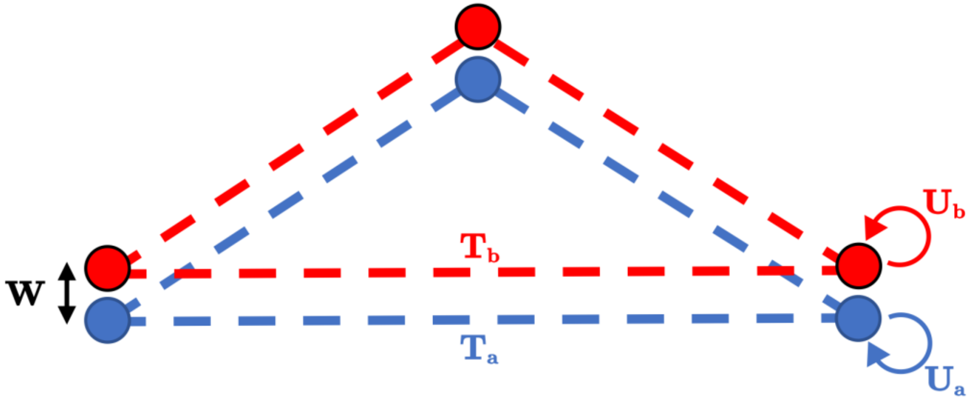
Andrea Richaud

How does a binary mixture separate in a three-well potential?

A two-step mechanism

Full article: Scientific Reports 8, 10242 (2018)

The model



$$\hat{H} = -T_a \sum_{j=1}^{3} \left(A_{j+1}^{\dagger} A_j + A_j^{\dagger} A_{j+1} \right) + \frac{U_a}{2} \sum_{j=1}^{3} N_j (N_j - 1)$$
$$- T_b \sum_{j=1}^{3} \left(B_{j+1}^{\dagger} B_j + B_j^{\dagger} B_{j+1} \right) + \frac{U_b}{2} \sum_{j=1}^{3} M_j (M_j - 1)$$
$$+ W \sum_{j=1}^{3} N_j M_j$$

Conserved quantities:

$$\sum_{j=1}^{3} N_j = N$$

$$\sum_{j=1}^{3} M_j = M$$

The target

Determine the **ground state** of Hamiltonian $\widehat{H}$ according to model parameters T_a, T_b, U_a, U_b and W.

Especially: the **degree of miscibility**.

$$\hat{H} = -T_a \sum_{j=1}^{3} \left(A_{j+1}^{\dagger} A_j + A_j^{\dagger} A_{j+1} \right) + \frac{U_a}{2} \sum_{j=1}^{3} N_j (N_j - 1)$$
$$- T_b \sum_{j=1}^{3} \left(B_{j+1}^{\dagger} B_j + B_j^{\dagger} B_{j+1} \right) + \frac{U_b}{2} \sum_{j=1}^{3} M_j (M_j - 1)$$
$$+ W \sum_{j=1}^{3} N_j M_j$$

The Continuous Variable Picture

Ground state of Hamiltonian $\widehat{H}$ → **Minimum** of effective potential V_*

$$V_* = -2NT\left(\sqrt{x_1x_2} + \sqrt{x_2x_3} + \sqrt{x_3x_1} + \sqrt{y_1y_2} + \sqrt{y_2y_3} + \sqrt{y_3y_1}\right) + \frac{UN^2}{2}\left(x_1^2 + x_2^2 + x_3^2 + y_1^2 + y_2^2 + y_3^2\right) + WN^2\left(x_1y_1 + x_2y_2 + x_3y_3\right)$$

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

$$x_i = \frac{N_i}{N}; \quad y_i = \frac{M_i}{N}$$

A technique already successfully used in e.g.:

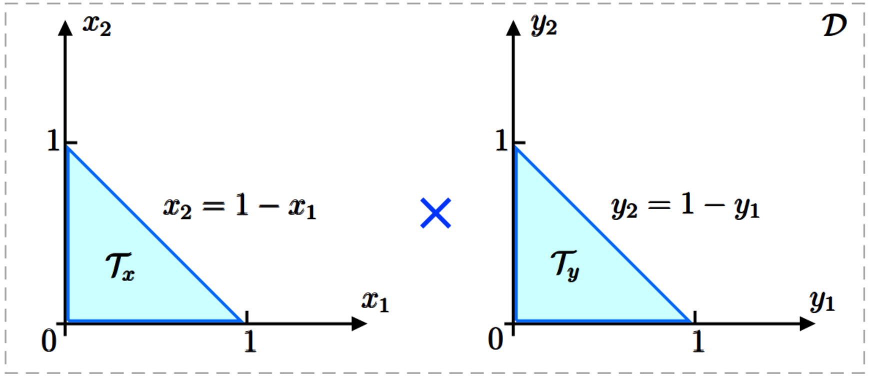
- F. Lingua and V. Penna, PRE 95, 062142 (2017);
- R. W. Spekkens and J. E. Sipe, PRA 59, 3868 (1999);

Search for the global minimum of V_*

$$V_*(x_1, x_2, \cancel{x_3}, y_1, y_2, \cancel{y_3}) = V_*\,(x_1, x_2, y_1, y_2)$$

$$\boxed{\begin{aligned} x_3 &= 1 - x_1 - x_2 \\ y_3 &= 1 - y_1 - y_2 \end{aligned}}$$

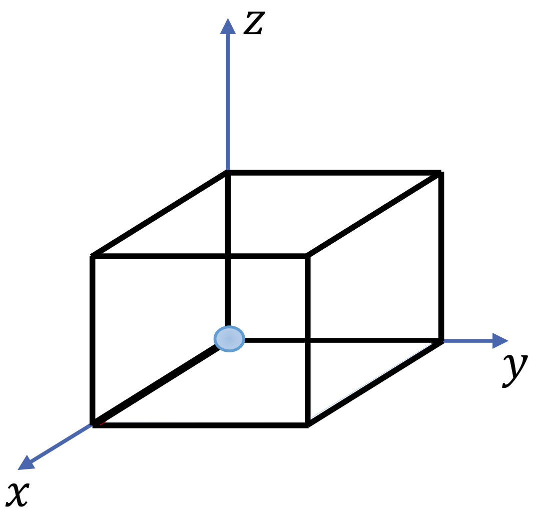
Domain of V_*:



How to explore it?

