Pair-Factorised Steady State model exhibits condensate's growth on monolayers

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Models of mass transport and condensation

Motivation:

- Cluster or atomic deposition, diffusion of atomic clusters on substrate surface, thin films growth, self-assembled quantum dots, etc.

Existing models:

- Balls-in-Boxes, Zero-Range Process (ultralocal rules of dynamics → stationary state factorises → condensates occupy single sites), Solid-on-Solid, etc.
- The models aim at describing particle/mass condensation: critical density, size and shape of the condesate, fluctuations, etc.

Pair-Factorised Steady State (PFSS)

M particles at N sites, set of occupation numbers $\{m_1, \dots, m_N\}$.

A particle at a site *i* hops with a rate $u(m_i | m_{i+1}, m_{i-1})$ (can be assymetric).

Master eq. $$\frac{\mathrm{d}P(\vec{m},t)}{\mathrm{d}t} = \sum_{\vec{m}'} \left[W(\vec{m}' \to \vec{m}) P(\vec{m}',t) - W(\vec{m} \to \vec{m}') P(\vec{m},t) \right],$$

In steady-state: $$\sum_{\vec{m}'} P(\vec{m}) W(\vec{m} \to \vec{m}') = \sum_{\vec{m}'} P(\vec{m}') W(\vec{m}' \to \vec{m})$$

one obtains: $$P(\vec{m}) = \frac{1}{Z} \prod_{i=1}^{N} g(m_i, m_{i+1}) \delta_{m_1 + \cdots + m_N, M},$$

The stationary state is pair factorised.

Assume weights: $$g(m,n) = K(|m-n|) \sqrt{p(m)p(n)},$$

B Waclaw, J Sopik, W Janke and H Meyer-Ortmanns, J. Stat. Mech. (2009) P10021

B Waclaw, J Sopik, W Janke and H Meyer-Ortmanns, PRL 103 (2009) 080602

Known 1D results

Assume P(m) is a probability of a microstate.

Canonical:
$$Z(N,M)=\sum_{\{m_i\}}\prod_i g(m_i,m_{i+1})\delta_{\sum_i m_i,M}$$

Grand-can.:
$$Z_N(z)=\sum_M Z(N,M)z^M=\sum_{\{m_i\}} z^{\sum_i m_i}\prod_i g(m_i,m_{i+1})$$

In 1D case, the partition function takes the form:

$$Z_N(z)=\sum_{m_1,\ldots,m_N} T_{m_1m_2}T_{m_2m_3}\cdots T_{m_Nm_1}=\mathrm{Tr}\,T(z)^N,$$

where $T_{mn}=z^{(m+n)/2}g(m,n)$

So solving 1D problem is equivalent to the eigenproblem:

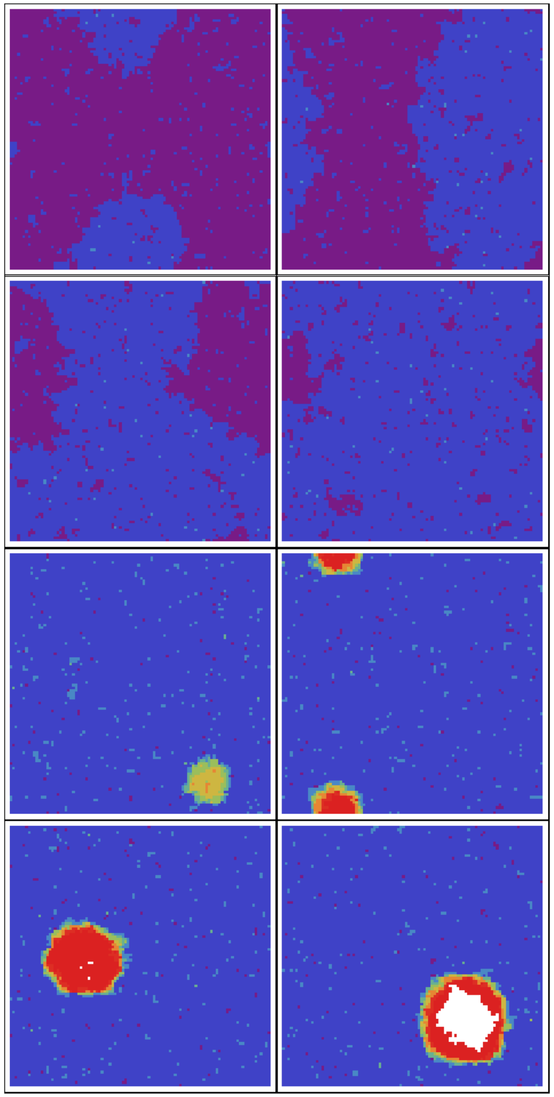
$$\sum_n T_{mn}\phi_n=\lambda_{\max}\phi_m,$$

