

Dynamic wetting with two competing adsorbates

Christian Gogolin

Universität Würzburg

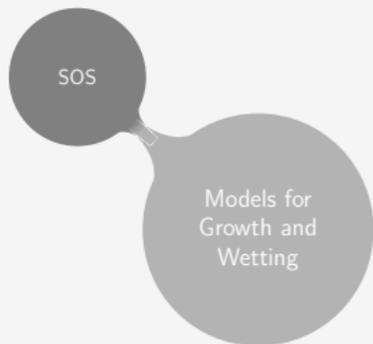
2009-02-06

Outline

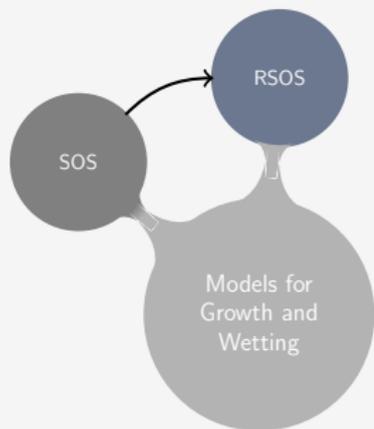


Models for
Growth and
Wetting

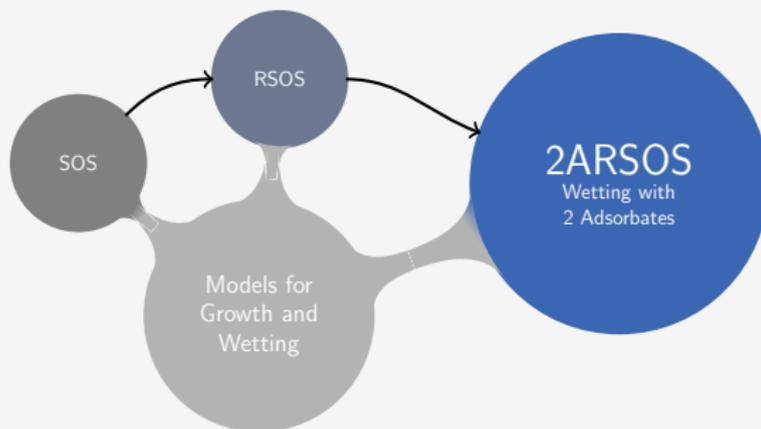
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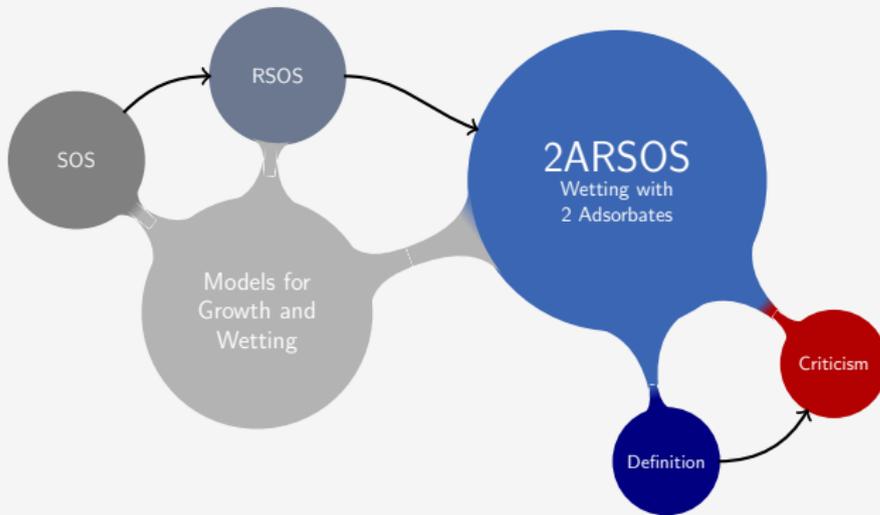
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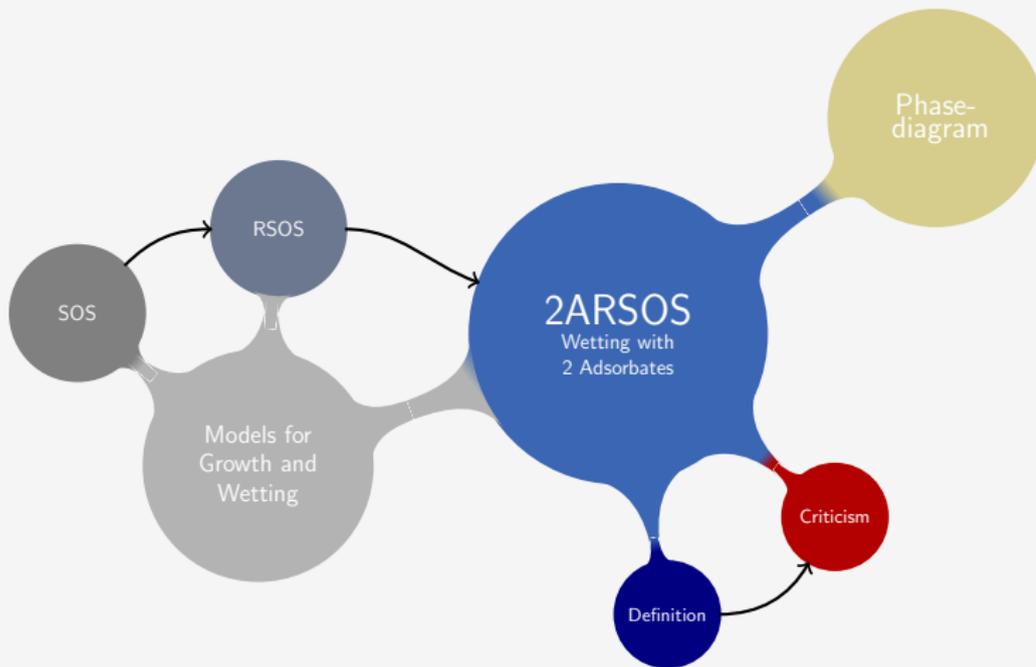
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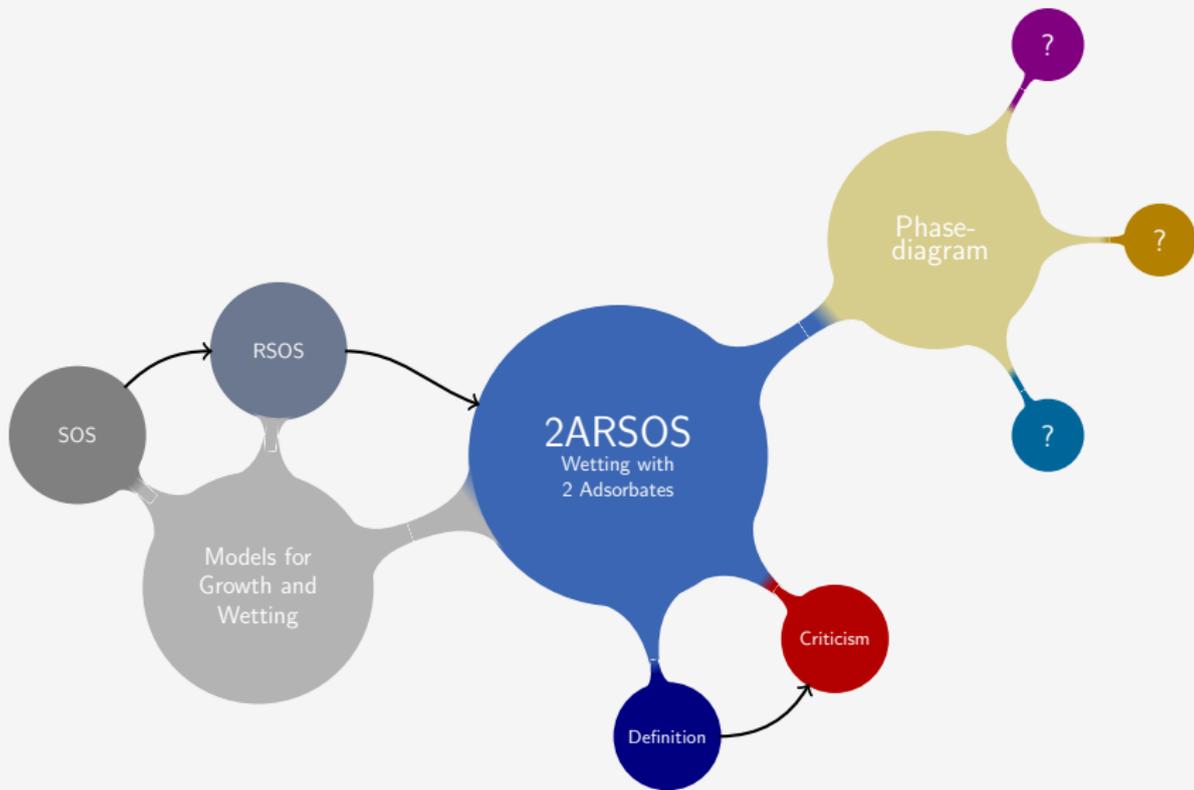
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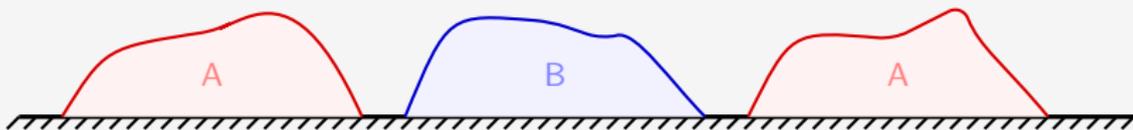


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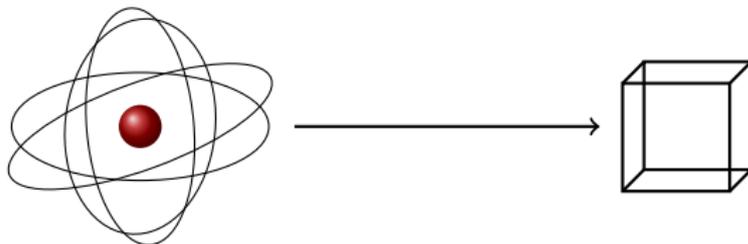
Deposition models

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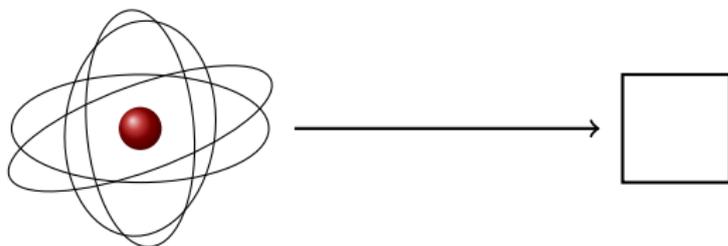
Description of Deposition processes

A rough approximation



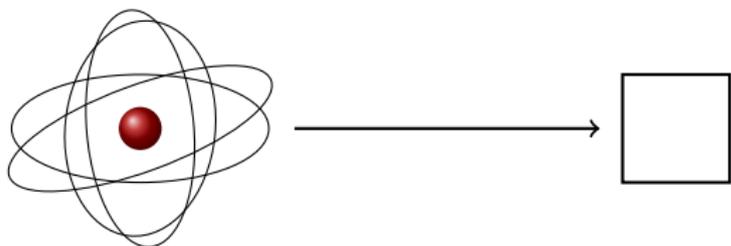
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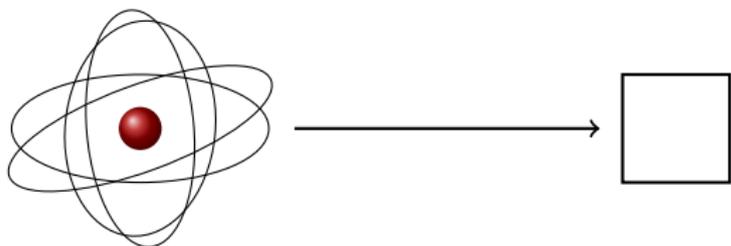


Aim:

- Make it **simple** (toy model).

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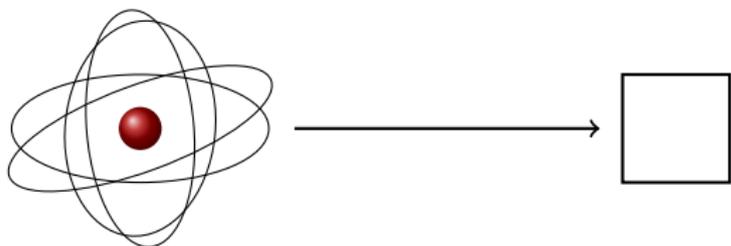


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- Study only the **dominating** effects.

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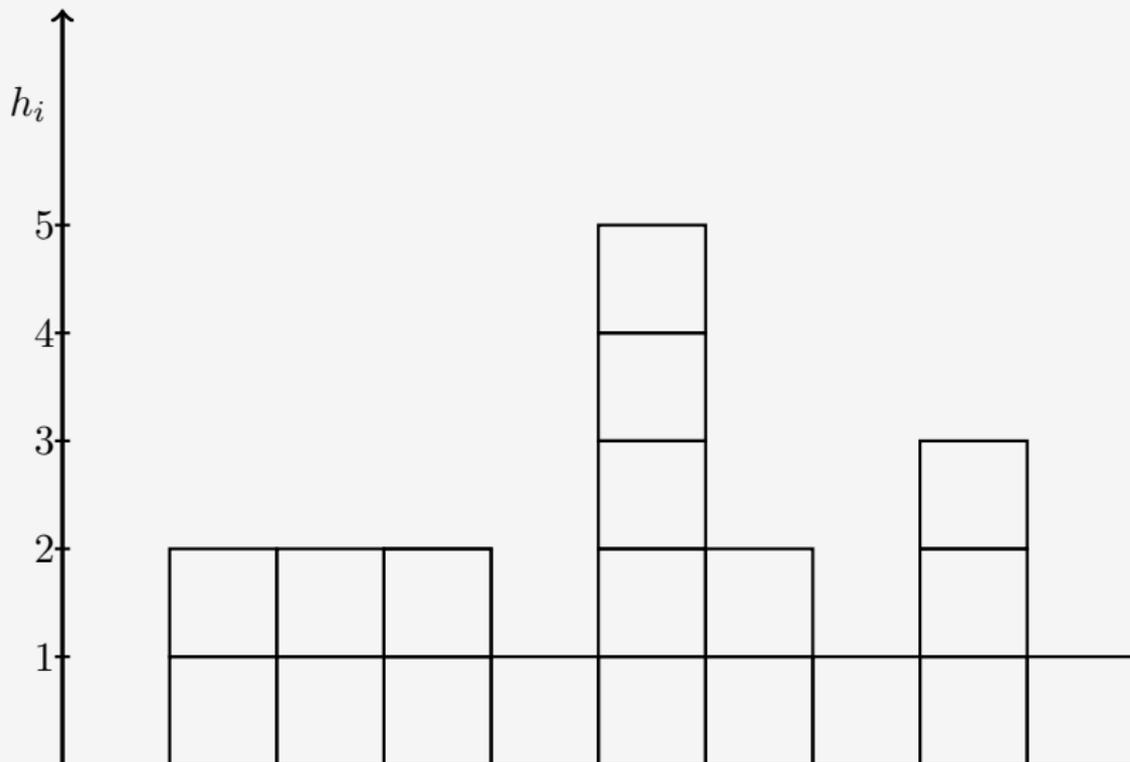
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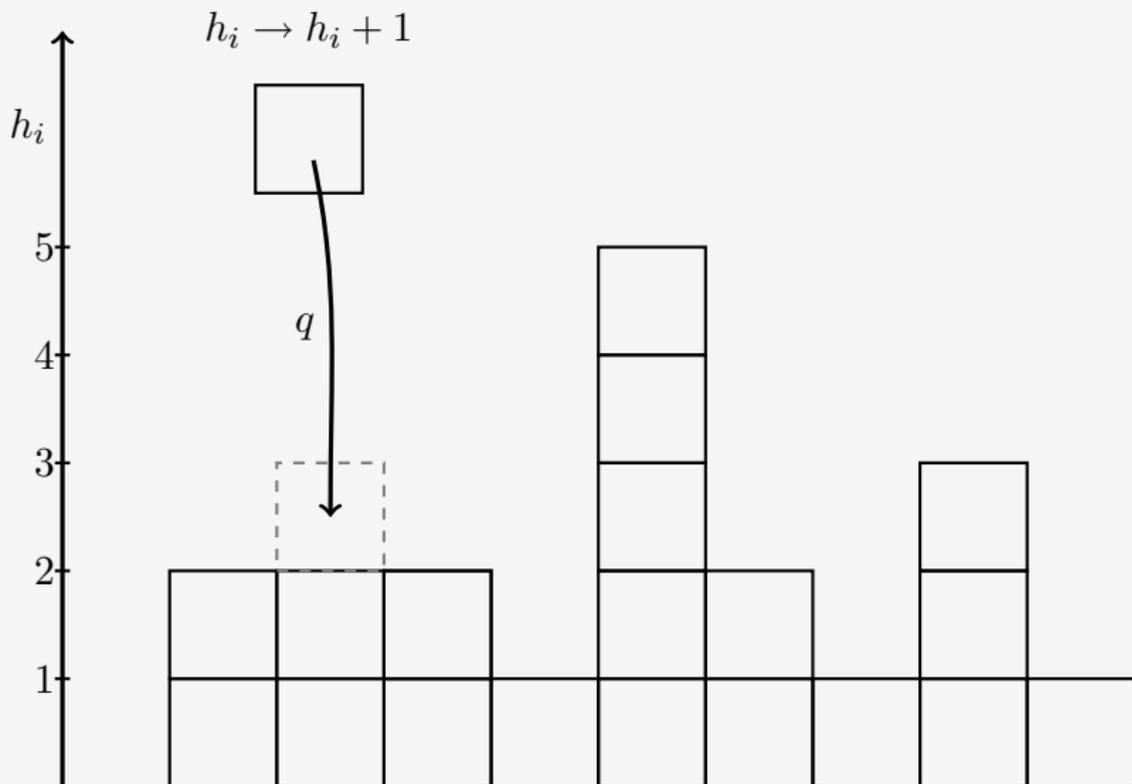
Aim:

- Make it **simple** (toy model).
- Study only the **dominating** effects.
- Gain insight in the **fundamental** properties.

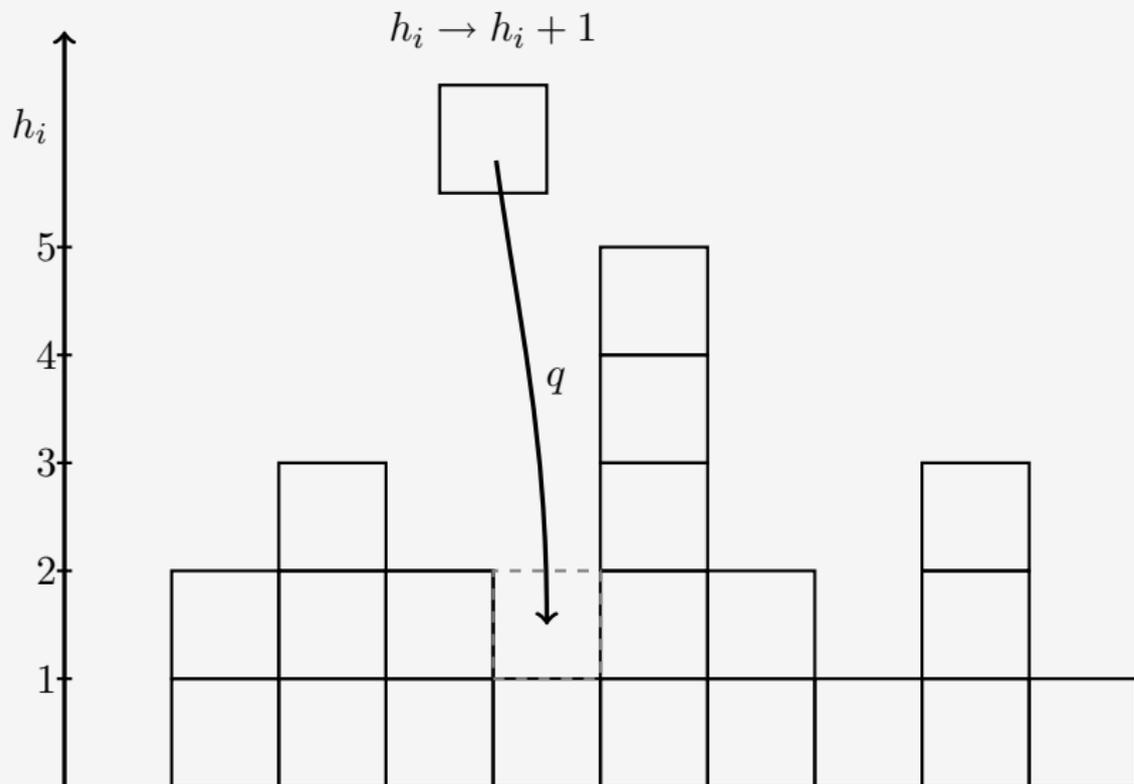
(SOS) solid-on-solid deposition



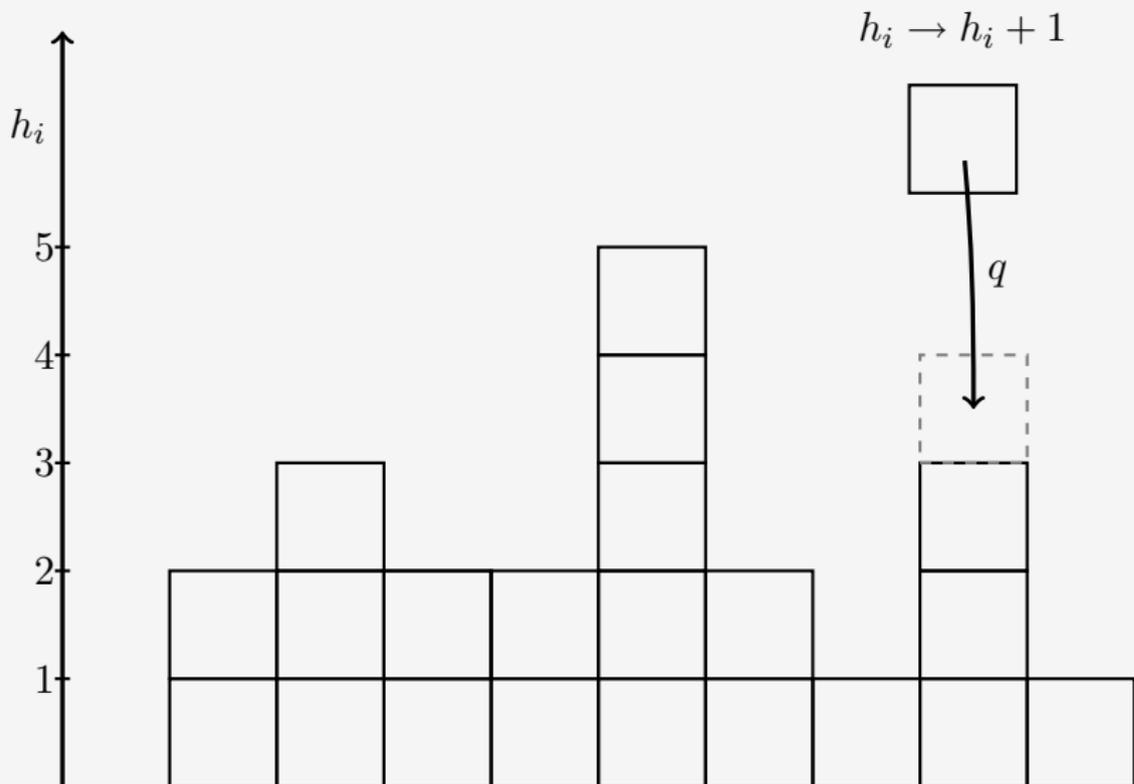
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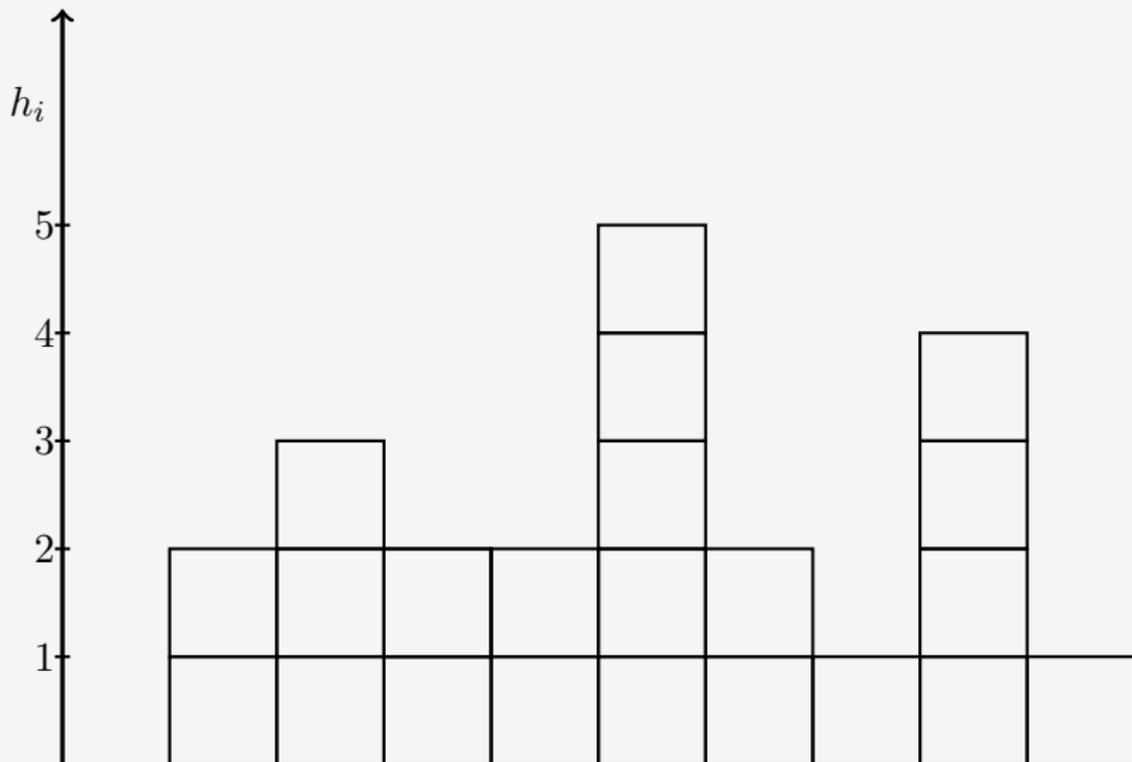
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(RSOS) restricted solid-on-solid deposition

RSOS constraint

$$|\Delta h_{\langle i,j \rangle}| = |h_i - h_j| \leq 1$$

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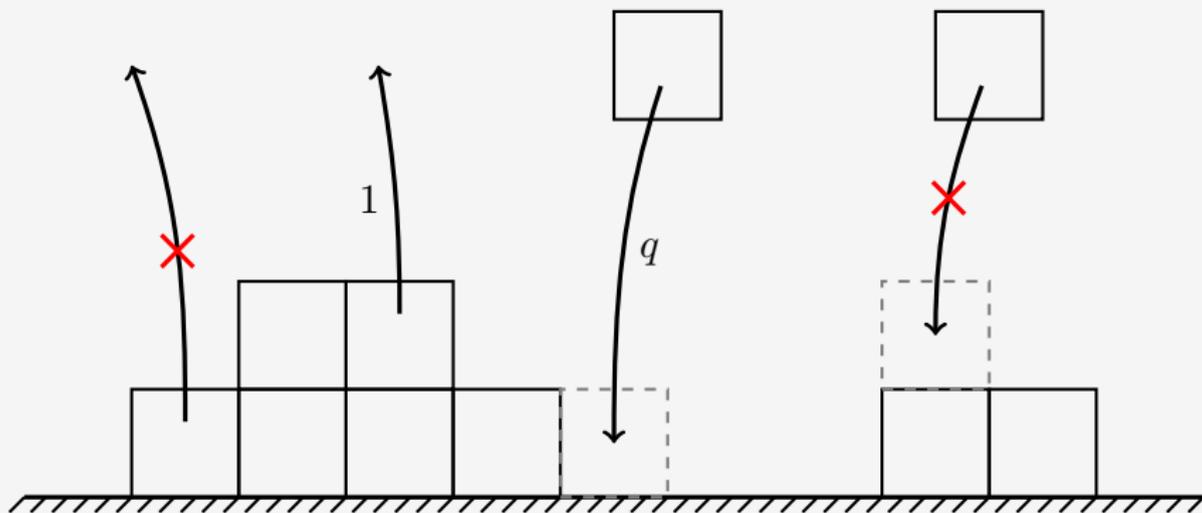


(RSOS) restricted solid-on-solid deposition

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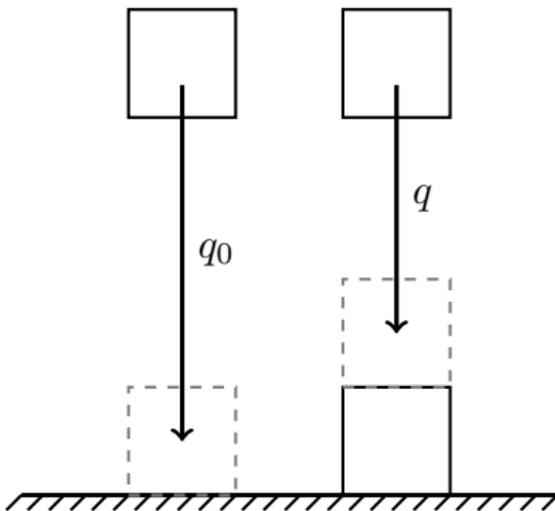
$$h_i \rightarrow h_i - 1 \quad h_i \rightarrow h_i + 1$$



Taking different binding energies into account

Different deposition rate on the substrate

$q_0 > q$ adhesive
 $q_0 < q$ repulsive



Deposition with two competing adsorbates

How to include multiple species?