A simpler example: a cubic domain

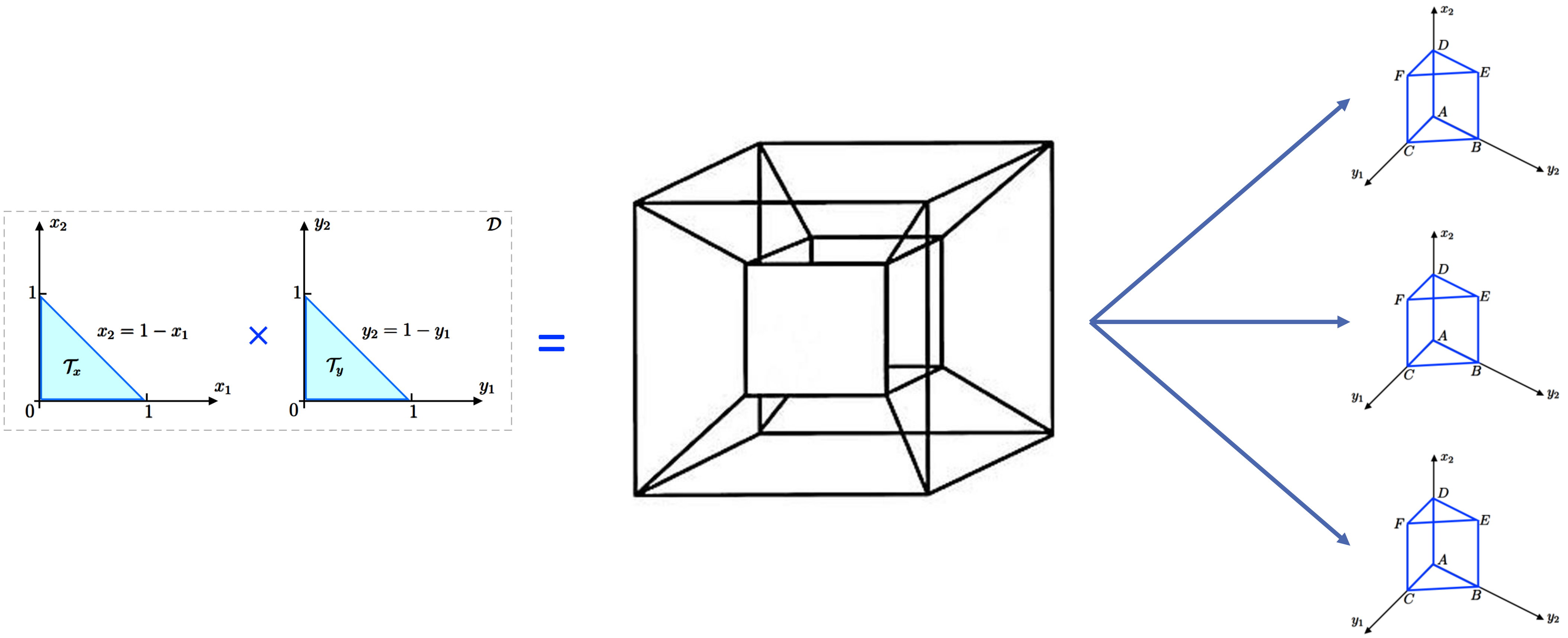
To find the **global minimum** of a function $f(x, y, z)$ defined on a cubic domain, one has to look:



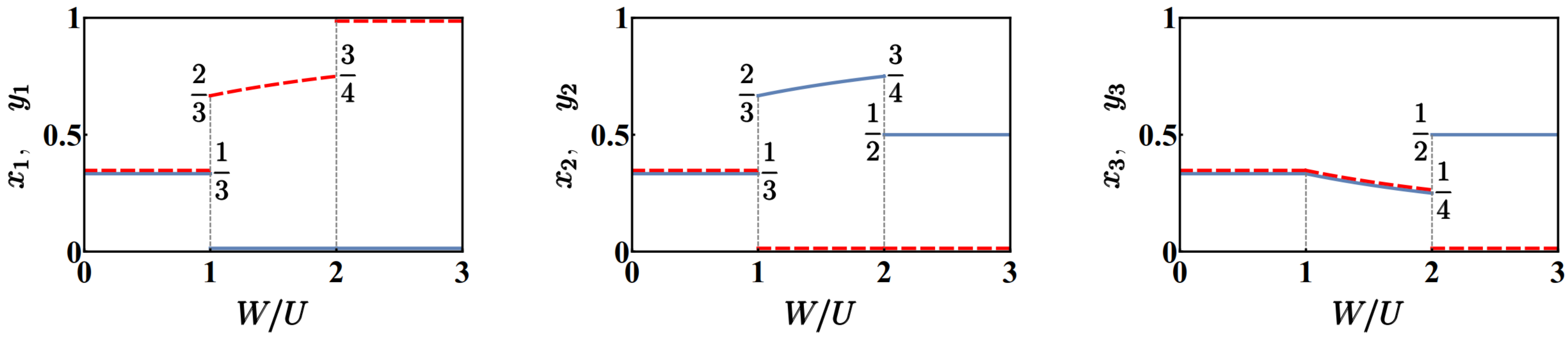
- **Inside** the cube: $\left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right) = \vec{0}$
- On each of the 6 **faces**, e.g. $\left(\frac{\partial f_{z=0}}{\partial x}, \frac{\partial f_{z=0}}{\partial y}\right) = \vec{0}$
- On each of the 12 edges, e.g. $\frac{\mathrm{d} f_{y=z=0}}{\mathrm{d}x} = 0$
- On each of the 8 vertices, e.g. $f(0,0,0)$