Lennard - Jones

$$g(m,n) = \exp(-J|m-n|)$$
$$\exp\left(\frac{U}{4}\left[\left(\frac{\sigma}{m+1}\right)^3 + \left(\frac{\sigma}{n+1}\right)^3 - \left(\frac{\sigma}{m+1}\right)^9 - \left(\frac{\sigma}{n+1}\right)^9\right]\right)$$

A layer of thickness ≈ σ builds up.
A condensate forms upon the layer.

σ tunes the thickness (almost) linearly!



Densities: 0.2, 0.5, 0.7, 0.9, 1.1, 1.2, 1.5, 1.8

σ = 1

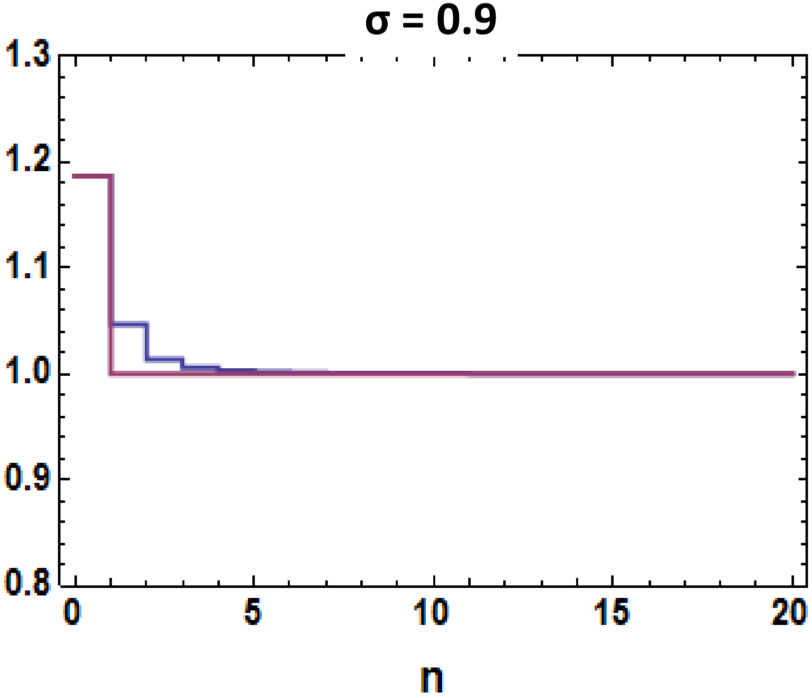
J=1, U=6

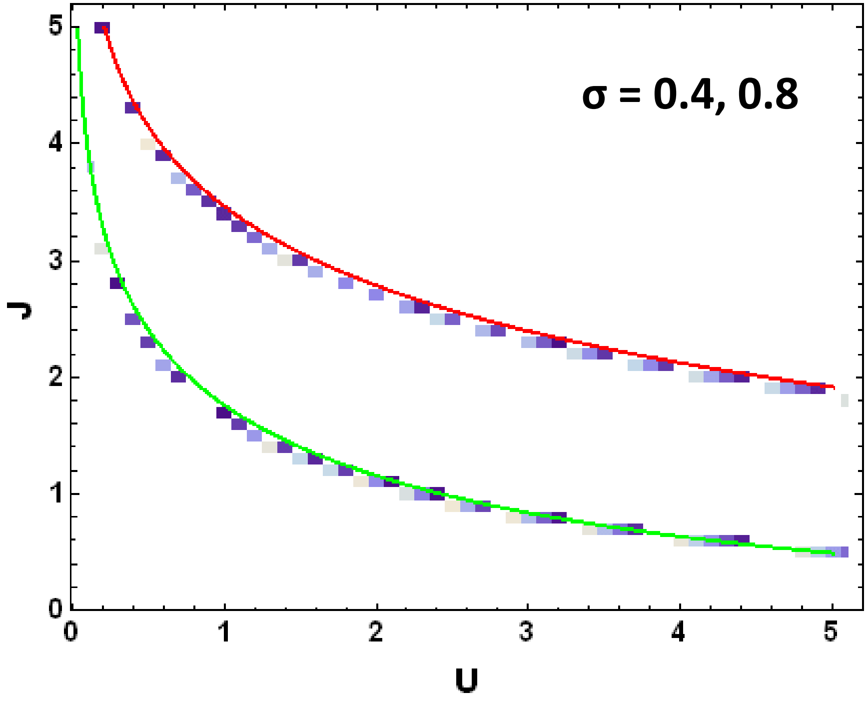
3-9 LJ surface in: R. Hentschke, Macromol. Theory Simul. 6,287-316 (1997)

