$$

$$\Omega_k = \frac{1}{\hbar}\sqrt{2T(1-c_k)[2T(1-c_k)+2u-2w]}.$$

Collapse

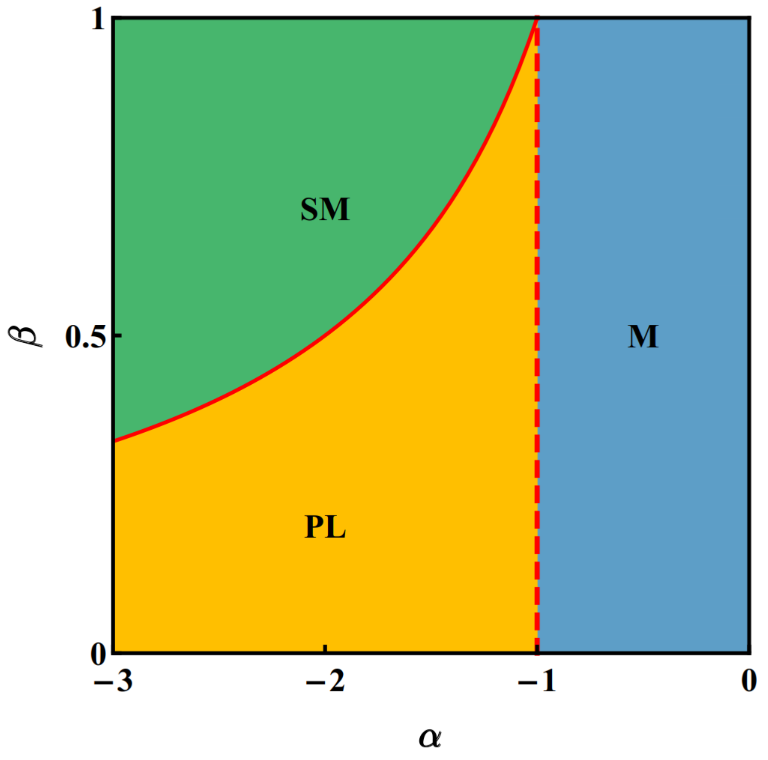
$$\omega_2 > 0, \quad \omega_3 > 0, \quad \Omega_2 > 0, \quad \Omega_3 > 0$$



$$\alpha > -\sqrt{\left[1 + C_L\frac{T_aL}{U_aN_a}\right]\left[1 + C_L\frac{T_bL}{U_bN_b}\right]}$$

where $C_L = 1 - \cos(2\pi/L)$

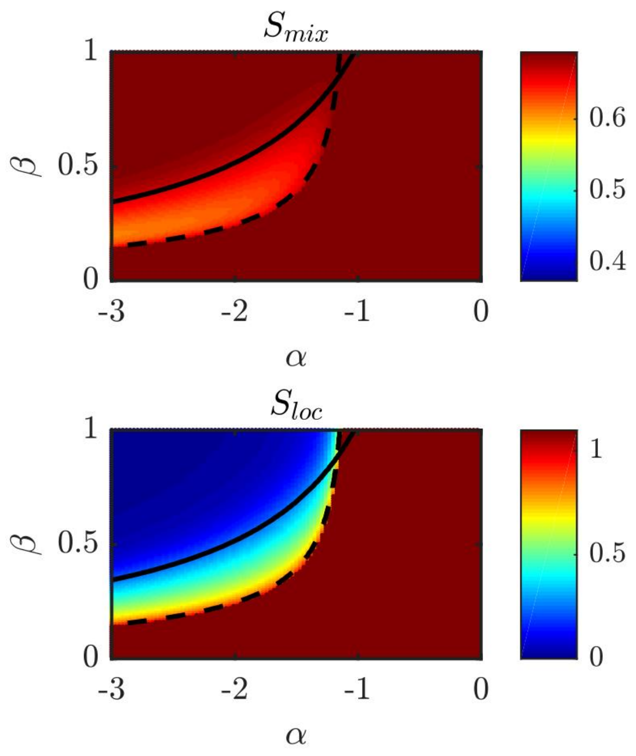
Conclusions



$$\alpha = \frac{W}{\sqrt{U_a U_b}}, \qquad \beta = \frac{M}{N}\sqrt{\frac{U_b}{U_a}}$$

Same mechanism of supermixed soliton formation in all 1D ring lattices, whatever the number of lattice sites.