$$\min\{f\} = \min\{\dots, \dots, \dots\}$$

Search for the global minimum of V_*



Result for T=0

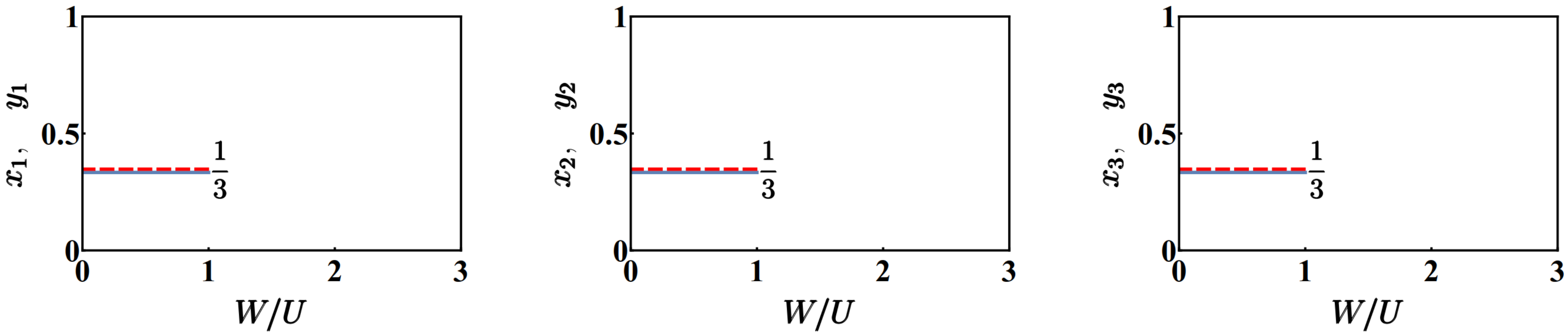


Site 1

Site 2

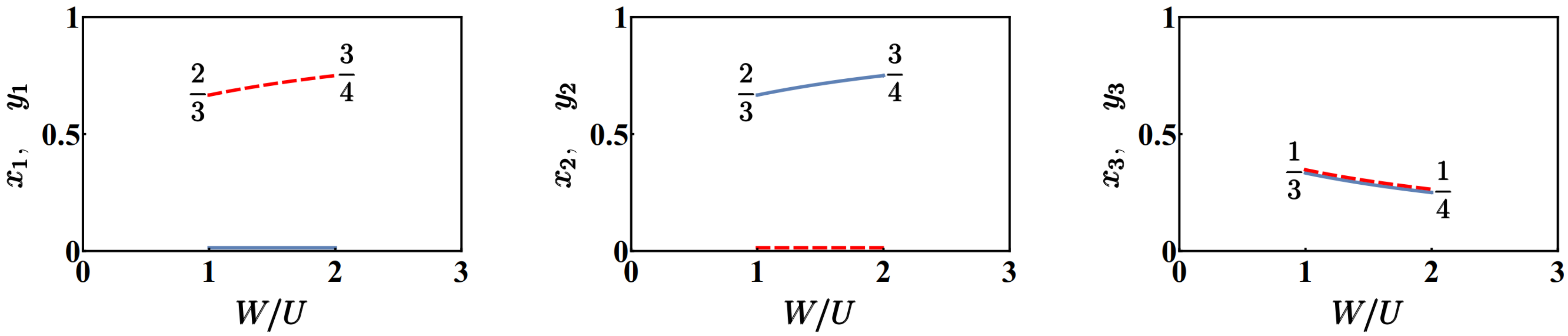
Site 3

Result for T=0



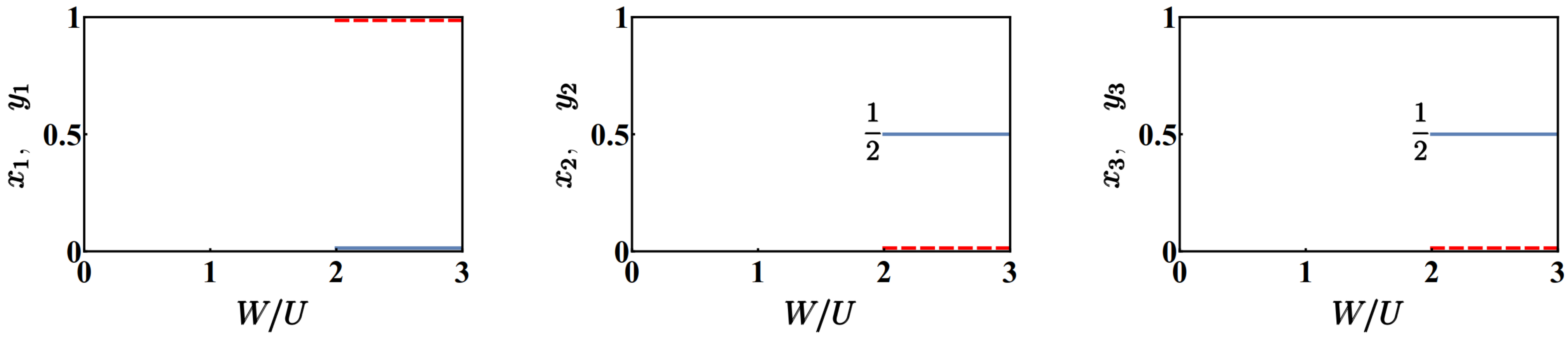
$$\frac{W}{U} < 1 \quad \rightarrow \quad \text{Uniform and completely mixed phase}$$

Result for T=0



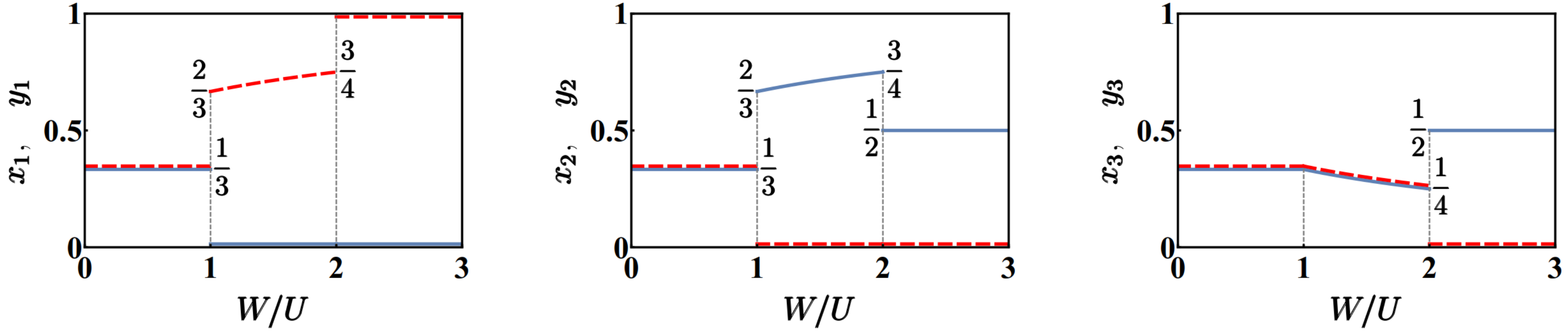
$$\frac{W}{U} \in (1,2) \quad \rightarrow \quad \text{Partially mixed phase}$$

Result for T=0



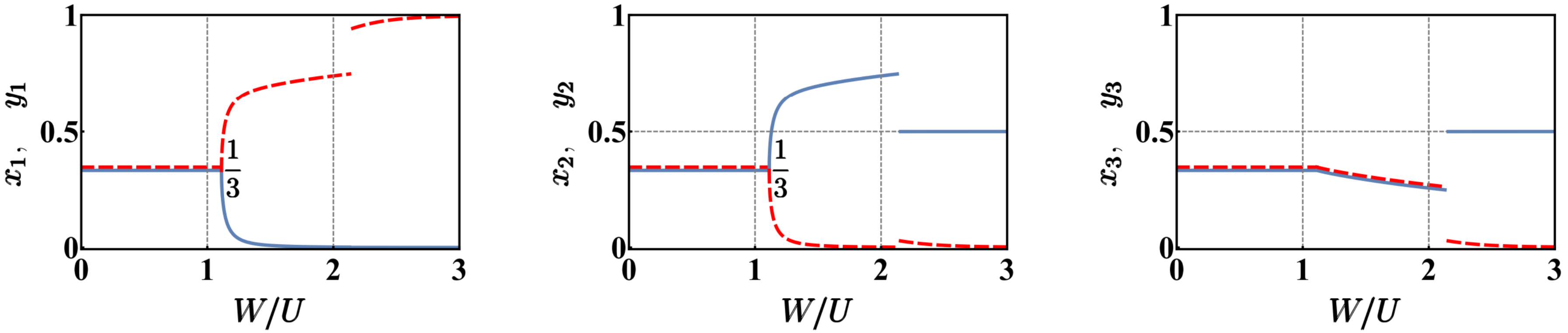
$\frac{W}{U} > 2 \quad \rightarrow \quad$ Completely demixed phase

Result for T > 0



T=0

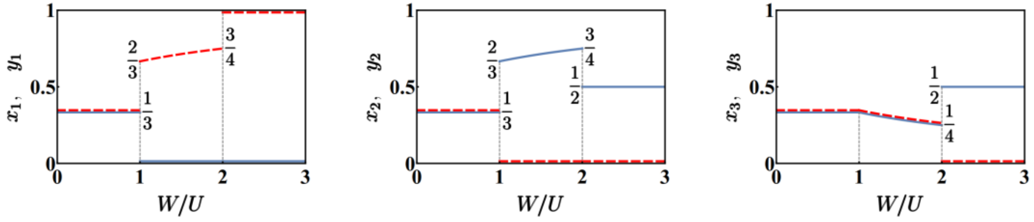
Let's switch on the tunnelling processes:



T>0

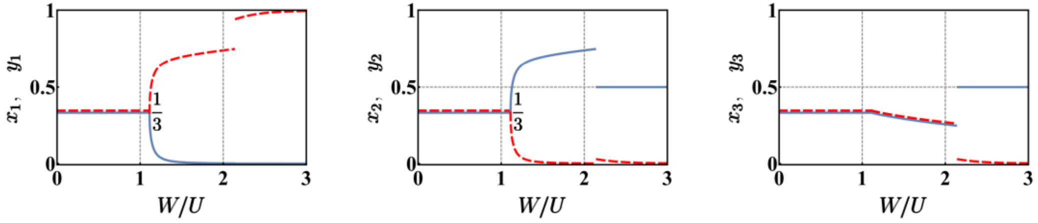
Comparison

T=0



- Analytical expression;
- Both transitions are abrupt;
- Transitions exactly @ W/U=1 and W/U=2;