Good 1D approximations, σ<1

Instead of $\exp\left[\frac{U}{2}\left[\left(\frac{\sigma}{m+1}\right)^3 - \left(\frac{\sigma}{m+1}\right)^9\right]\right]$

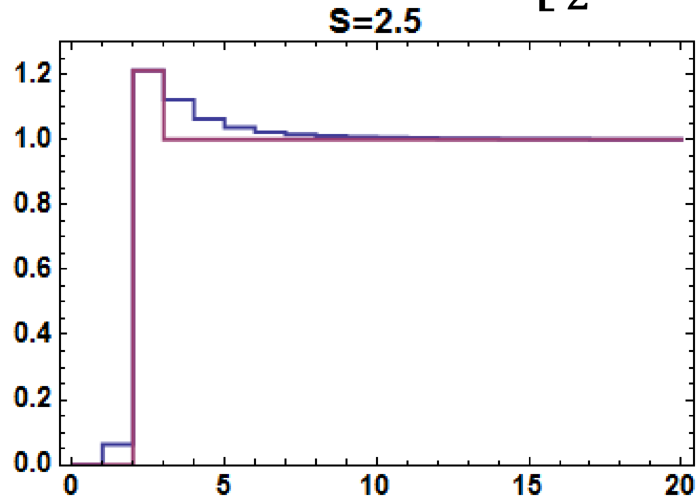
use $\exp\left[\frac{U'}{2}\delta(n,0)\right]$ with $U' = U(\sigma^3 - \sigma^9)$