Treat them equally

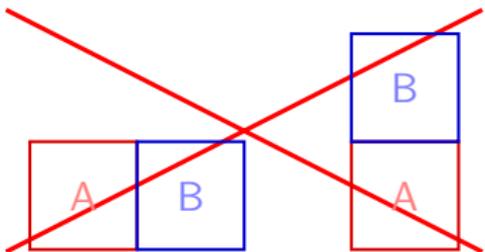


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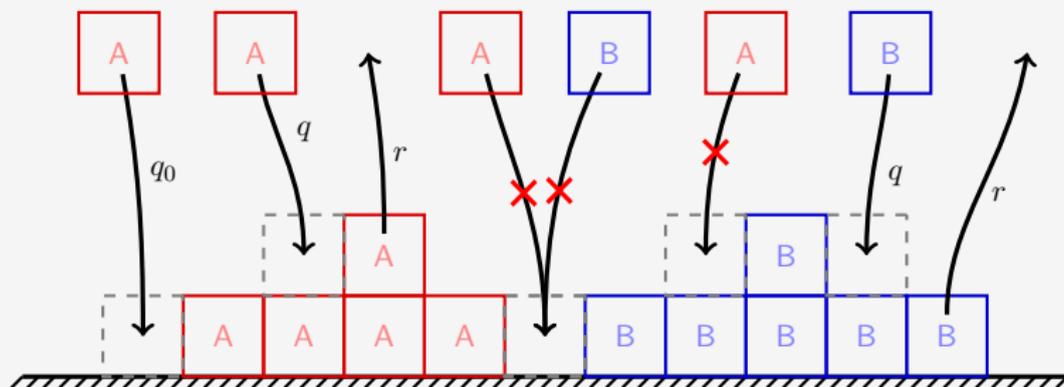
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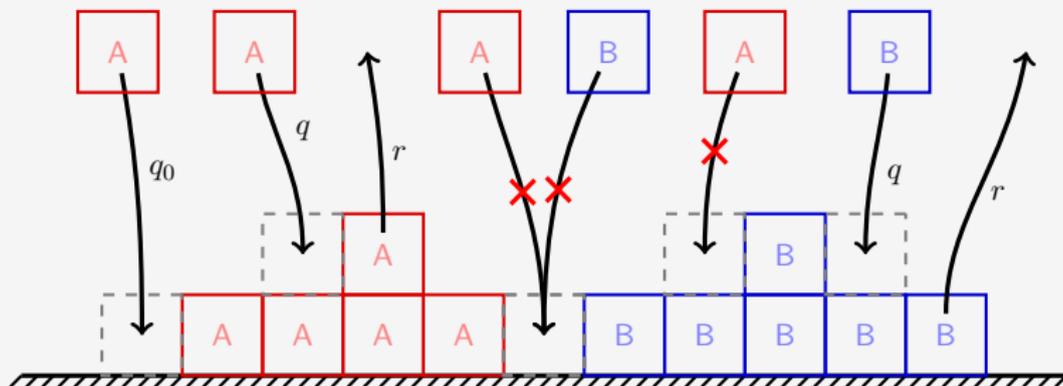
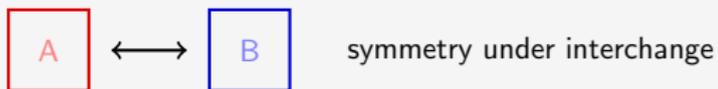
A and B may not touch



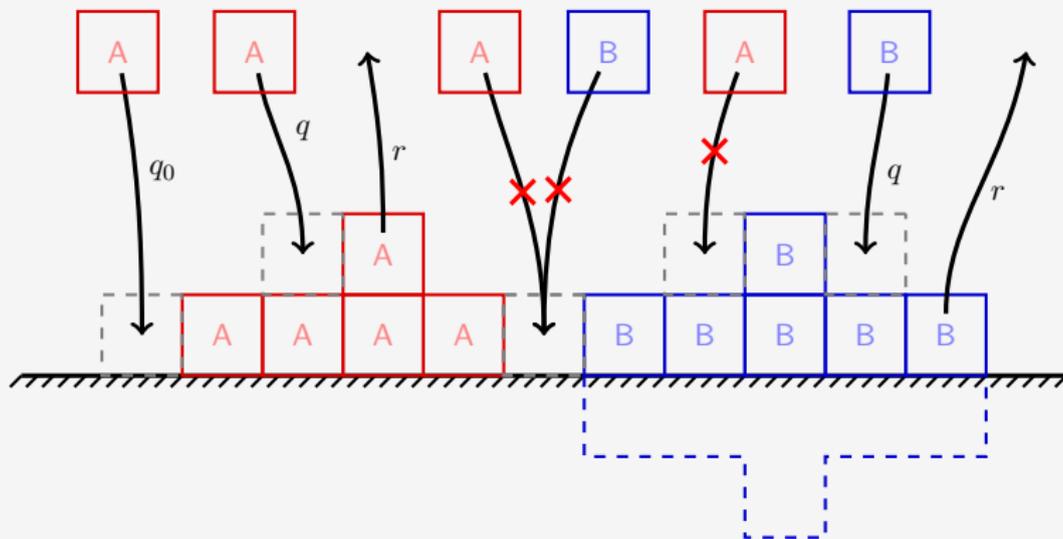
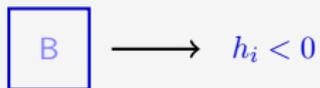
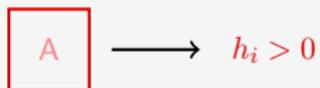
(2ARSOS) two adsorbates restricted solid-on-solid



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(2ARSOS) two adsorbates restricted solid-on-solid



Criticism

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Cons:

- Only a toy model
- $A \leftrightarrow B$ symmetry is rather unrealistic

Phase diagram

Quantities to characterize the state of the model

Occupation balance

$$b = \frac{1}{N} \sum_{i=1}^N h_i$$

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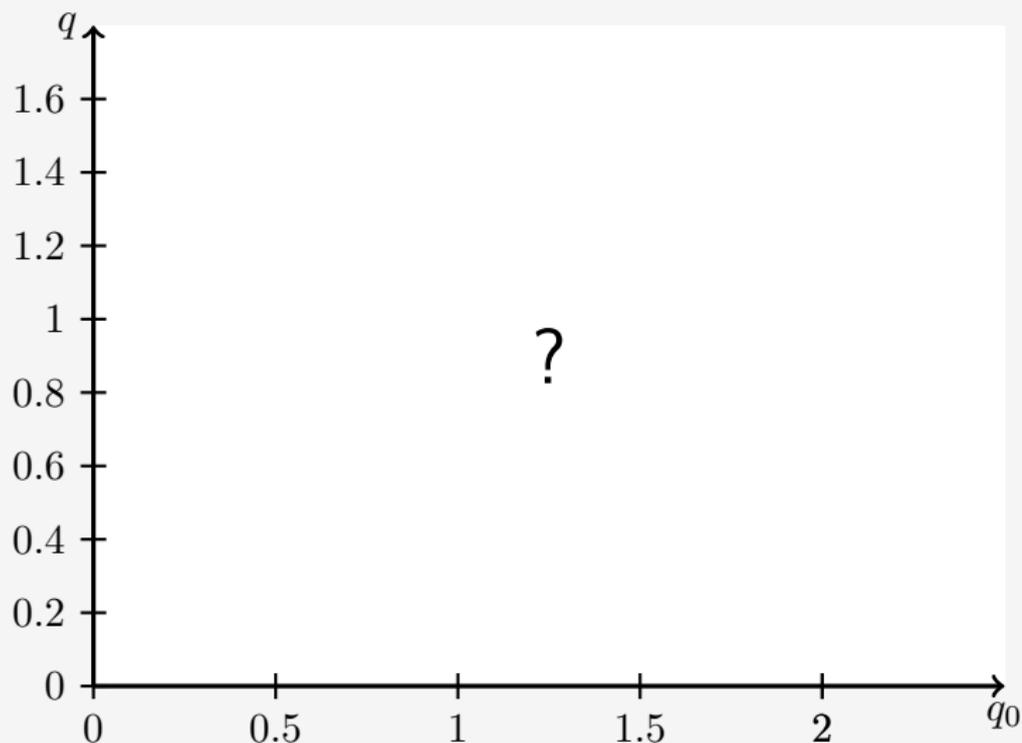
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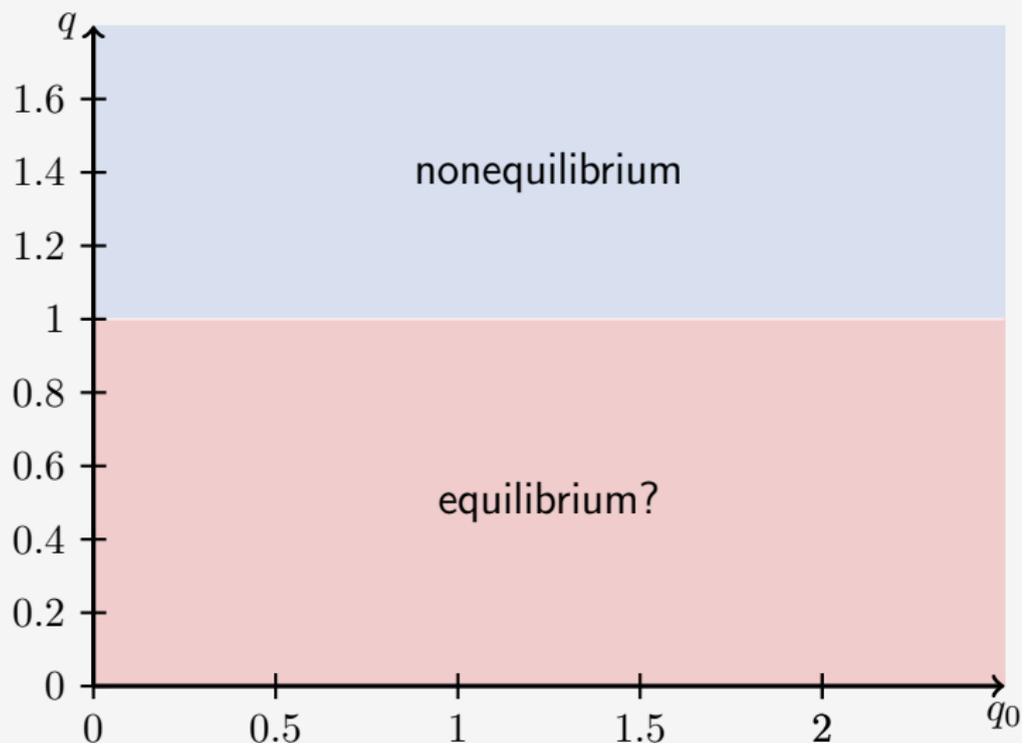
Density of unoccupied sites

$$\rho^{(0)} = \frac{1}{N} |\{h_i | h_i = 0\}| = \frac{1}{N} \sum_{i=1}^N \delta_{h_i,0} = \frac{N^{(0)}}{N}$$

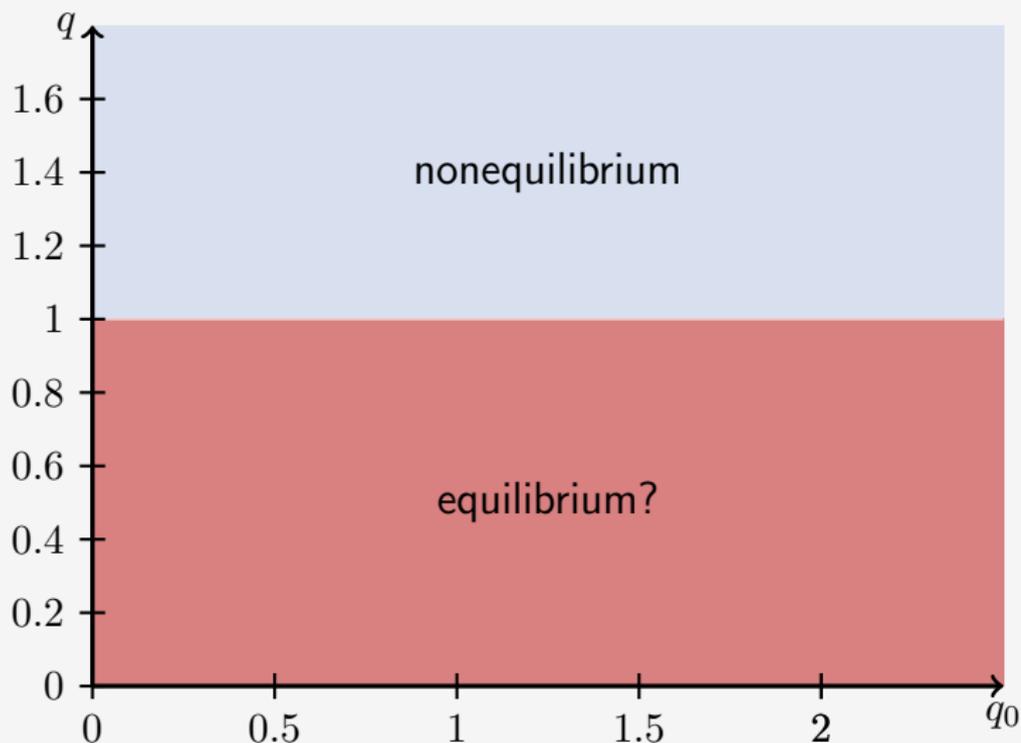
Phase diagram



Phase diagram



Phase diagram



The stationary probability distribution

$$P(\{h_i\}_{i=1}^N) = \frac{1}{Z_N} \exp\left[-\sum_{i=1}^N V(h_i)\right]$$
$$V(h) = \begin{cases} -\ln(q/q_0) & h = 0 \\ -|h| \ln(q) & h \neq 0 \end{cases}$$

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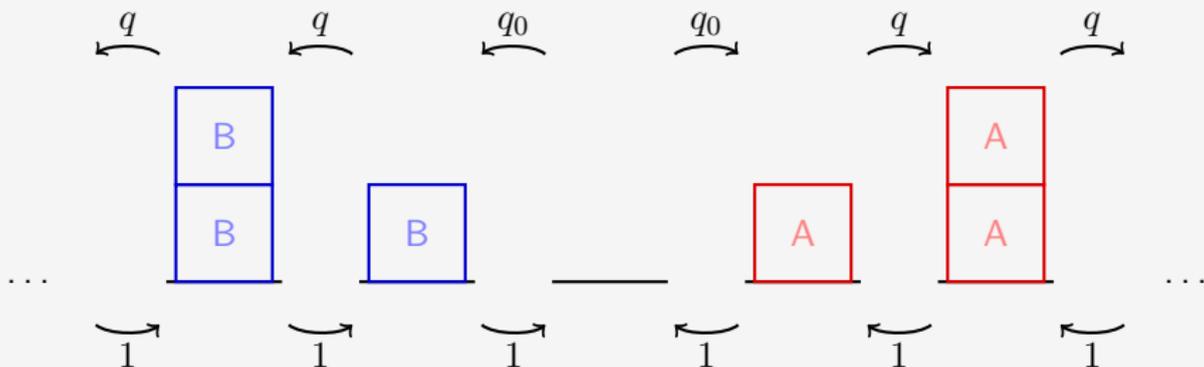
Check without the RSOS constraint