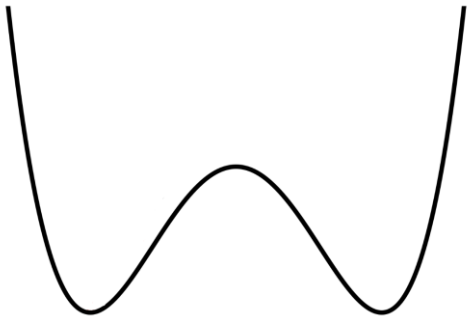
T>0

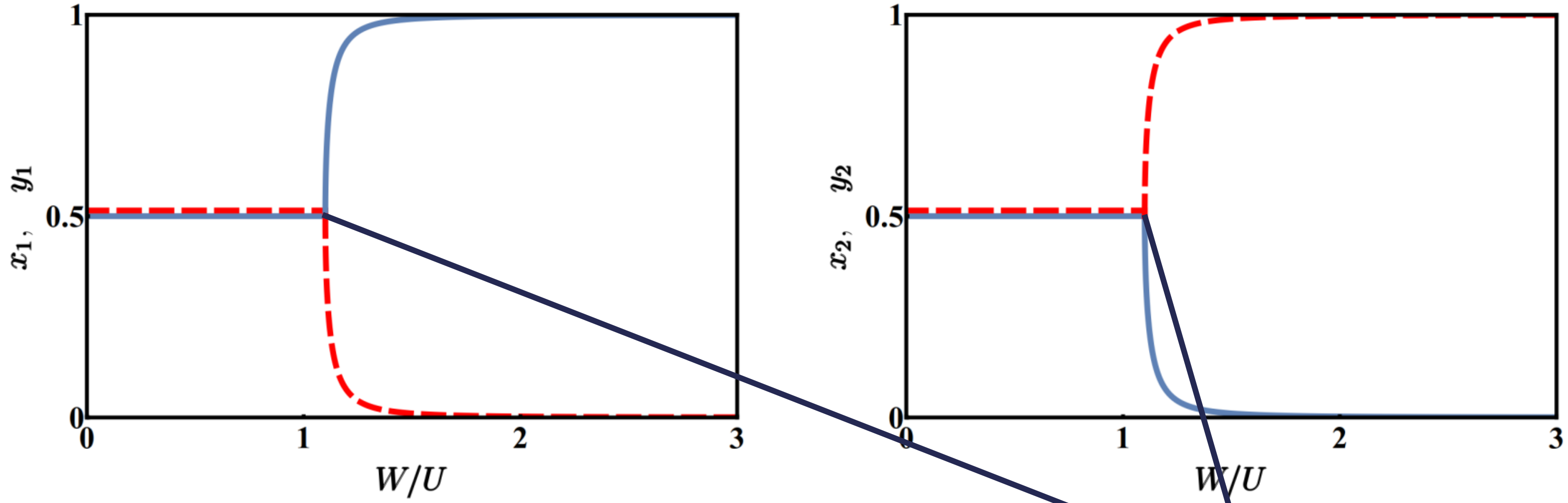


- Not fully analytic (just first border!);
- First transitions is continuous, second abrupt;
- Transitions @ W/U$\gtrsim$1 and W/U $\gtrsim$ 2;

A new mechanism

Previous investigations have shown that in the **dimer** there is only one mixing-demixing phase transition.