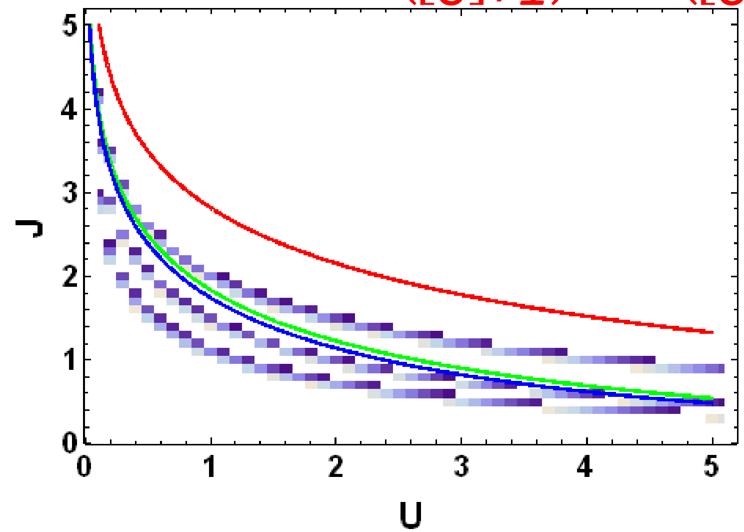


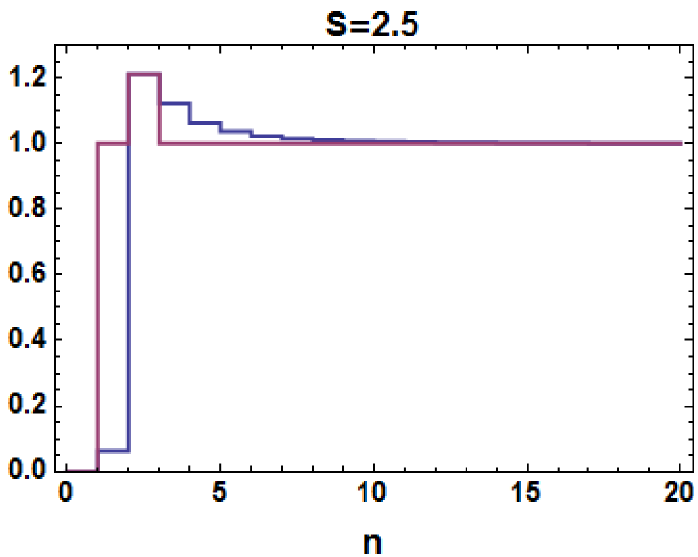


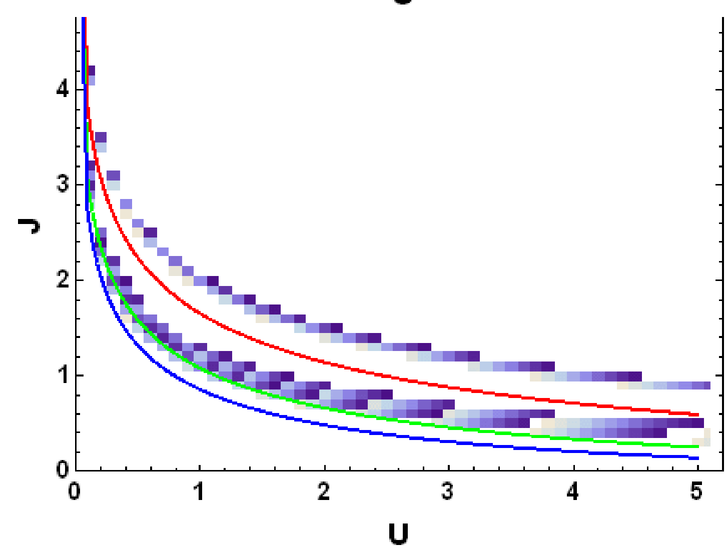
Bad 1D approximations, σ>1

Similarly take $\exp\left[\frac{U'}{2}\delta(n,0)\right]$ with $U' = U\left[\left(\frac{\sigma}{|\sigma|+1}\right)^{3} - \left(\frac{\sigma}{|\sigma|+1}\right)^{9}\right]$