N site system $\longleftrightarrow N$ one site systems

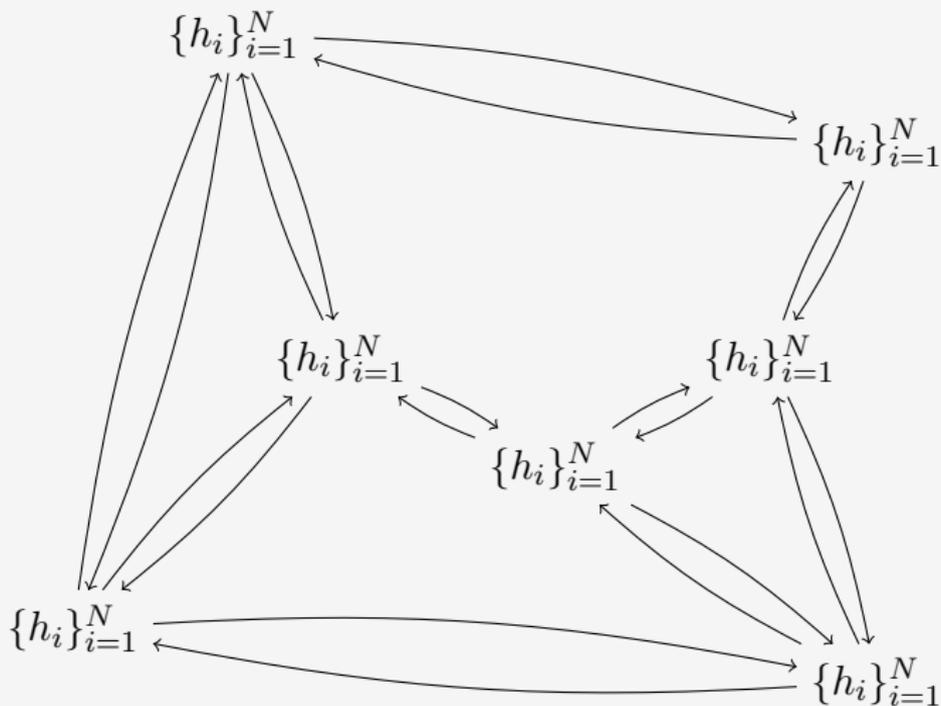
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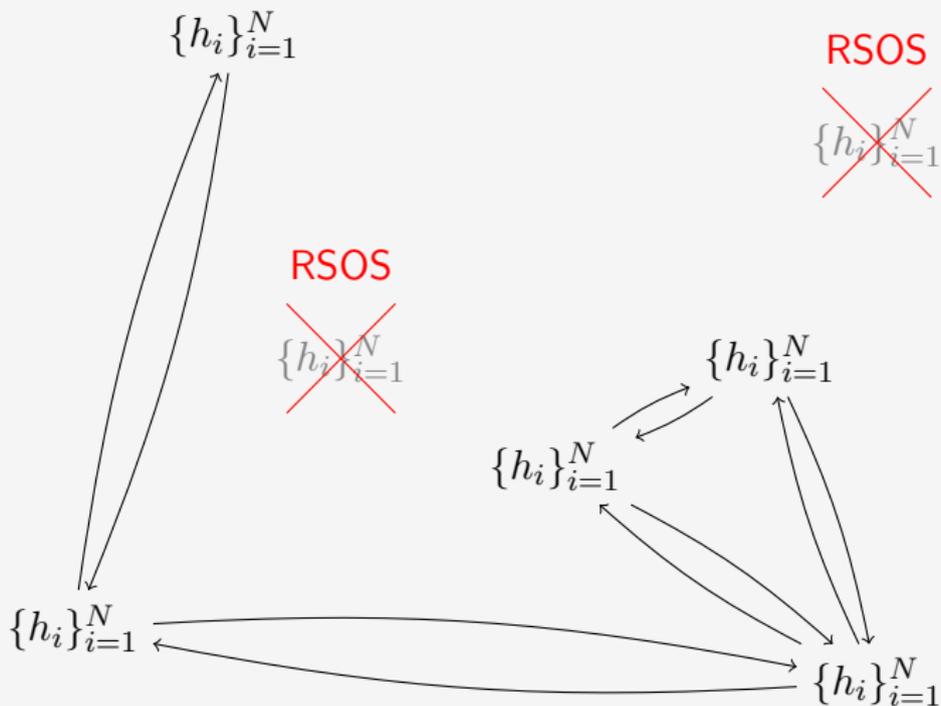
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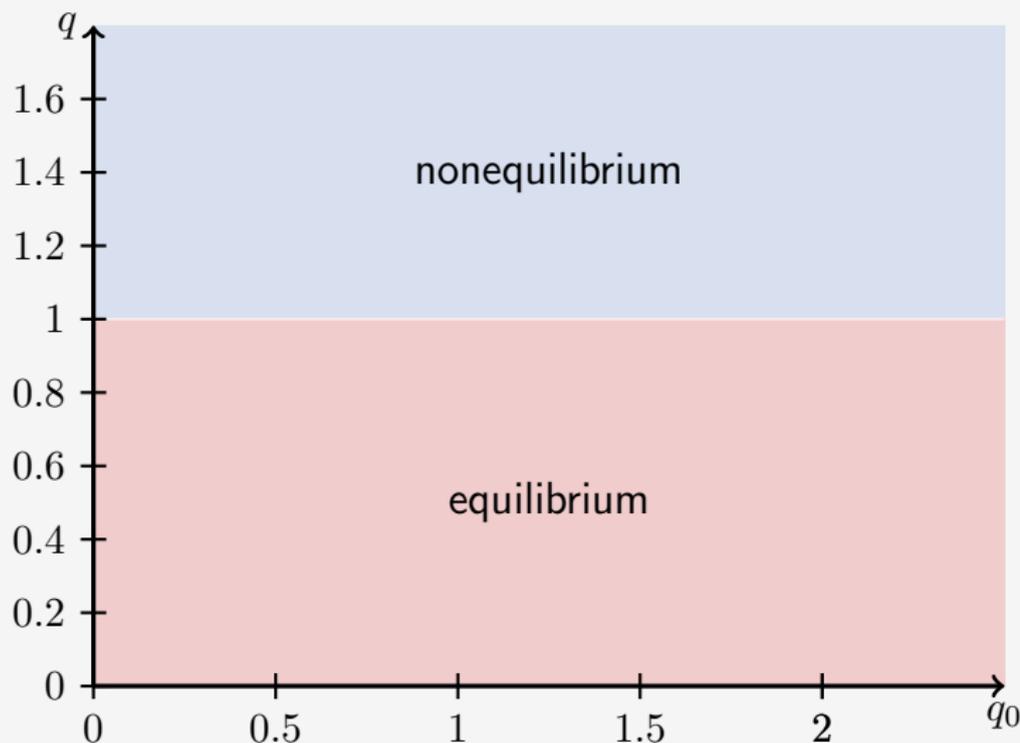
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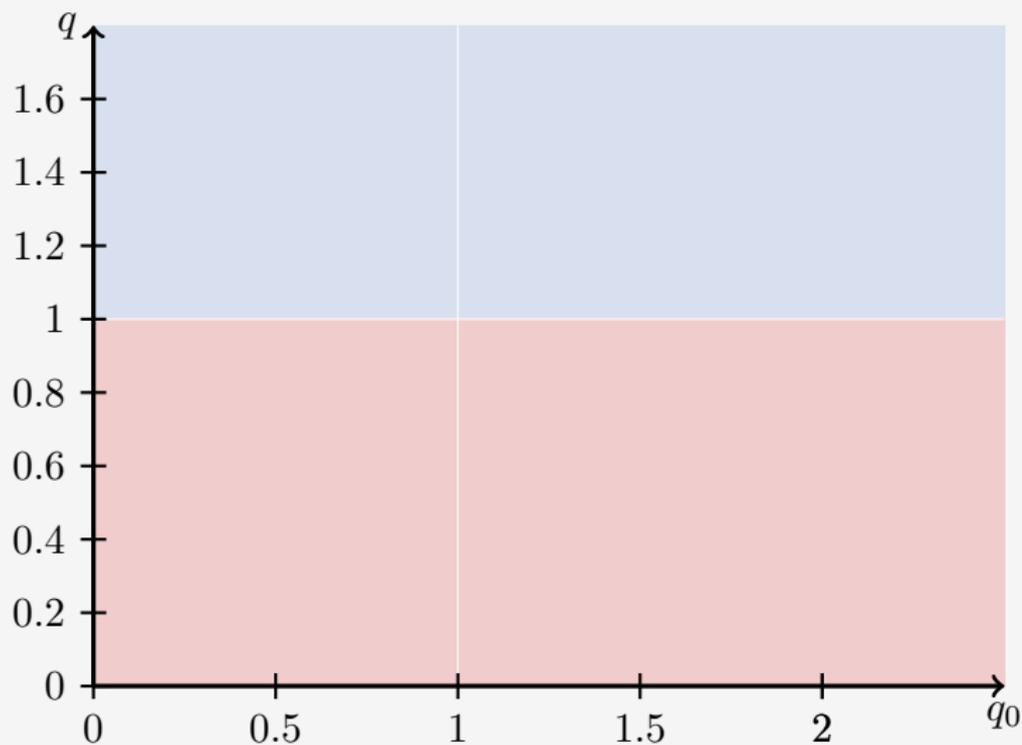
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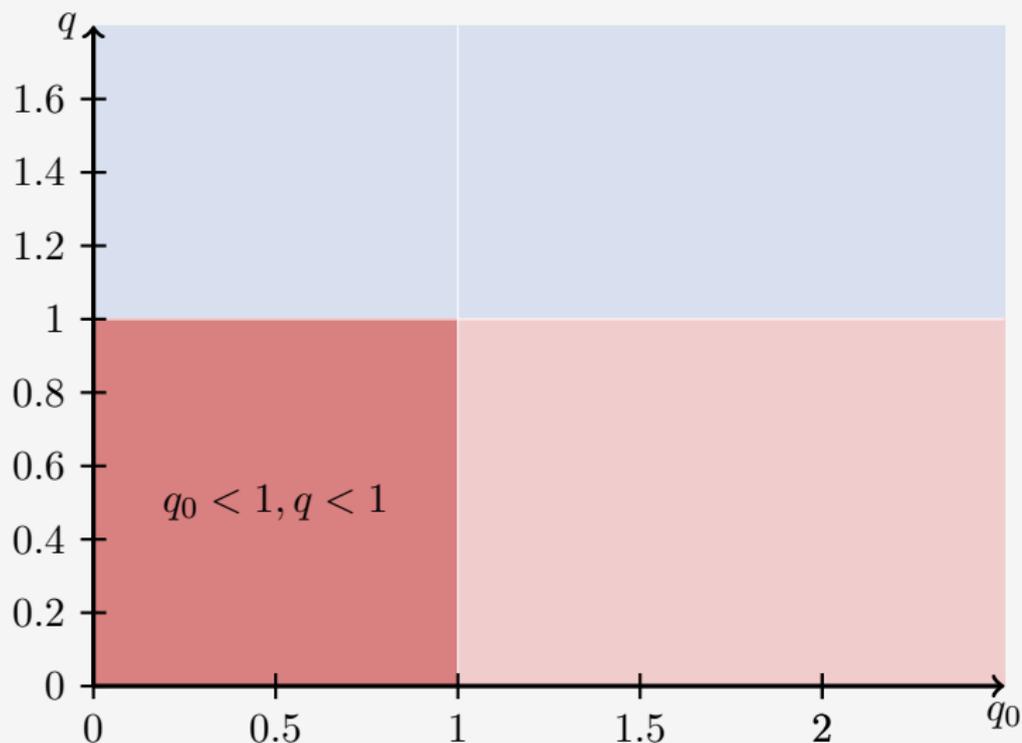
Phase diagram



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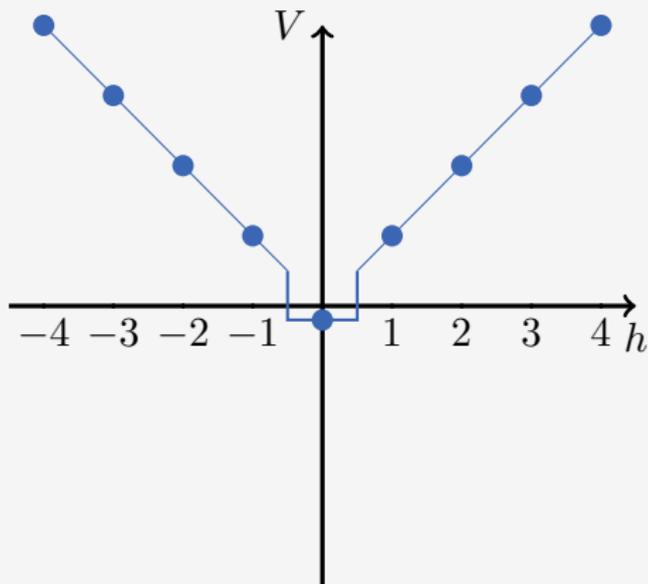


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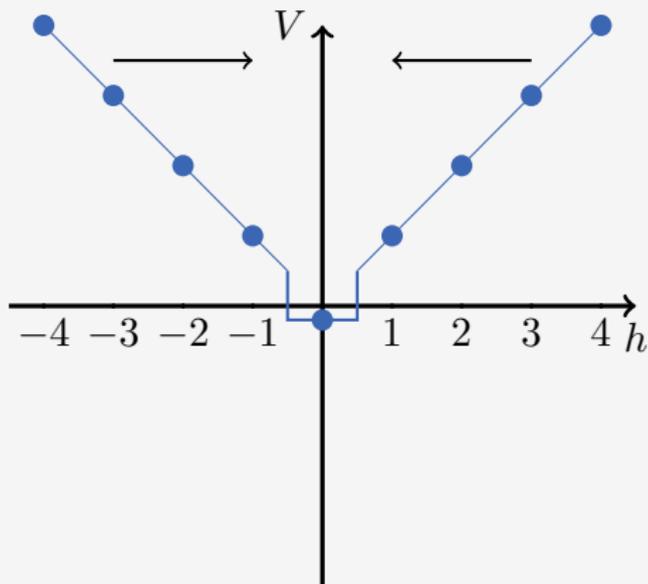
Unordered Phase

$$V(h) = \begin{cases} -\ln(q/q_0) & h = 0 \\ -|h| \ln(q) & h \neq 0 \end{cases}.$$