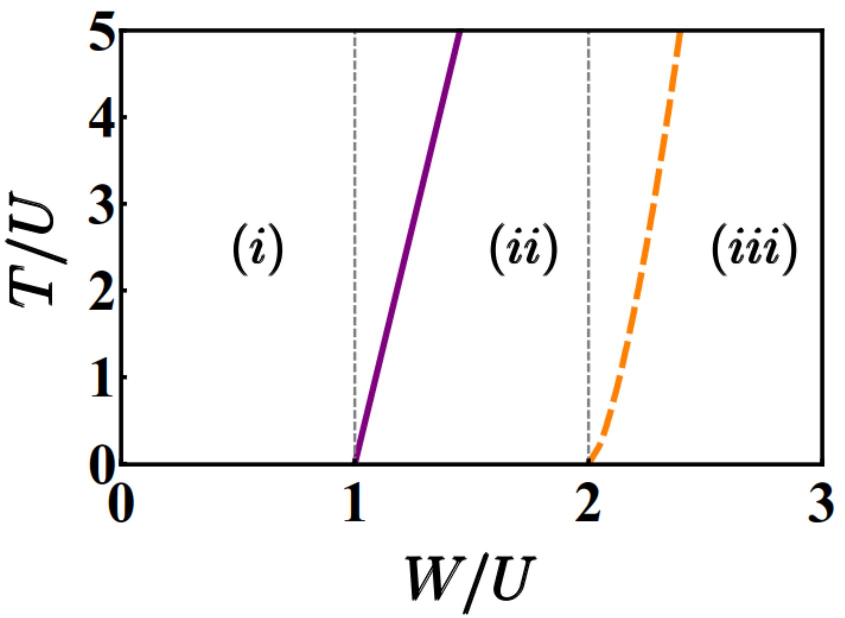




F. Lingua & V. Penna, PRE 95, 062142 (2017)

$$\frac{W}{U} = 1 + \frac{2T}{UN}$$

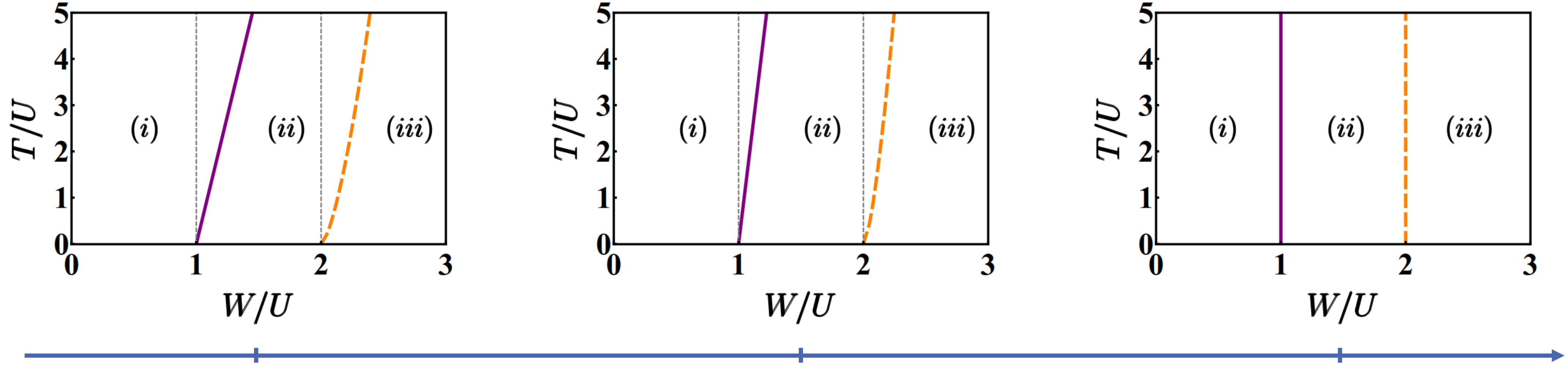
Phase diagram



$$\frac{W}{U} = 1 + \frac{9T}{2UN}$$

No known analytical expression

Phase diagram: thermodynamic limit



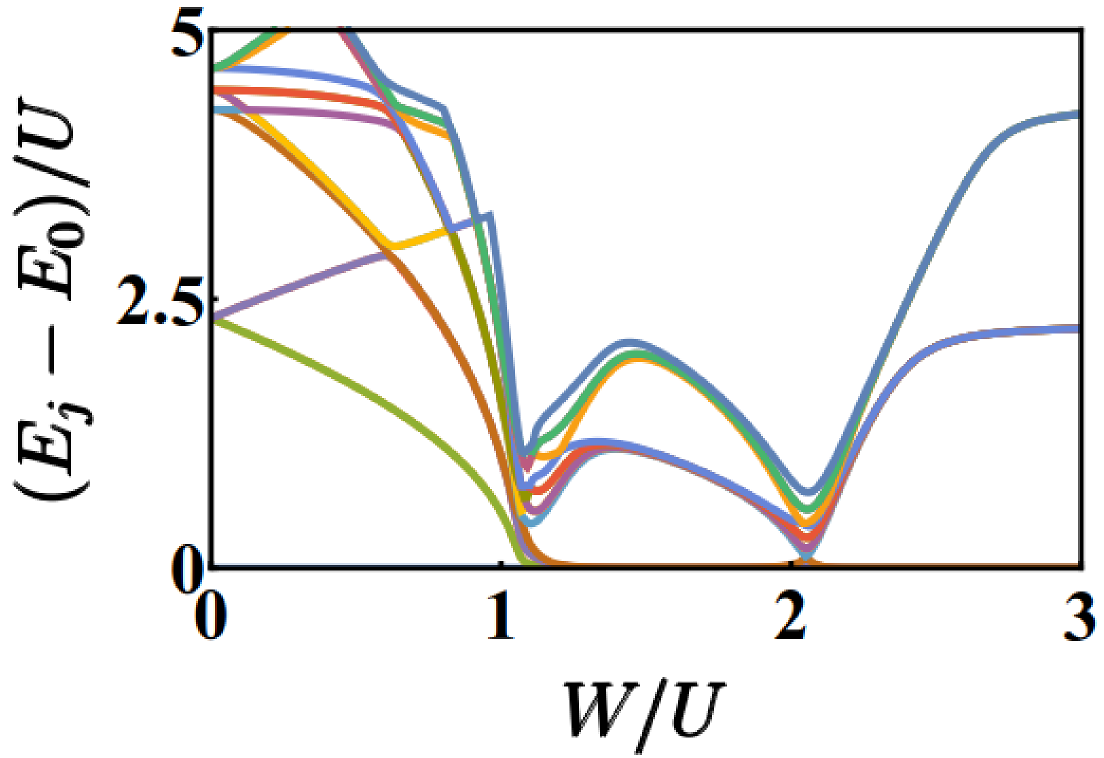
N=50 N=100 $N \to \infty$

$$\frac{W}{U} = 1 + \frac{9T}{2UN}$$

No known analytical expression

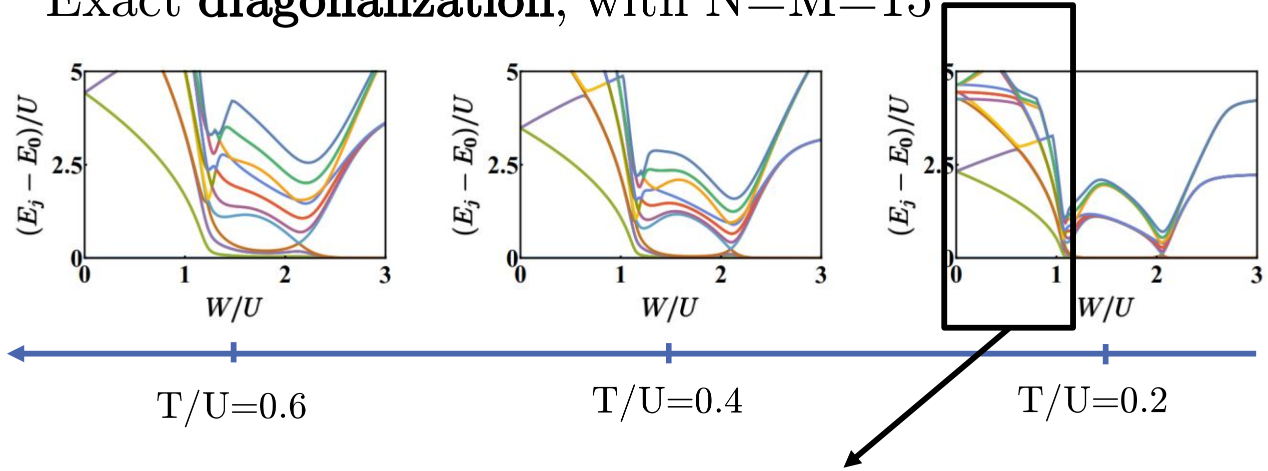
Energetic fingerprint

Exact **diagonalization**, with N=M=15



Energetic fingerprint

Exact **diagonalization**, with N=M=15



Increasing T/U:

- Transition gets smoother;
- Critical points move rightward;

The expression of the **characteristic frequencies** in the uniform phase has been obtained within the **Bogoliubov** approximation scheme followed by the Dynamical Algebra method (see V. Penna, A. Richaud, PRA 96, 053631 (2017)).

$$\omega_1 = \sqrt{T(9T + 2UN + 2WN)}$$

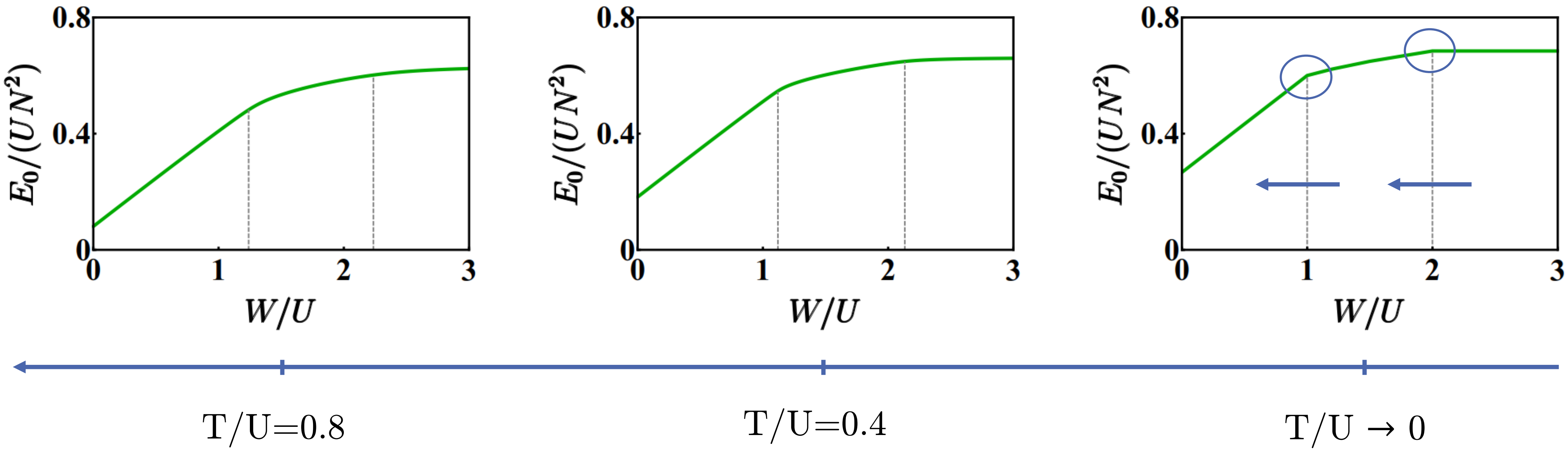
$$\omega_2 = \sqrt{T(9T + 2UN - 2WN)}$$

$$\longrightarrow \boxed{\frac{W}{U} < 1 + \frac{9T}{2UN}}$$

Collapse of Bogoliubov frequencies herald mixing-demixing phase transition!