1D approximations

For these approximations one can solve

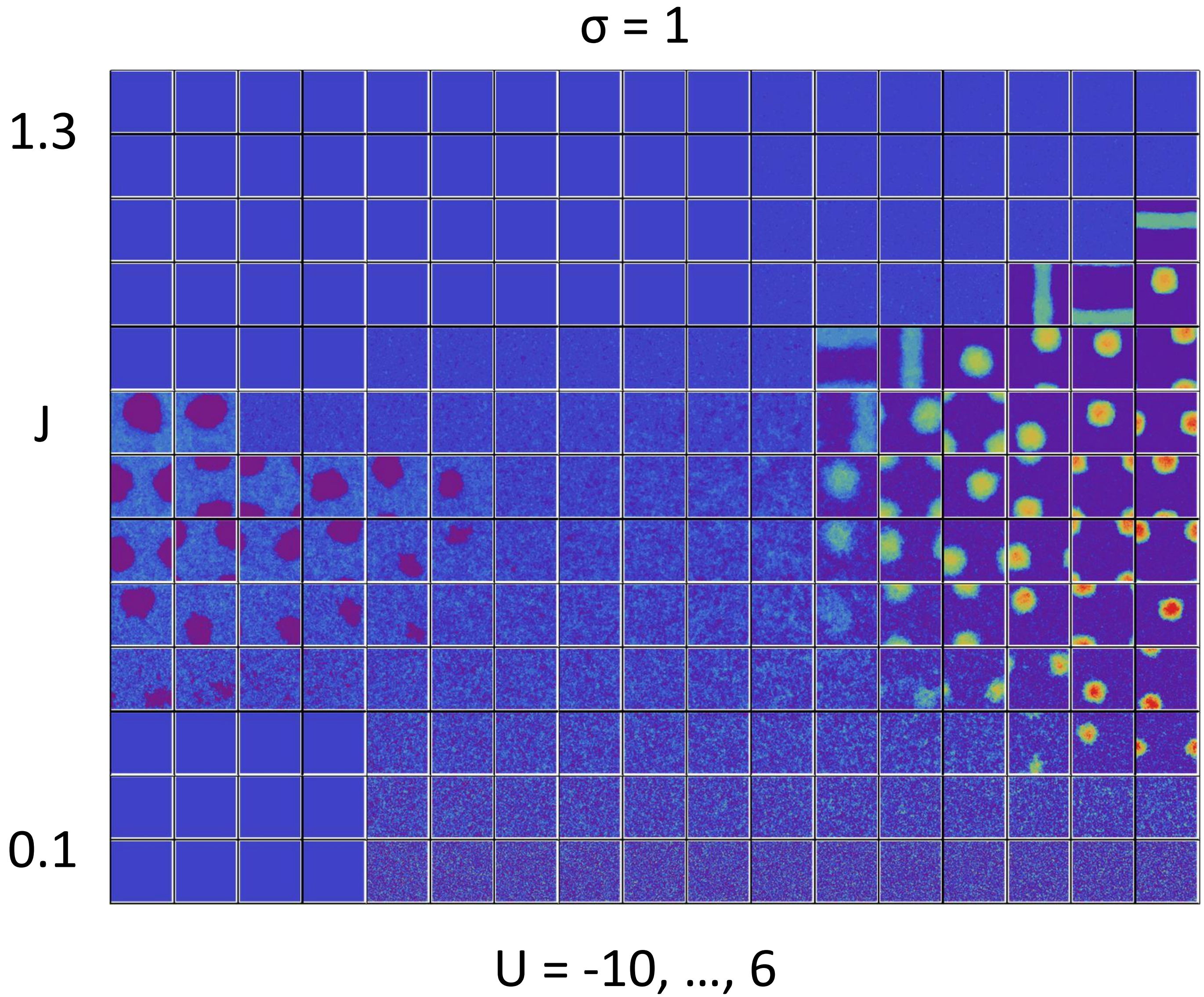
$$\sum_n g(m,n)\varphi_n = \lambda_{max}\,\varphi_m$$

and calculate the **critical density**

$$\rho_{c(\sigma)} = \frac{\sum_n^{\infty} m\,\varphi_m{}^2}{\sum_n^{\infty}\,\varphi_m{}^2} = \rho_{c(0)} + \sigma$$