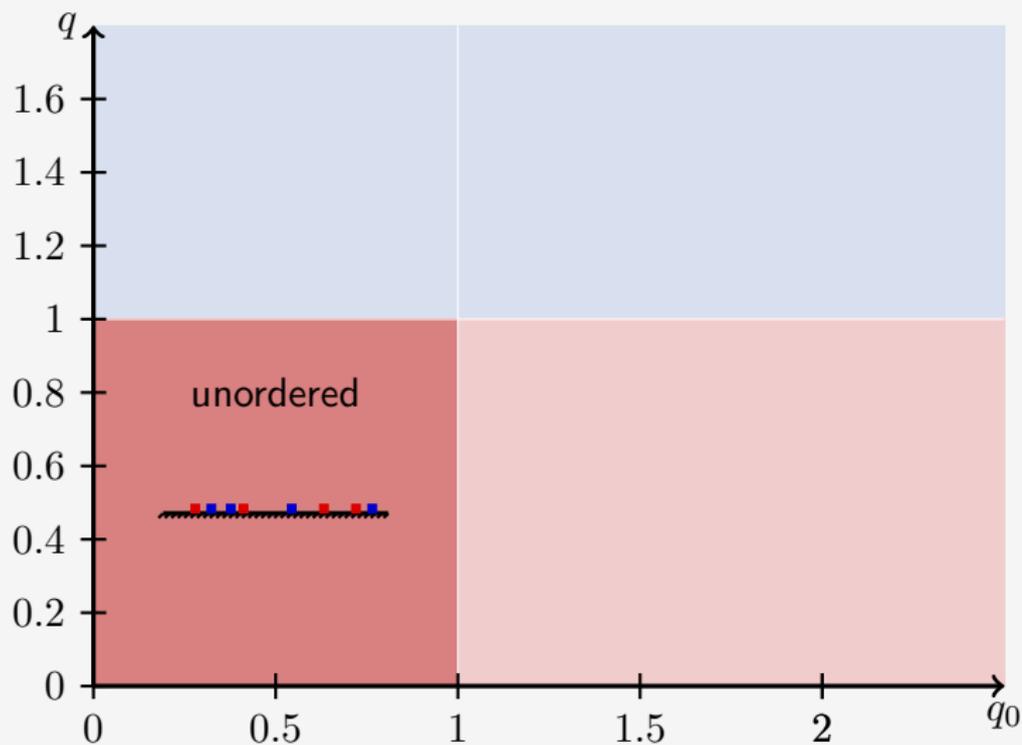


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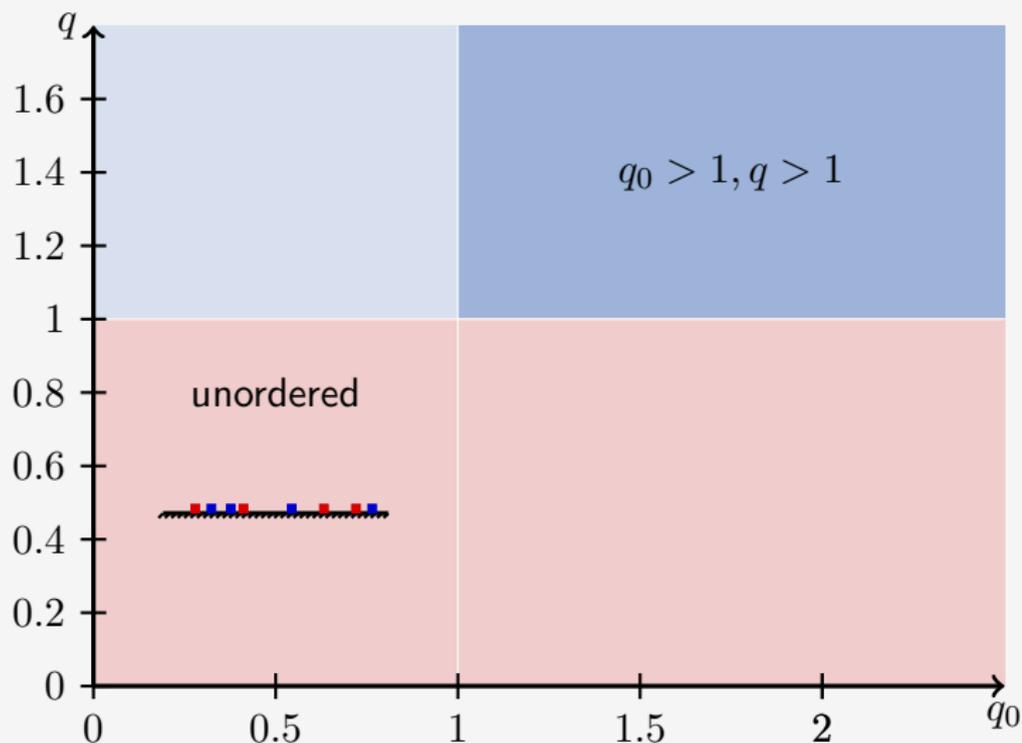
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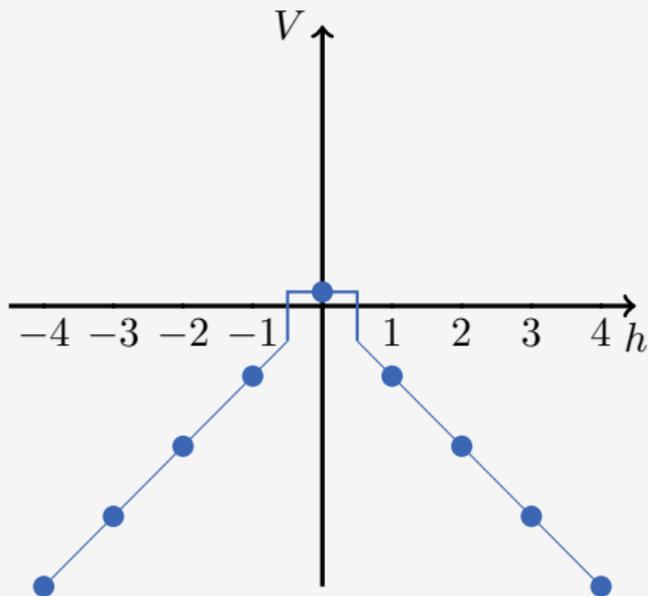


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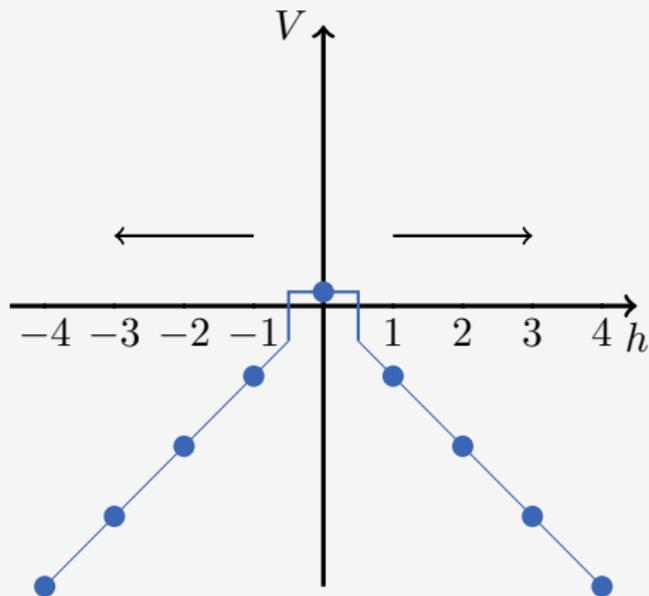
Competing growth

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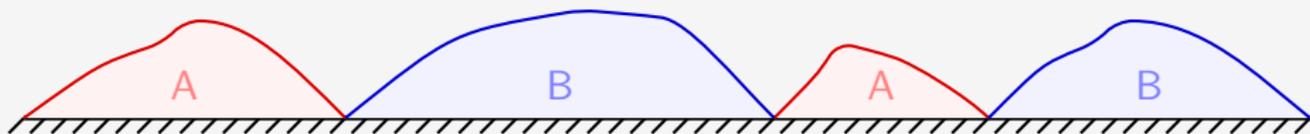


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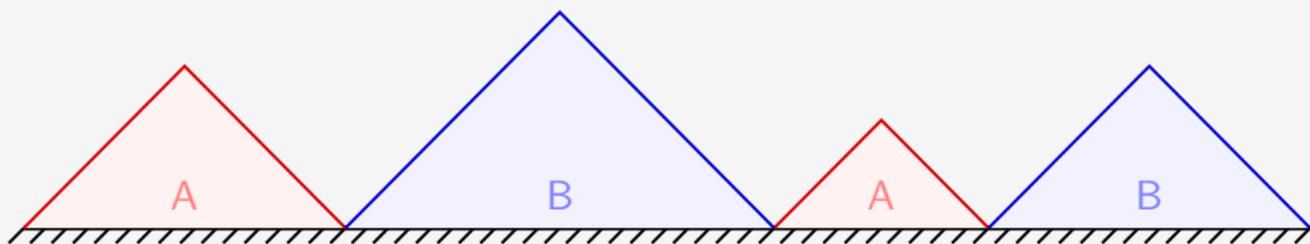
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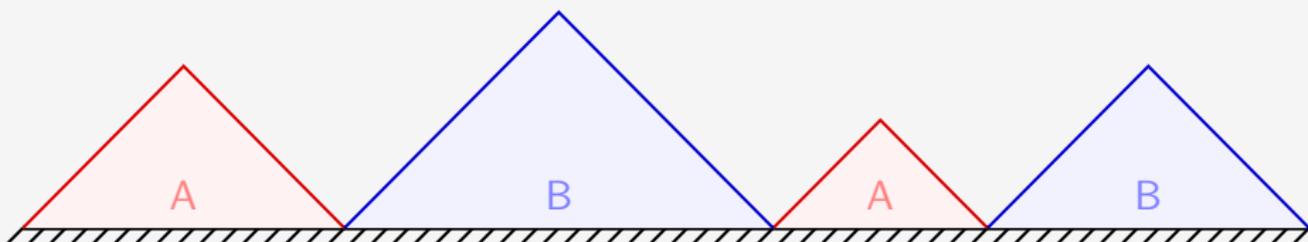


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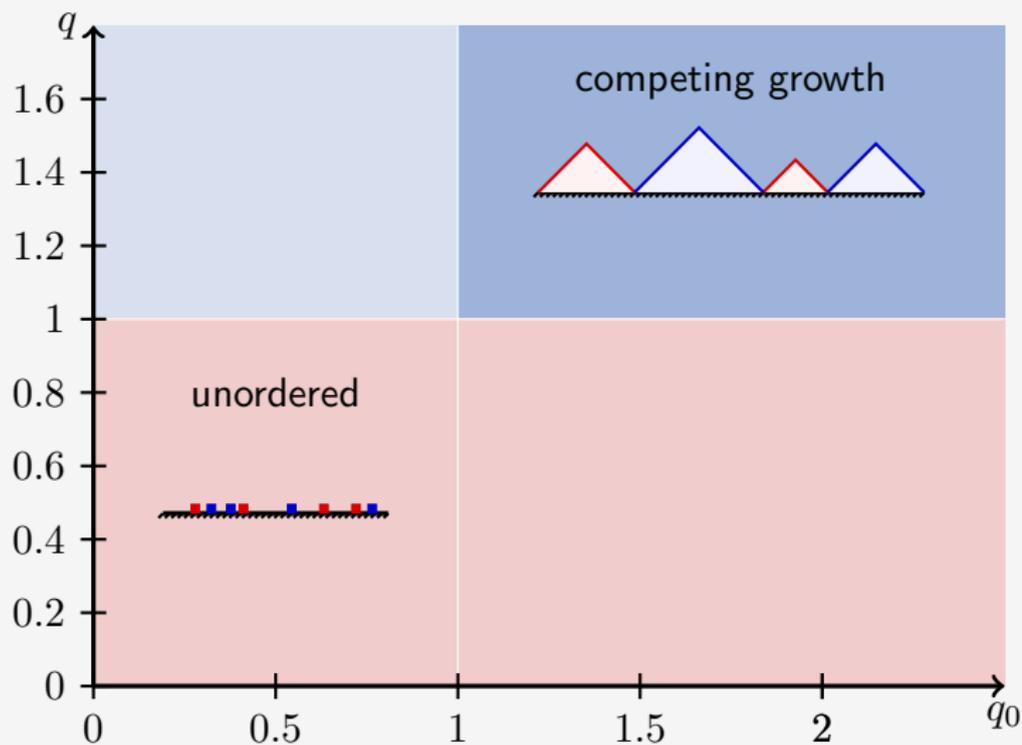


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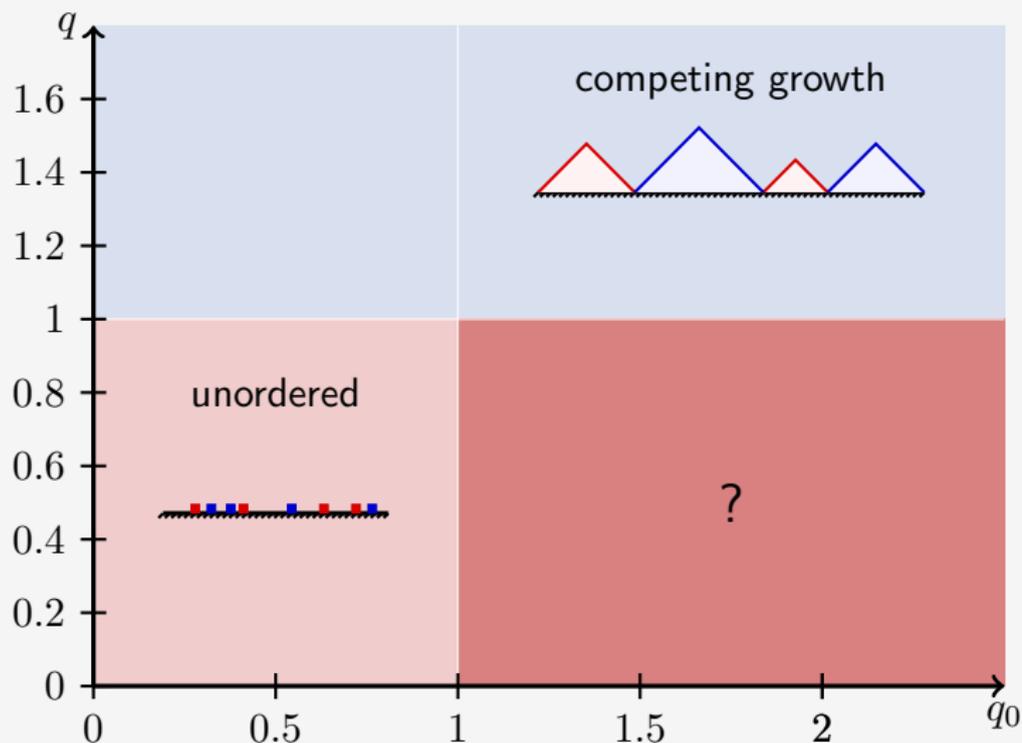
- RSOS constraint prevents real growth
- Island borders become immobilized
- Displacement time: $T_d \sim e^{\alpha N}$



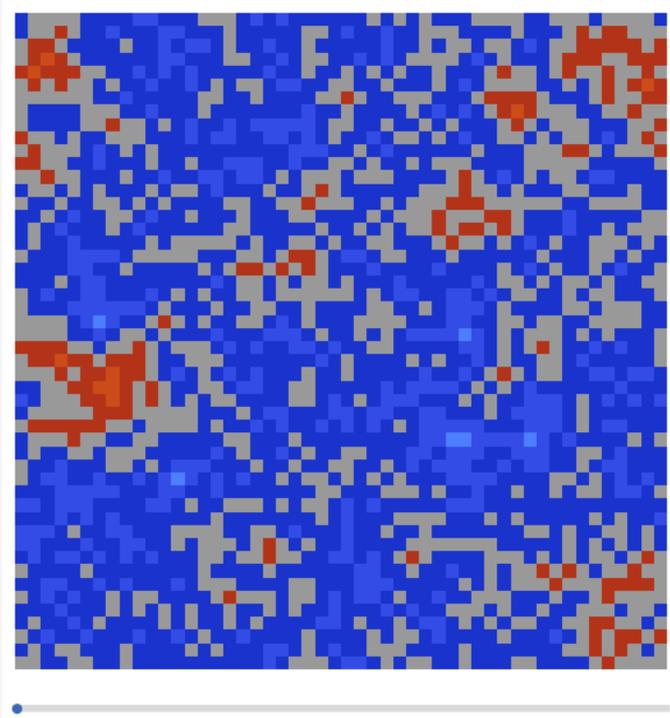
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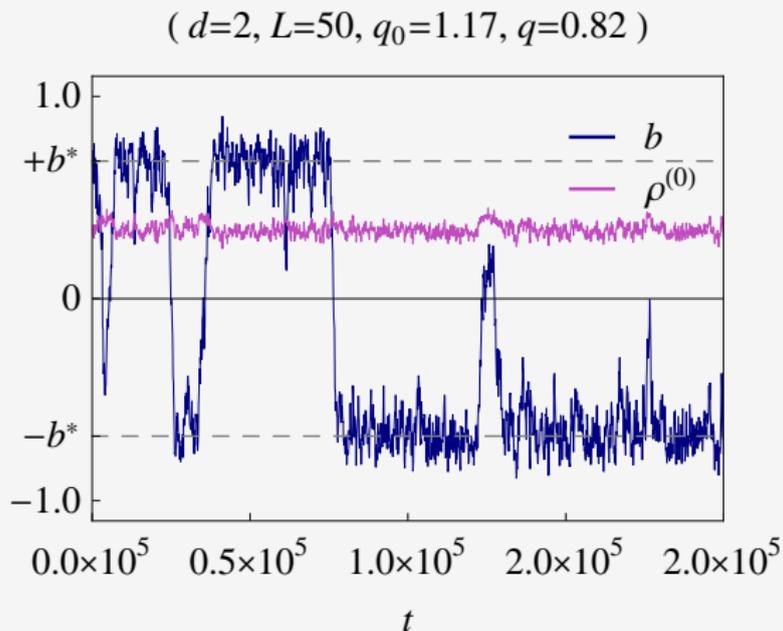
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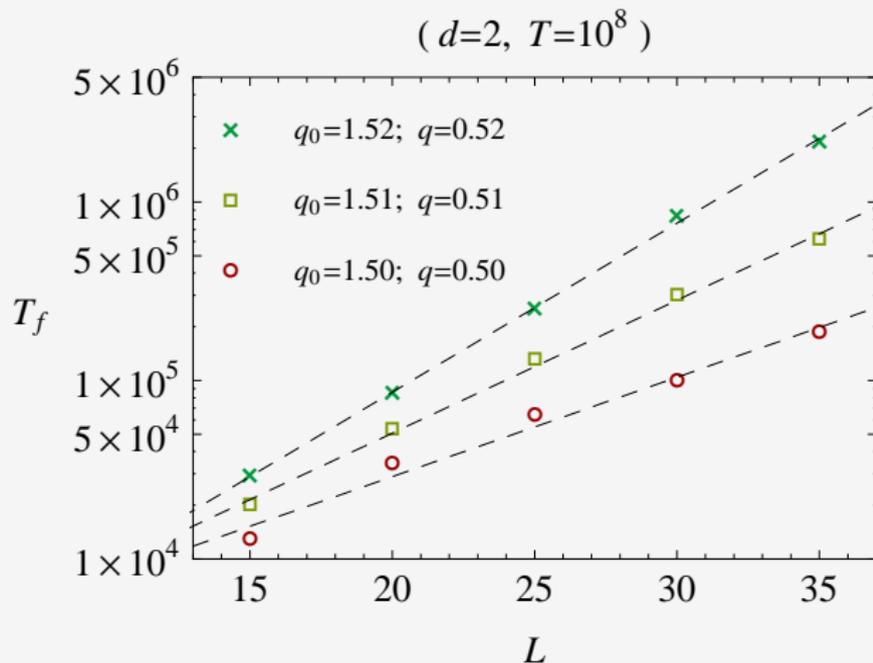
Adhesive case in 2+1-dimensions