Conclusions



$$\alpha = \frac{W}{\sqrt{U_a U_b}}, \qquad \beta = \frac{N_b}{N_a}\sqrt{\frac{U_b}{U_a}}$$

Quantum indicators $\hat{S}_{mix}$ and $\hat{S}_{loc}$ can be conveniently used to determine the phase of the system.

$$\tilde{S}_{mix} := \sum_{\vec{n},\vec{m}}^{Q} |c(\vec{n},\vec{m})|^2 S_{mix}(\vec{n},\vec{m}),$$

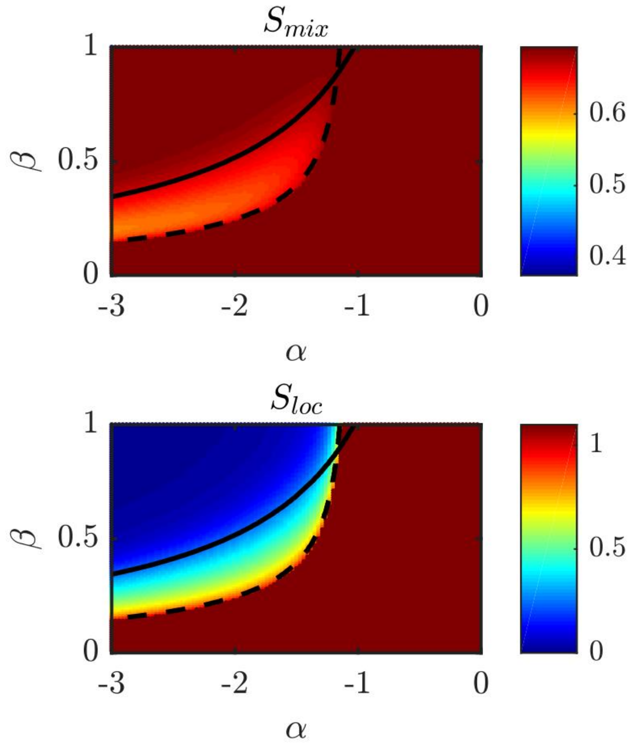
$$\tilde{S}_{loc} := \sum_{\vec{n},\vec{m}}^{Q} |c(\vec{n},\vec{m})|^2 S_{loc}(\vec{n},\vec{m})$$

$$S_{mix} = -\frac{1}{2}\sum_{j=1}^{L}\left(x_j \log\frac{x_j}{x_j+y_j} + y_j \log\frac{y_j}{x_j+y_j}\right)$$

$$c(\vec{n},\vec{m}) = \langle \vec{n},\vec{m}|\psi_0\rangle$$

$$S_{loc} = -\sum_{j=1}^{L}\frac{x_j+y_j}{2}\log\frac{x_j+y_j}{2}.$$

Conclusions



$$\alpha = \frac{W}{\sqrt{U_a U_b}}, \qquad \beta = \frac{N_b}{N_a}\sqrt{\frac{U_b}{U_a}}$$

Transition lines can be extimated analytically, as they correspond to the collapse of the Bogoliubov spectra.

Future work

Extend the study of the mechanism of Soliton formation to more complex lattice topologies, like:

Future work

Go beyond the point-like approximation wells which is typical of the Bose-Hubbard model, i.e. study this phenomena in terms of the GPE.

Explore the possible dynamical regimes of the supermixed solitons.

Thanks for your attention!