Number of monolayers grows linearly with σ

2D phase diagrams



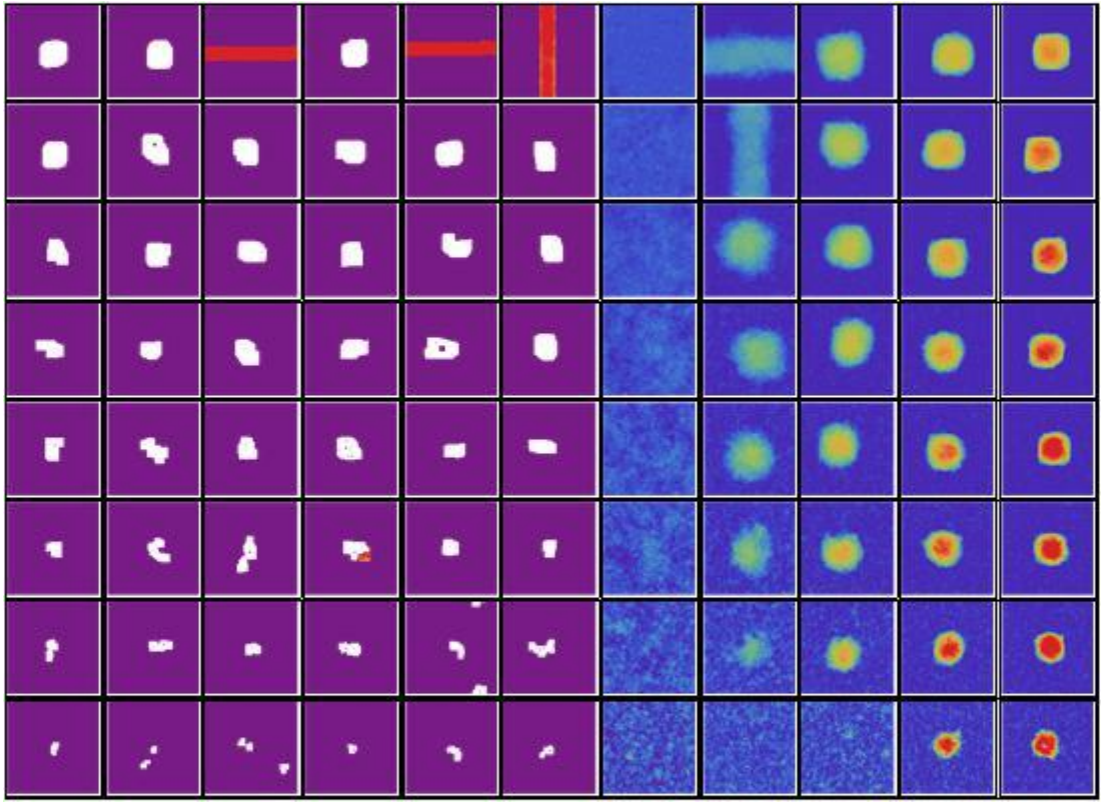
2D phase diagrams

σ = 3

0.9

J

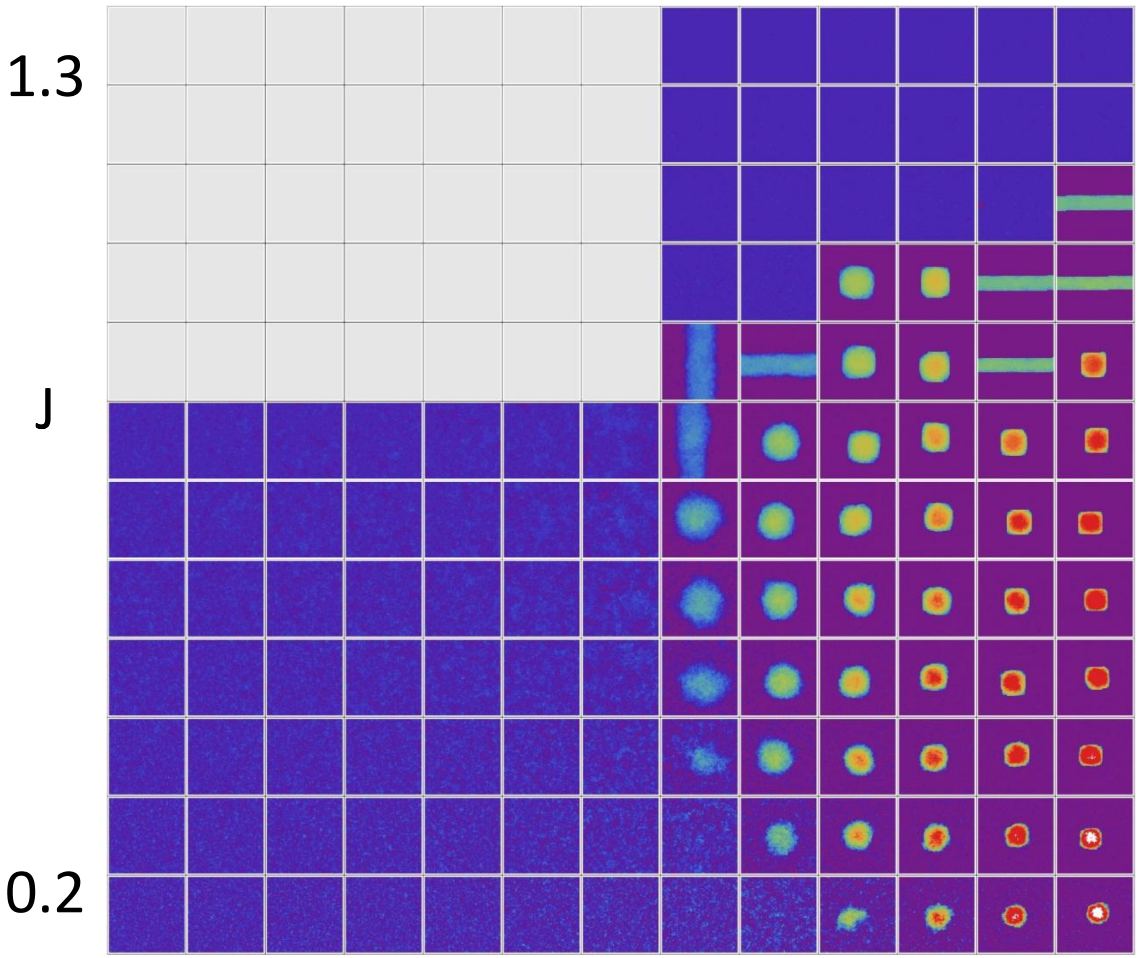
0.2



U = -6, ..., 4

2D phase diagrams

σ = 0.9



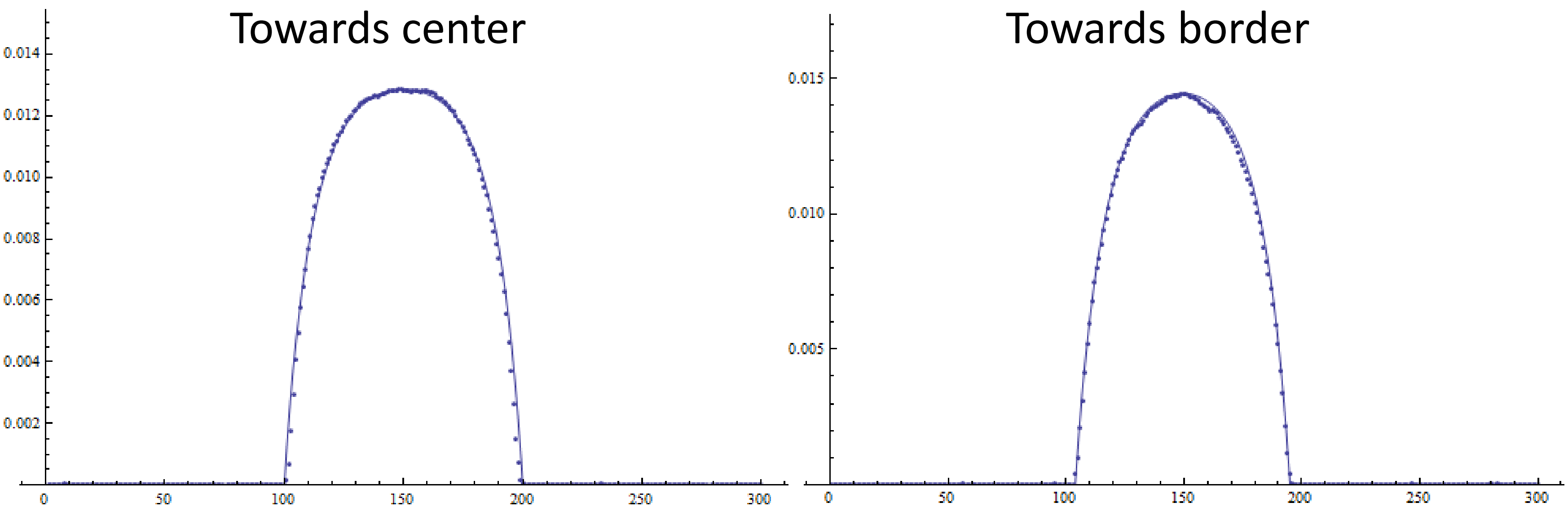
U = -6, ..., 6

2D condensate's shapes

In 1D width of the condensate $\sim \sqrt{N}$

And the shape $h(t) = \frac{w}{2v} \ln \frac{\tilde{K}(v)}{\tilde{K}(vt)}$ (t – normalised position, w and v depend on J and U)

$$K(|m-n|) = \exp(-J|m-n|)$$



Sections of 2D condensate can be fitted with 1D shape.

Larger flattening of the top for the same J values than in 1D.

Conclusions

- The model can exhibit growth of the condensate on monolayers (reminding of Stranski-Krastanov growth)
- Number (thickness) of monolayers connected with the σ parameter of Lennard-Jones potential
- 2D condensates behave very much like 1D

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