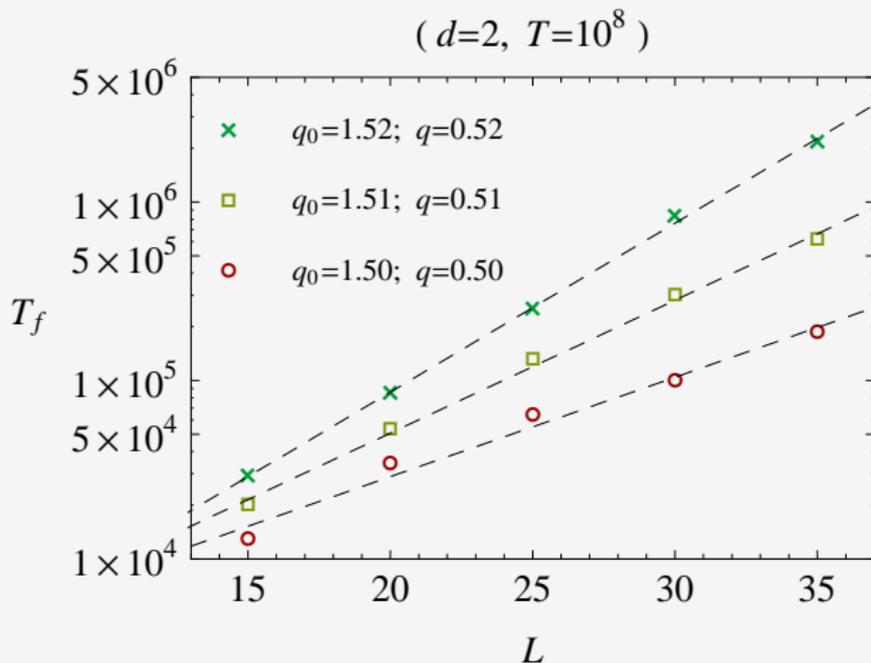
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Scaling of the flipping time

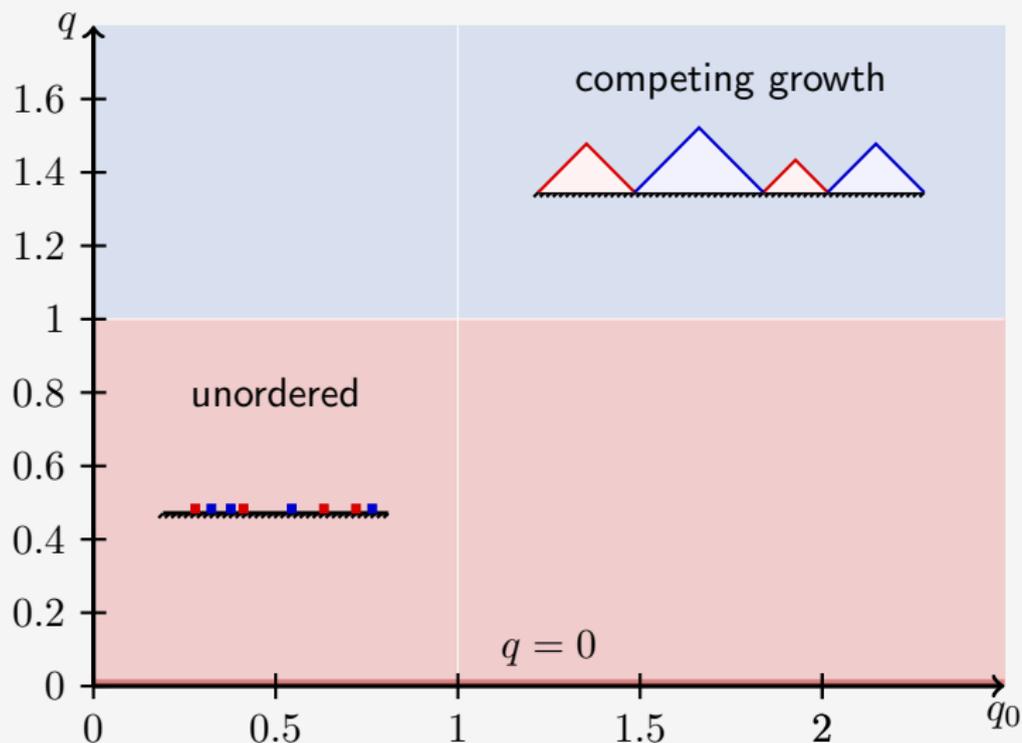


Scaling of the flipping time



$\Rightarrow A \leftrightarrow B$ symmetry is spontaneously broken

Phase diagram



The case $q = 0$

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$$P(\{h_i\}_{i=1}^N) = \frac{1}{Z_N} q_0^{(\sum_{i=1}^N |h_i|)} = \frac{1}{Z_N} q_0^{N^{(+)} + N^{(-)}}$$

The case $q = 0$

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$$m(N^{(+)}, N^{(-)})$$

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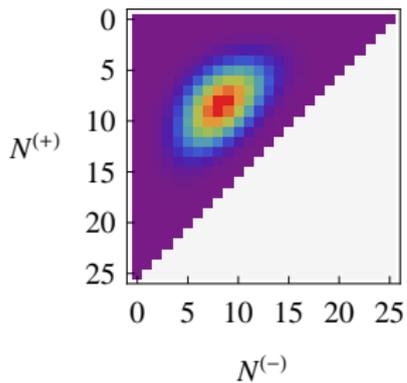
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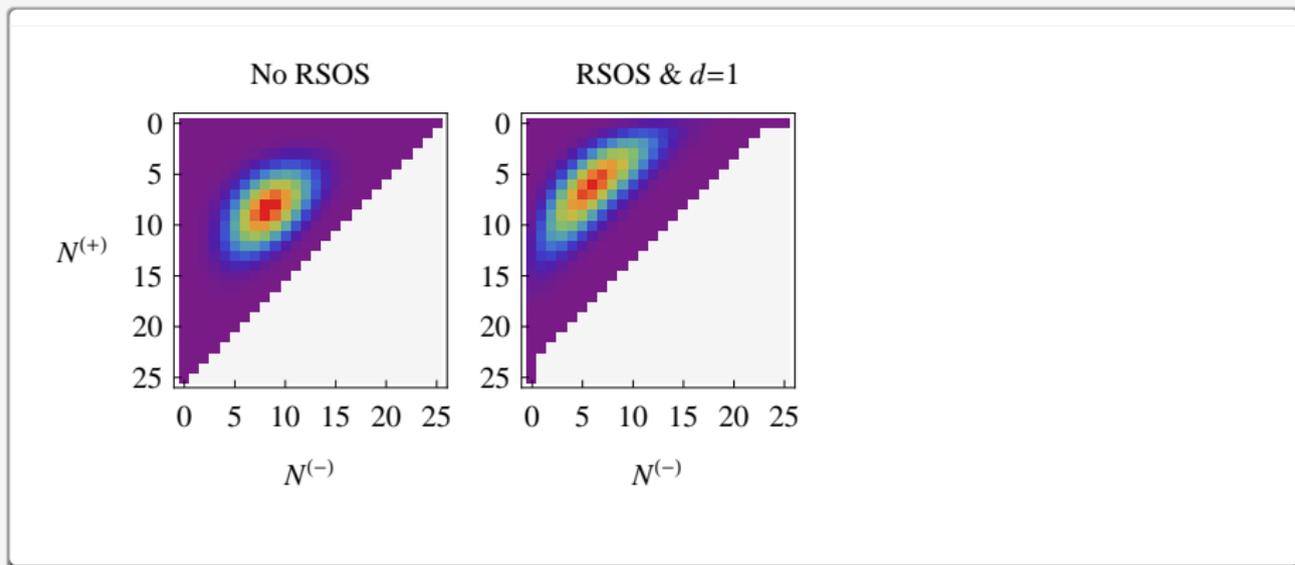
with RSOS: → computer

Multiplicities

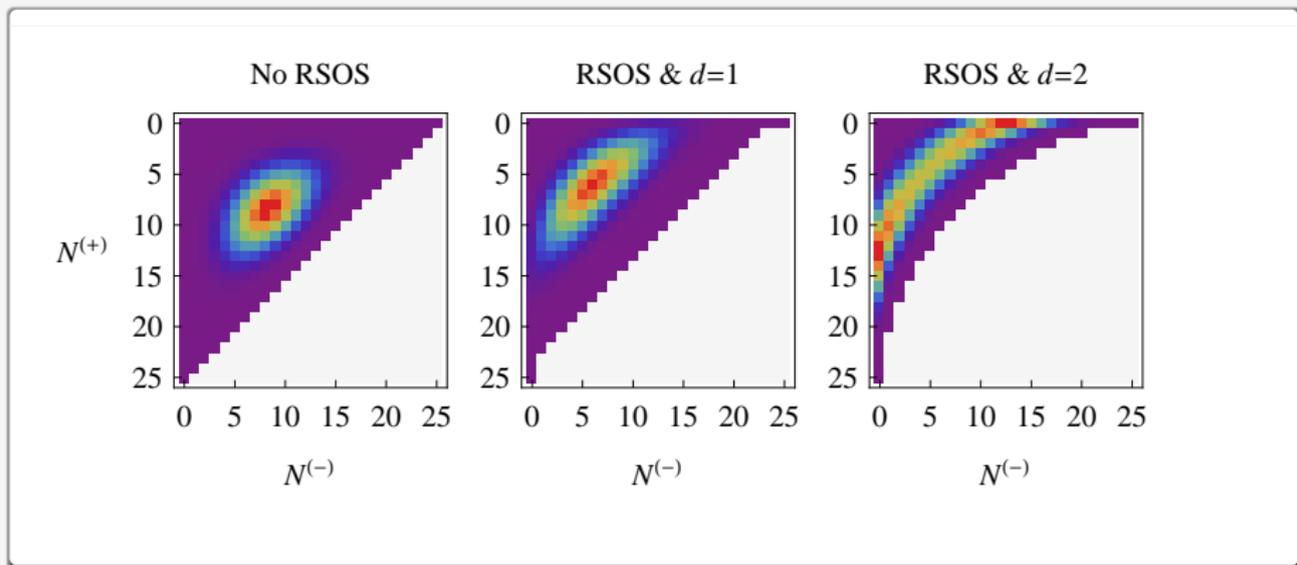
No RSOS



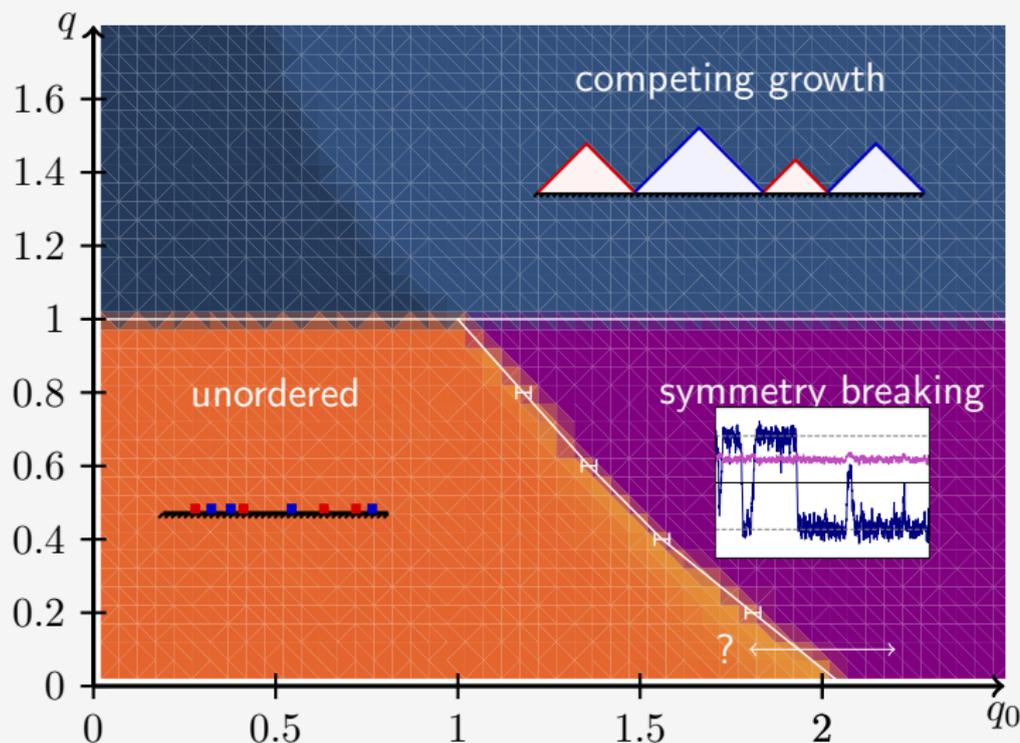
Multiplicities



Multiplicities



Phase diagram in 2+1-dimensions



■ Kinetic Ising at $q = 0$:

scaling law	2ARSOS	Ising
$\langle b \rangle \sim (q_0 - q_0^c(q))^\beta$	$\beta = 0.125(5)$	$1/8$
$b_t \sim t^{-\delta}$	$\delta = 0.06(2)$	0.058
$\rho_t^{(0)} \sim t^{-\alpha}$	$\alpha = 0.45(10)$	$1/2$

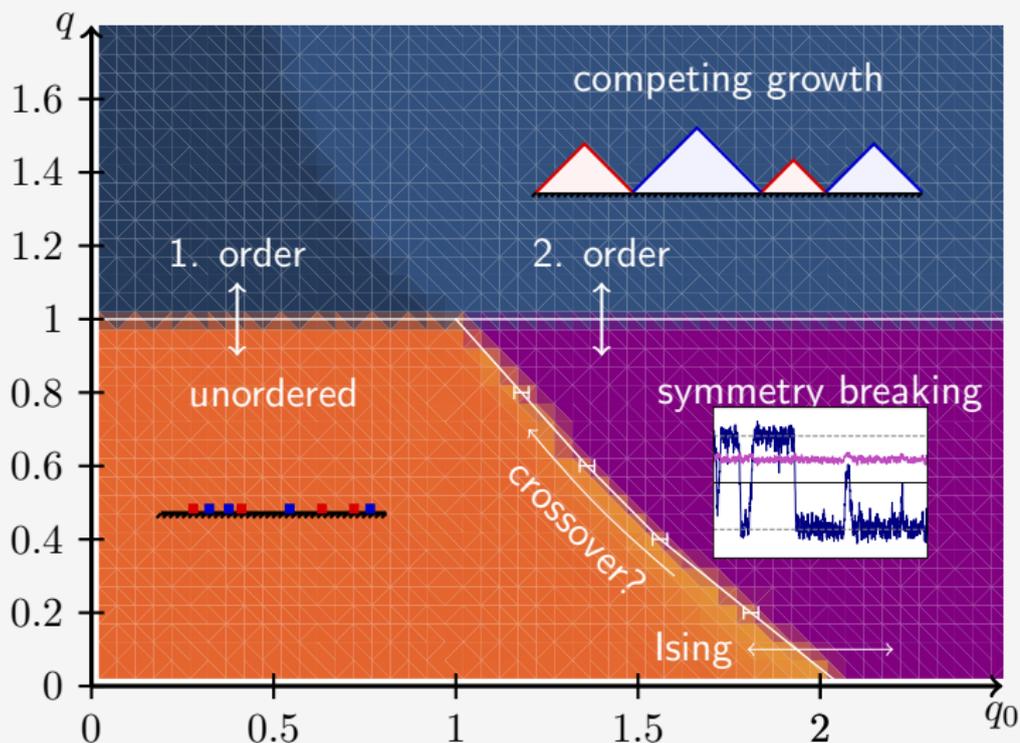
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■ Crossover for $q > 0$?

q	0	0.2	0.4	0.6	0.8	1
β	0.125(5)	0.14(1)	0.16(2)	0.19(3)	0.21(3)	-

The phase diagram in 2+1-dimensions



Thank you for your attention!