Ground-state energy

$$E_0 = \langle \psi_0 | \hat{H} | \psi_0 \rangle$$



Entanglement between the species

$$\hat{\rho}_0 = |\psi_0\rangle\langle\psi_0|$$

← Density matrix of the ground state

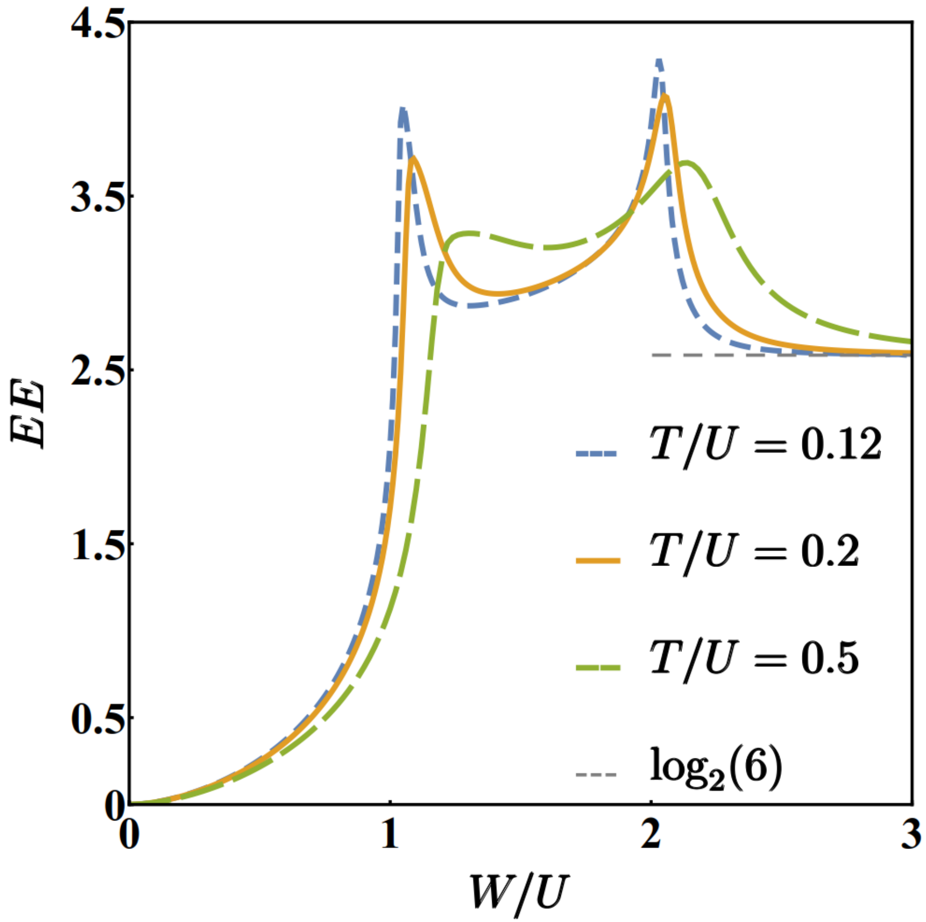
$$\downarrow$$

$$\hat{\rho}_{0,a} = \mathrm{Tr}_b\left(\hat{\rho}_0\right)$$

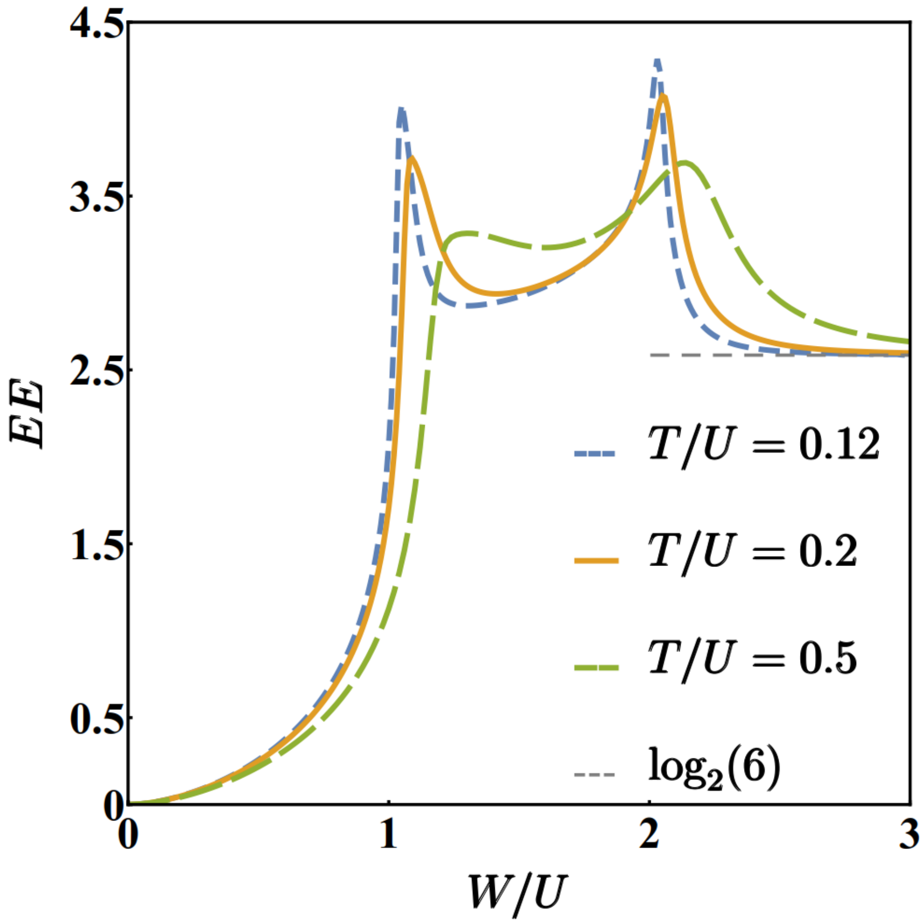
← Reduced density matrix

$$\downarrow$$

$$EE = -\mathrm{Tr}(\hat{\rho}_{0,a}\log_2\hat{\rho}_{0,a}) = -\sum_{j=0}\lambda_j \log_2 \lambda_j$$



Entanglement between the species



Observations:

- Peaks where transitions occur;

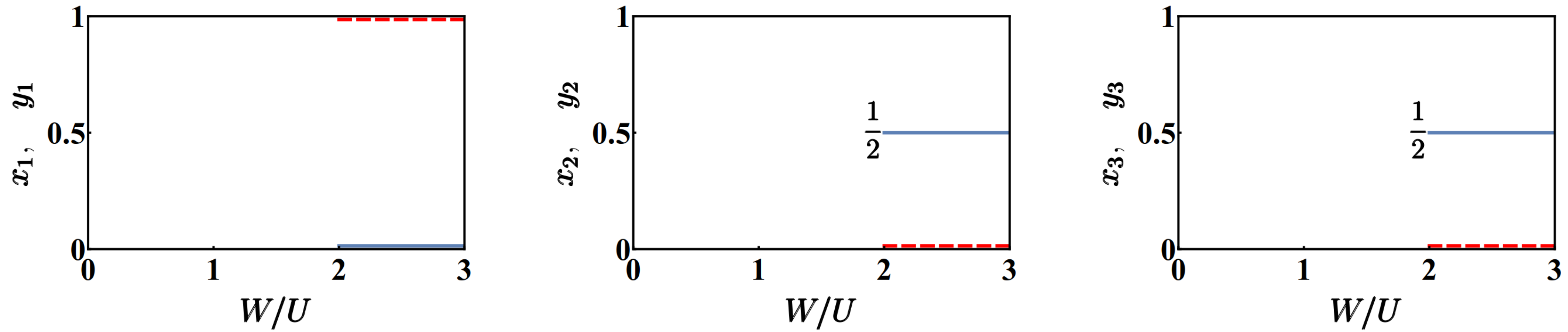
- Increasing **T/U**, transitions get smoother and shift rightward;