QUESTIONS ?

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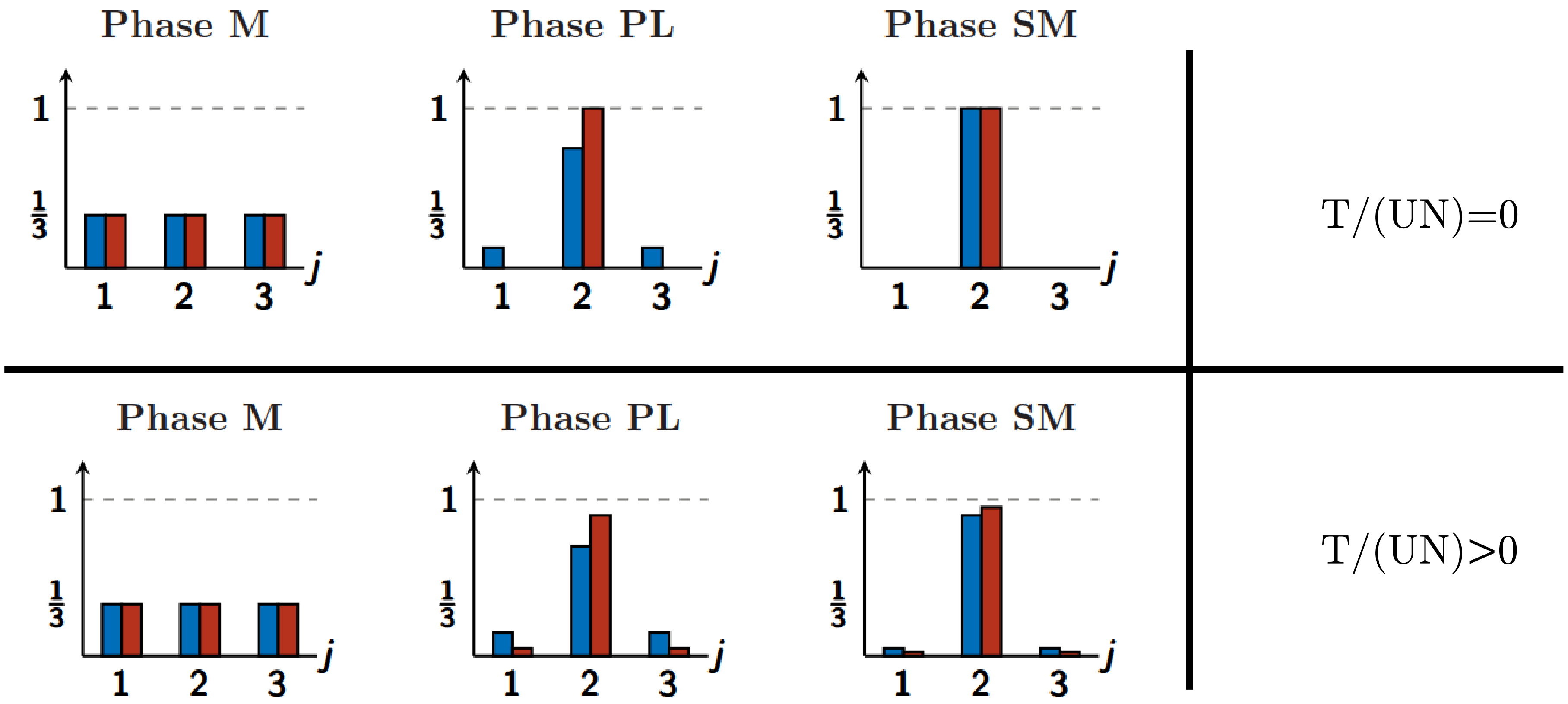
https://arxiv.org/abs/1903.09212