Literatur



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arXiv: 0809.2542v2, 2009.



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Model for nonequilibrium wetting transitions in two dimensions.

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H. Hinrichsen, R. Livi, D. Mukamel, and A. Politi.

Wetting under nonequilibrium conditions.

Phys. Rev. E, 68(4):041606, Oct 2003.

→ beamer slides: <http://www.cgogolin.de>

Simulation with random sequential updates

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	$h_i = 0$	$h_i > 0$	$h_i < 0$
Evaporate: $h_i \rightarrow h_i - \text{sgn}(h_i)$		r/n	r/n
Deposit A: $h_i \rightarrow h_i + 1$	q_0/n	q/n	
Deposit B: $h_i \rightarrow h_i - 1$	q_0/n		q/n

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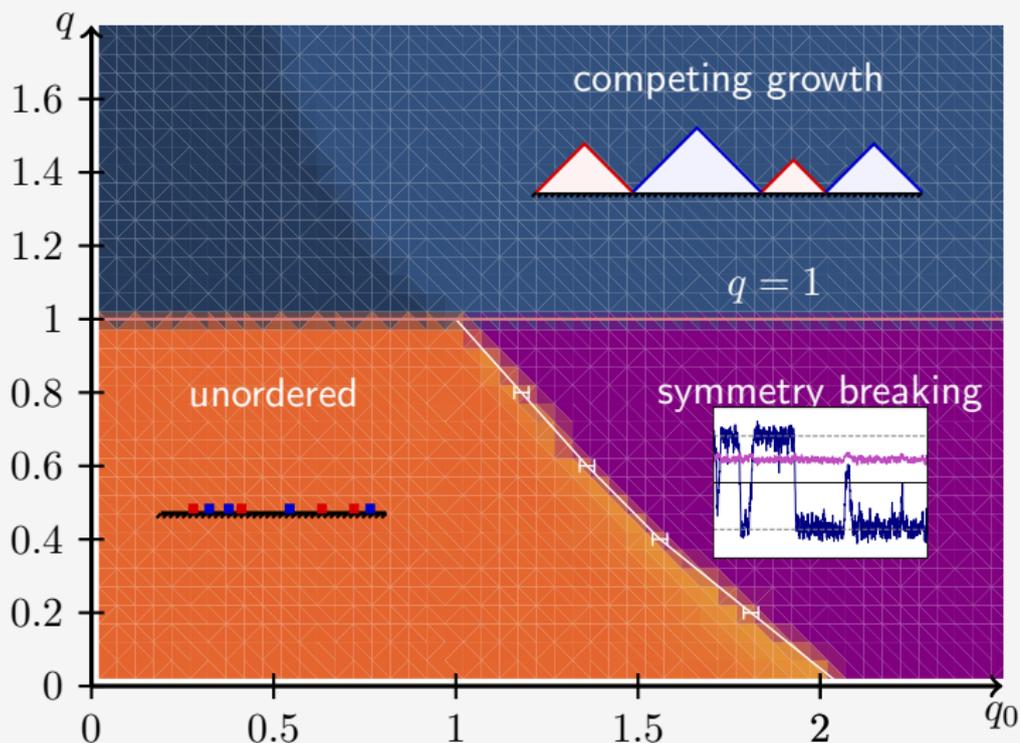
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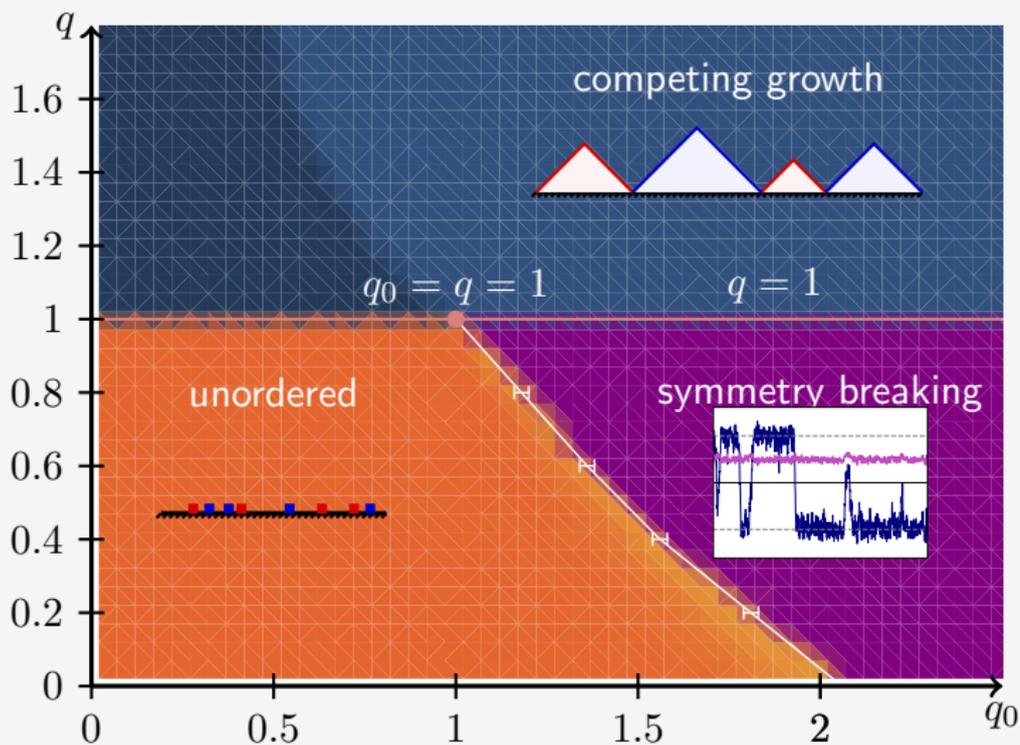
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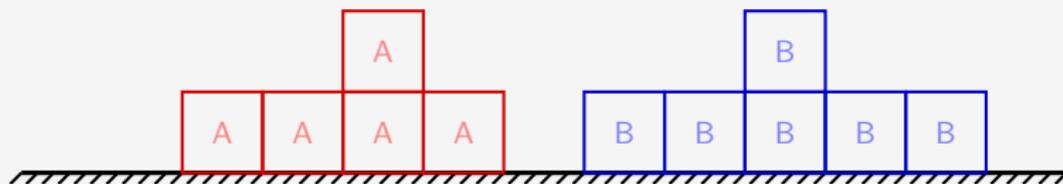
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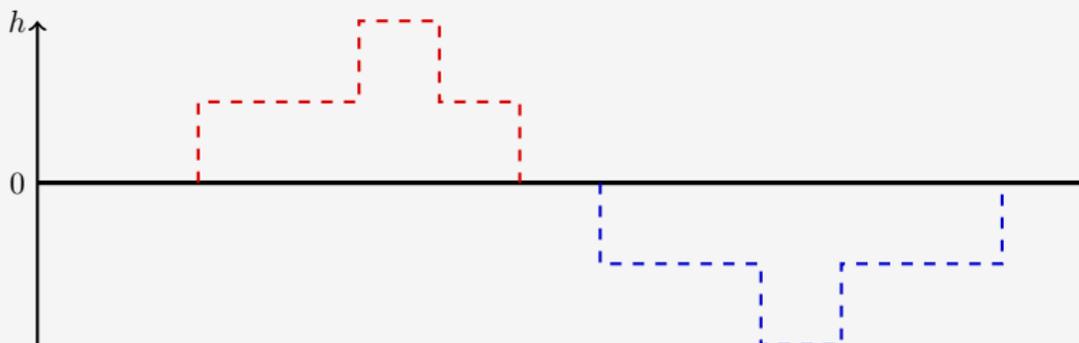
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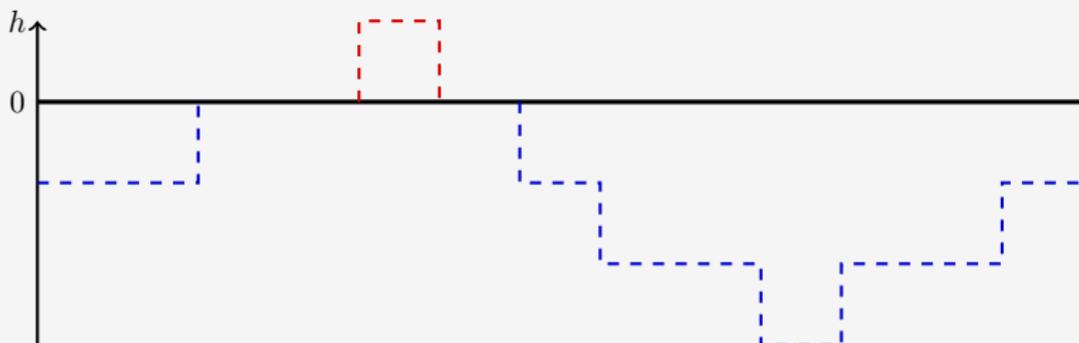
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The case $q = 1$ 

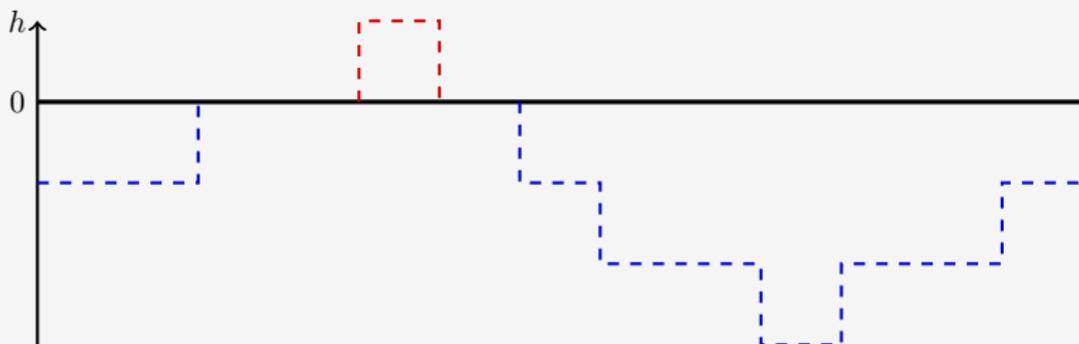
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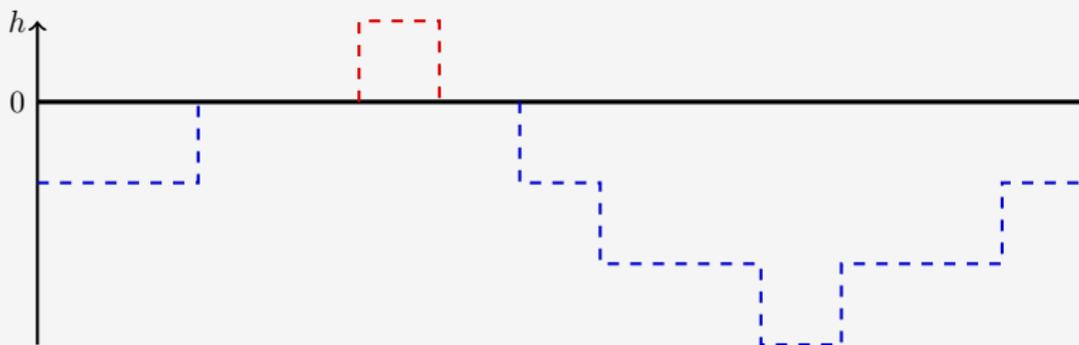
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- Discrimination of A and B becomes arbitrary

The case $q_0 = q = 1$ 

- Discrimination of A and B becomes arbitrary
- Surface fluctuates freely
- b does a random walk $\langle |b_t| \rangle \sim t^{-0.500(5)}$ $\langle \rho^{(0)} \rangle \sim t^{-0.50(1)}$

The phase boundary

The Binder cumulant as order Parameter:

$$U = 1 - \frac{1}{3} \frac{\langle b^4 \rangle}{\langle b^2 \rangle^2}$$

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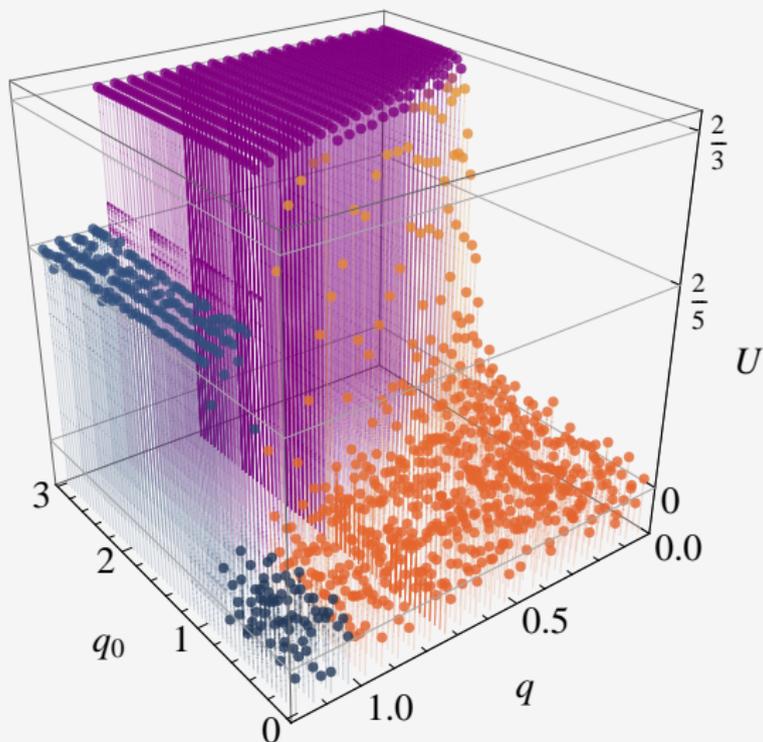
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Growing: $b \approx \pm v t$