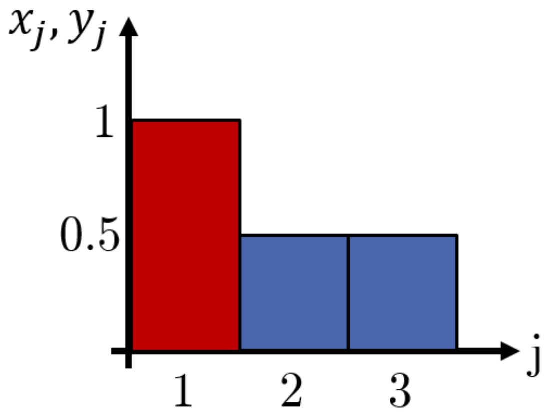
- For W/U=0, the species are decoupled, so EE=0;

- For W/U≫3, EE → $\boxed{\log_2(6)}$;

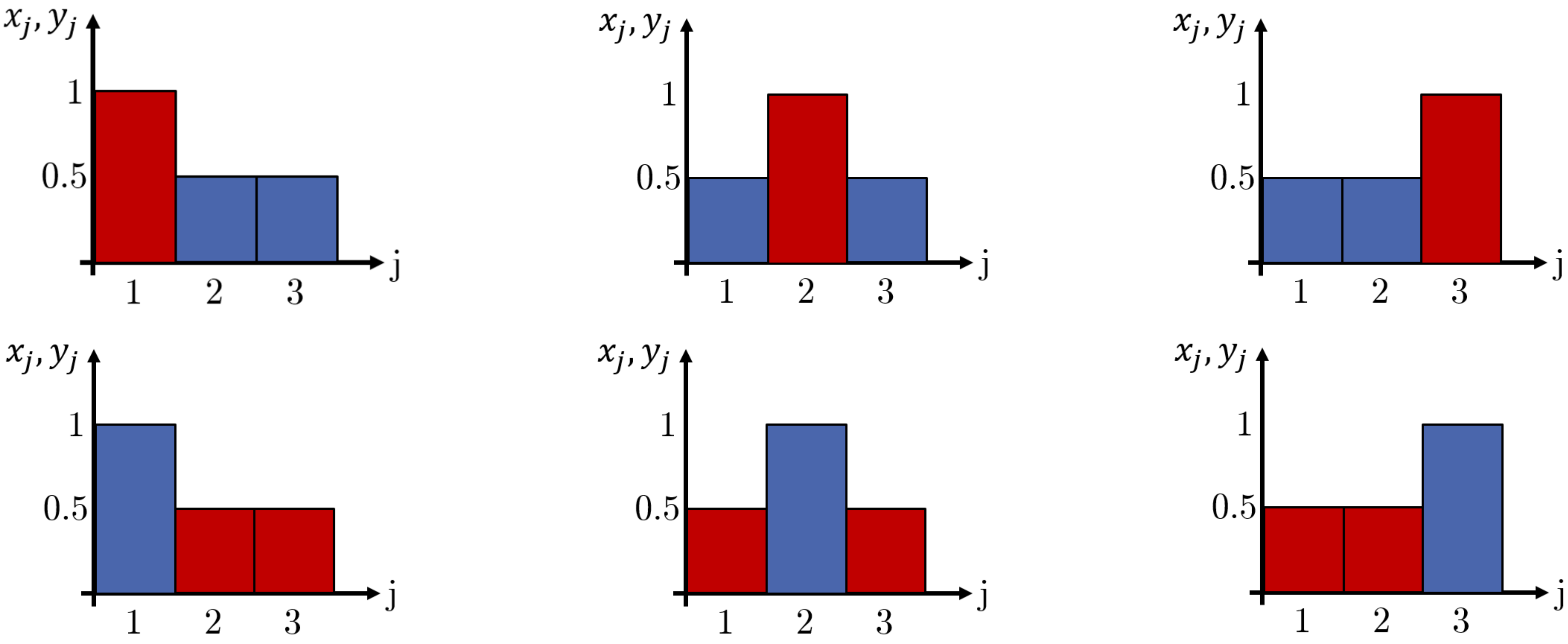
What's the meaning of this number?

A Schrodinger cat with 6 faces

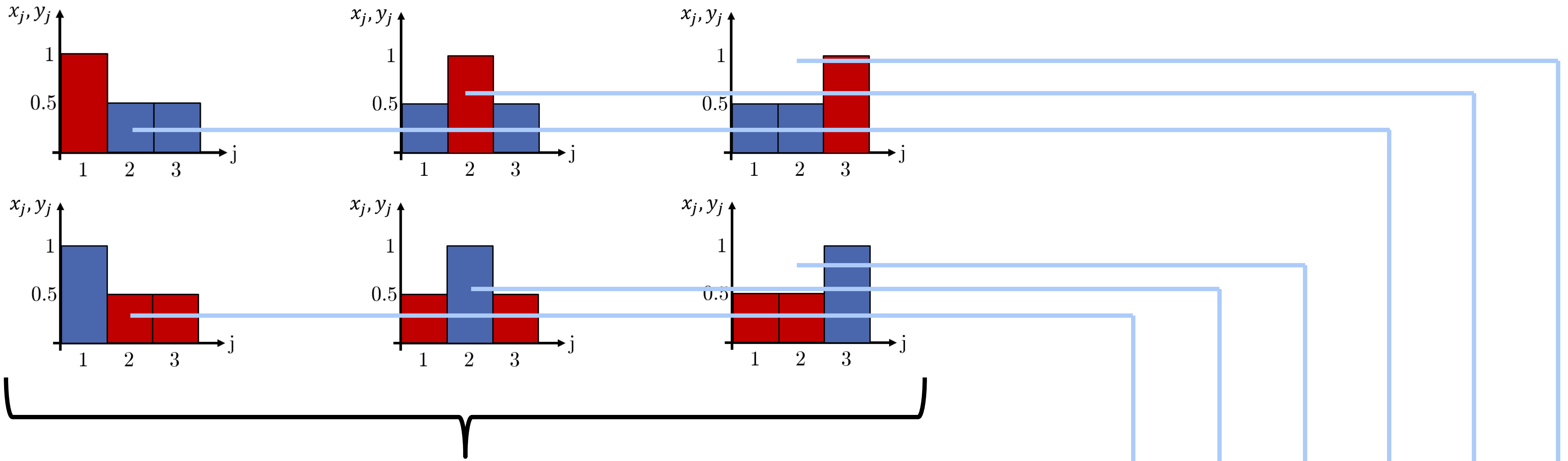




A Schrodinger cat with 6 faces



A Schrodinger cat with 6 faces

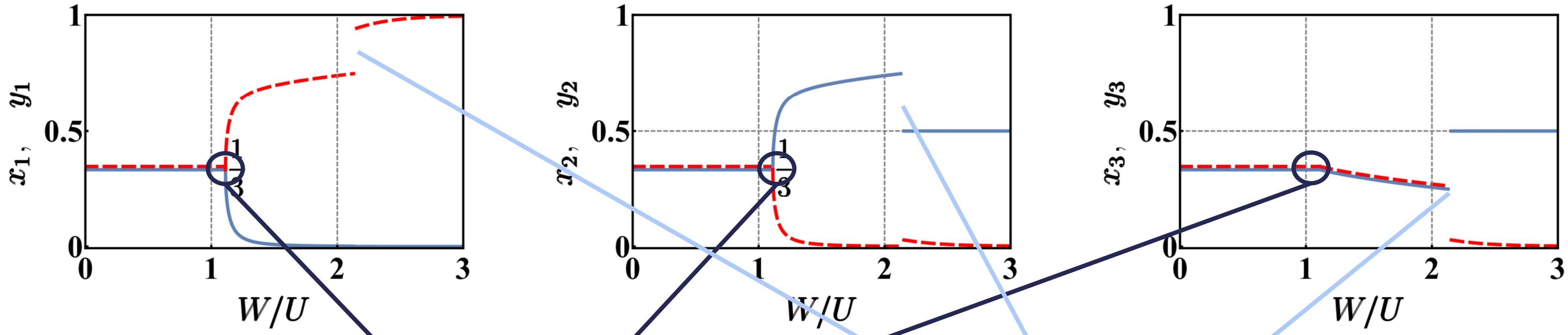


6 semiclassical distinct configurations

$$|\Psi_0\rangle = \frac{1}{\sqrt{6}}\left(|*\rangle + |*\rangle + |*\rangle + |*\rangle + |*\rangle + |*\rangle\right)$$

Recap

We have evidenced two different kinds of **mixing-demixing phase transitions**.