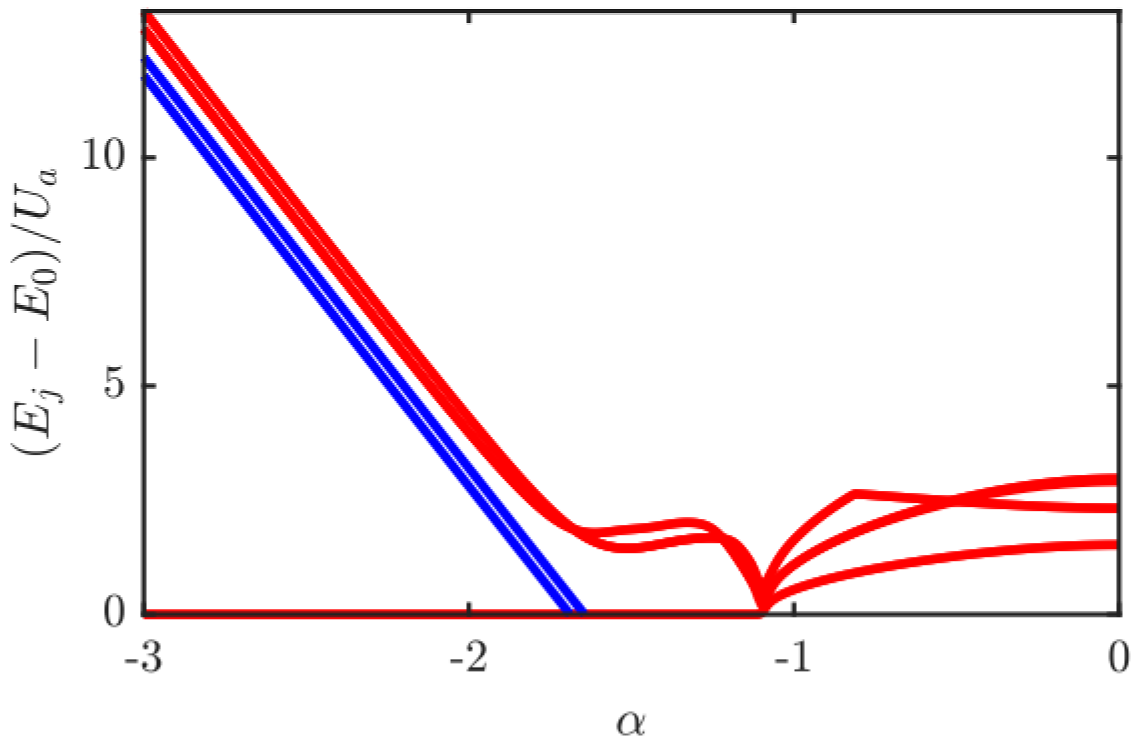
Minimum-energy configuration as a function of L

Phase	$(\vec{x}_*, \vec{y}_*)$	V_*
M	$x_{*,j} = 1/L \quad \forall j$ $y_{*,j} = 1/L \quad \forall j$	$V_*^{\mathrm{M}} = \frac{1}{2L}(\beta^2 + 2\alpha\beta + 1)$
PL	$x_{*,i} = [1-(L-1)\alpha\beta]/L$ $x_{*,j} = [1+\alpha\beta]/L \quad \forall j \neq i$ $y_{*,i} = 1, \;\; y_{*,j} = 0 \;\; \forall j \neq i$	$V_*^{\mathrm{PL}} = \frac{1}{2L}[1 + 2\alpha\beta$ $+\beta^2(L-(L-1)\alpha^2)]$
SM	$x_{*,i} = 1$ $x_{*,j} = 0 \quad \forall j \neq i$ $y_{*,i} = 1, \;\; y_{*,j} = 0 \;\; \forall j \neq i$	$V_*^{\mathrm{SM}} = \frac{1}{2}(\beta^2 + 2\alpha\beta + 1)$

Effect of non zero T/(UN)



Comparison with Bogolyubov (site-modes)



Comparison with Bogolyubov (momentum-modes)