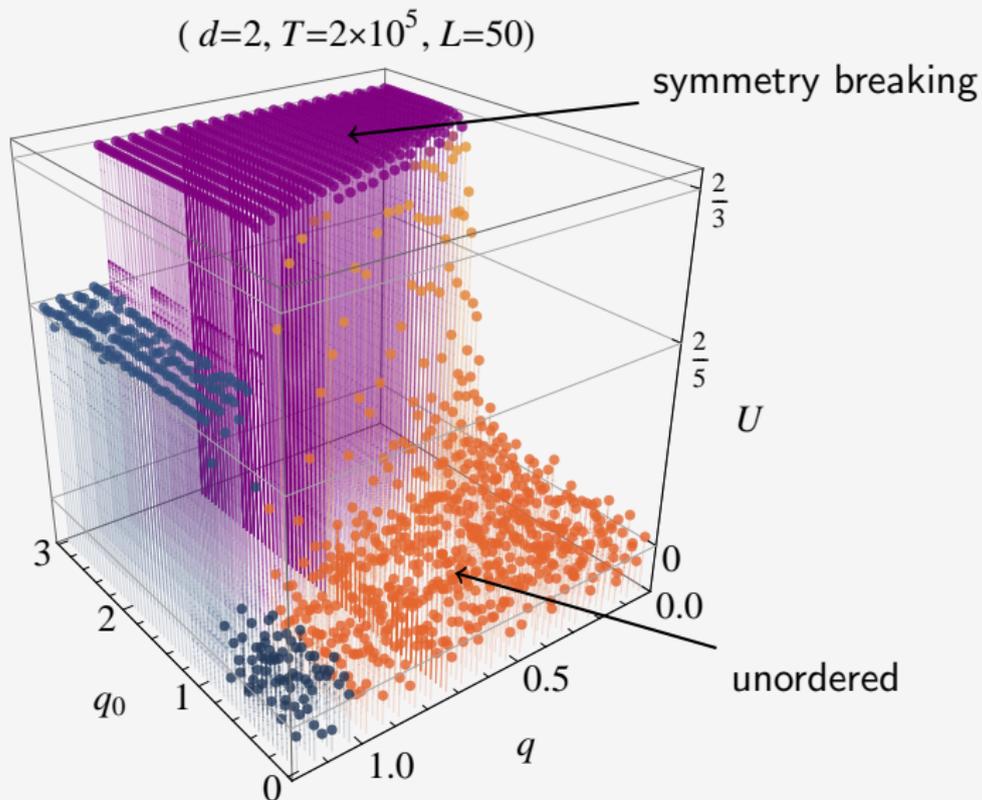
$$U \approx 1 - \frac{1}{3} \frac{1/T \int_0^T (v t)^4 dt}{\left(1/T \int_0^T (v t)^2 dt\right)^2} = \frac{2}{5}$$

Classification with the Binder cumulant

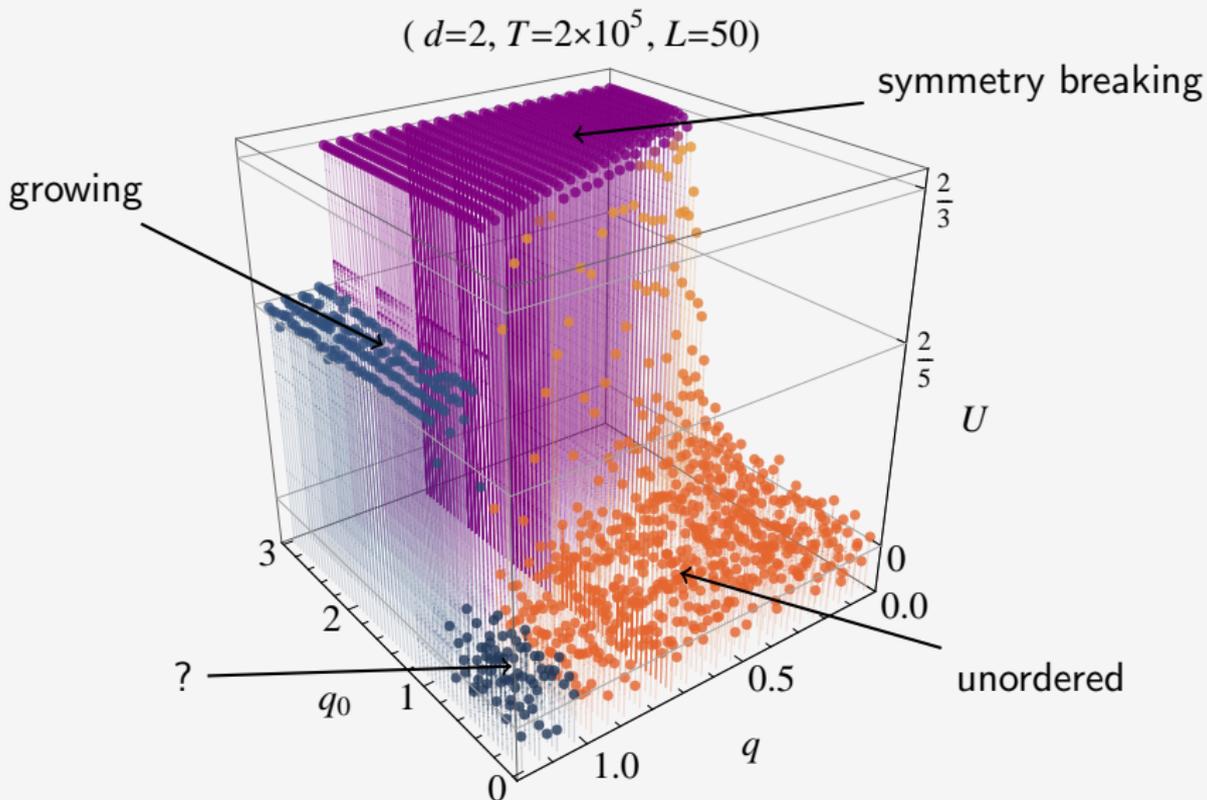
$(d=2, T=2 \times 10^5, L=50)$



Classification with the Binder cumulant

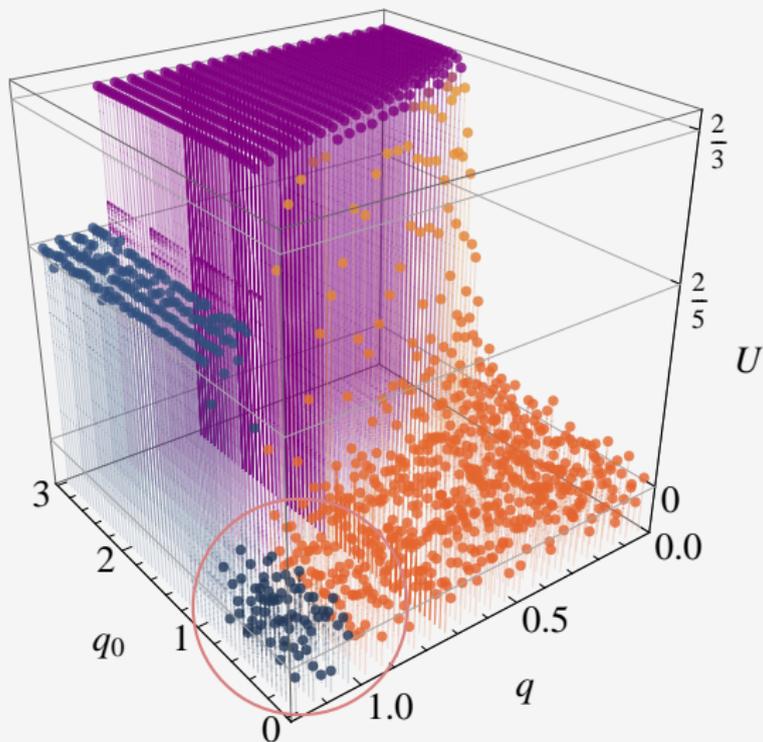


Classification with the Binder cumulant

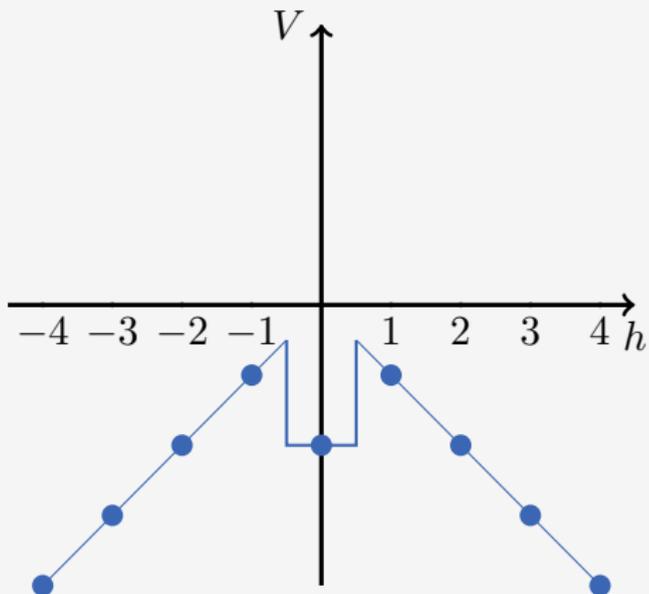


The strange region in the growing regime

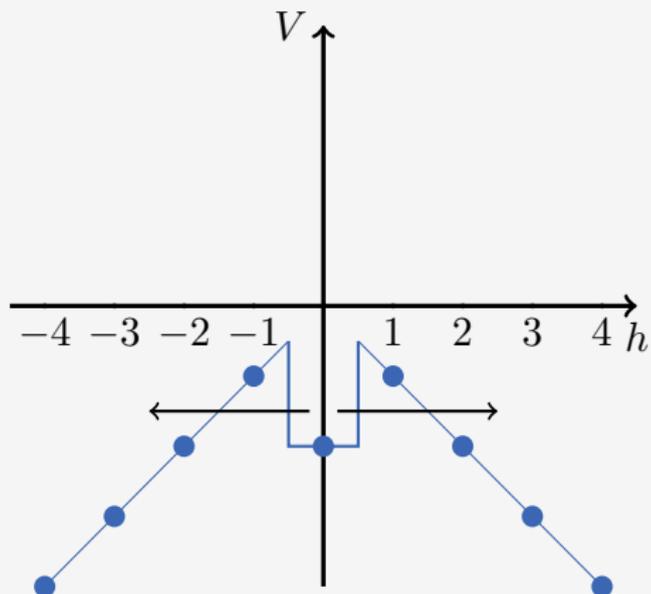
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Tunneling through a potential wall

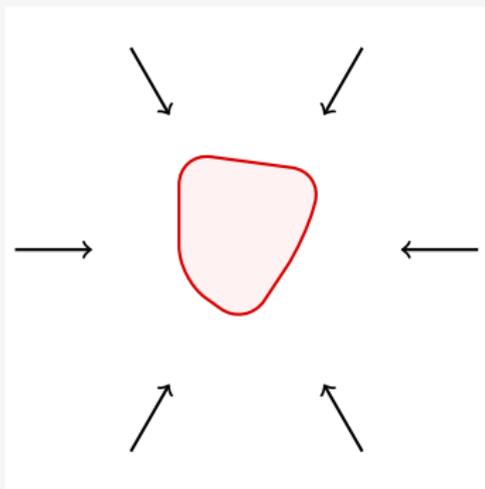


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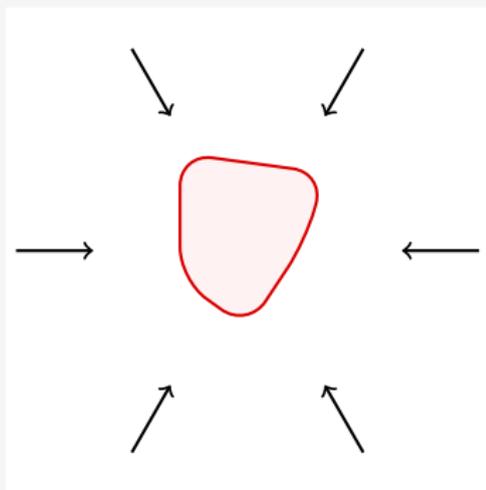
A lower critical droplet size

Small droplets shrink...

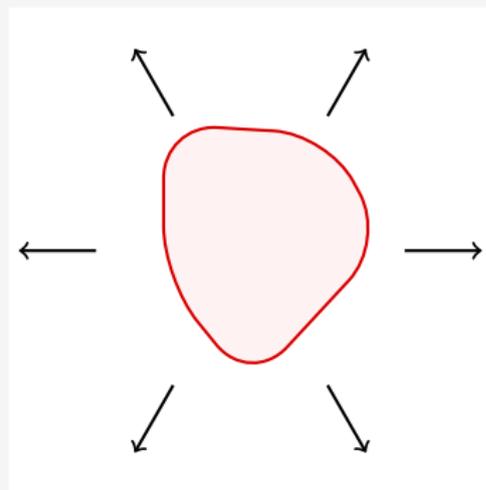


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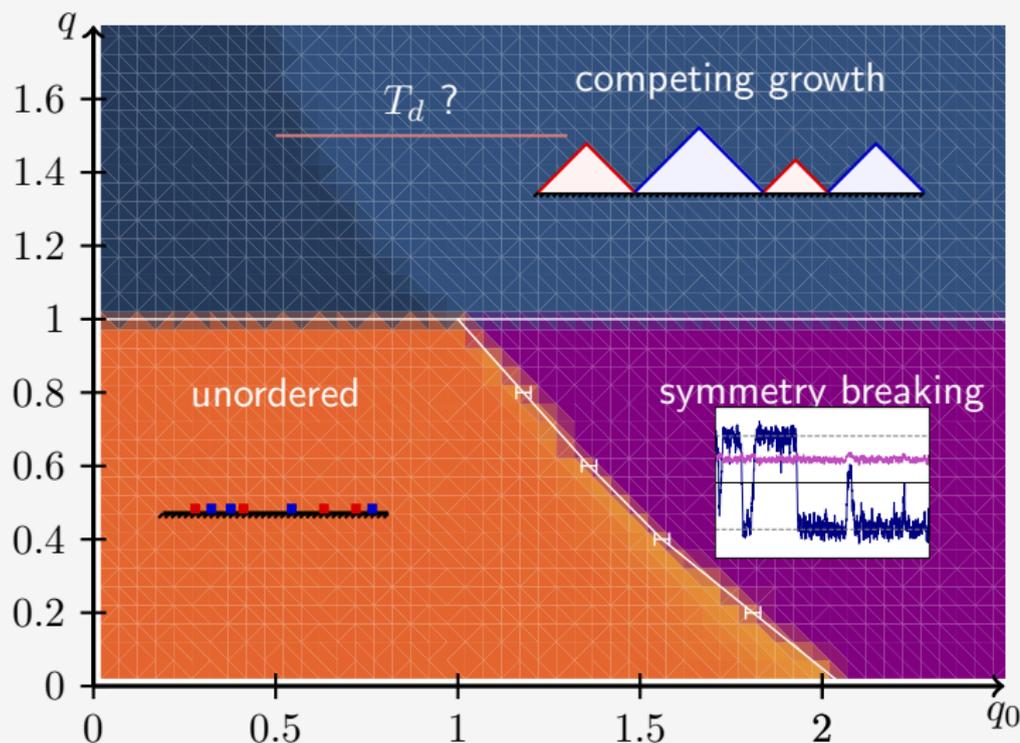
Small droplets shrink...



... while large droplets grow.



Phase diagram in 2+1-dimensions



Displacement time