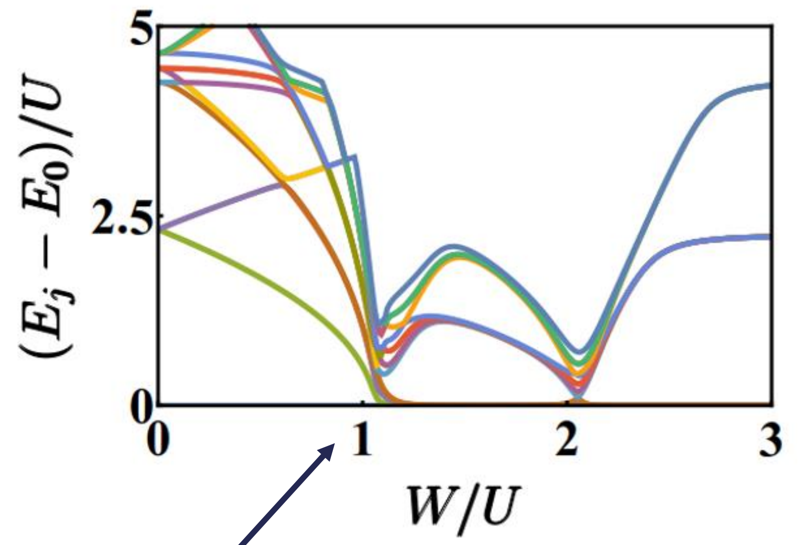


$$\frac{W}{U} = 1 + \frac{9T}{2UN}$$

$$\frac{W}{U} \gtrsim 2$$

Recap

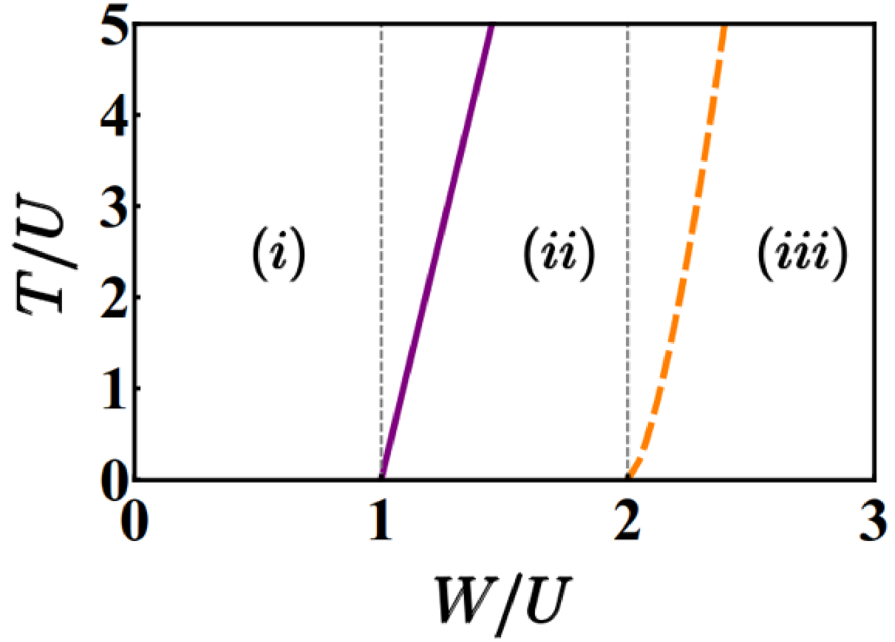
The three phases have a different **energetic fingerprint**:



The first mixing-demixing phase transitions is announced by the collapse of Bogoliubov frequencies (see V. Penna, A. Richaud, PRA 96, 053631 (2017))

Recap

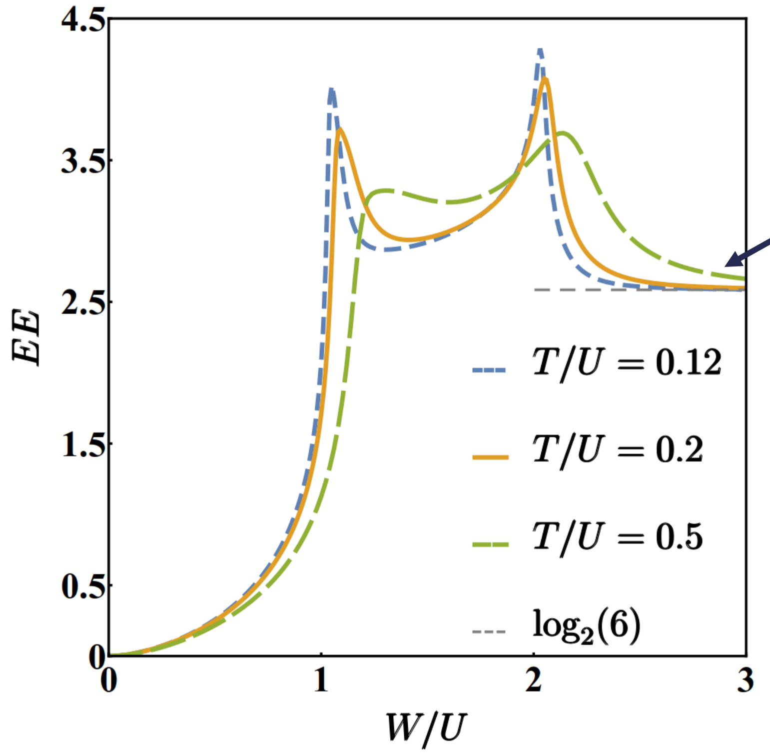
Phase diagram:



$$\frac{W}{U} = 1 + \frac{9T}{2UN}$$

Recap

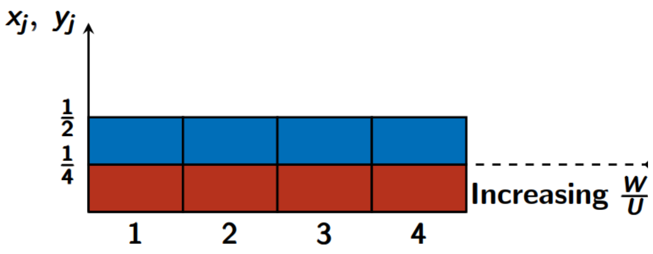
Entanglement entropy:



In the fully demixed phase, the ground state consists in a 6-faced Schrodinger's cat

Future work

Explore the phase separation mechanism in more complex lattice geometries. E.g.: the tetramer:



- How many intermediate phases?

- Structure of each of them?

Thanks for your attention!

QUESTIONS ?

Full article: `Scientific Reports 8, 10242 (2018)`

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