

Two dimensional spin-ice and the sixteen-vertex model

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PLAN of the talk

- **Introduction:**

- Geometrical frustration: Water **Ice**, Pyrochlore magnets (**3D spin ice**)
- Generic model: 2D **16-vertex model**
- Experiments: Artificial nano-arrays (**2D spin ice**)

- **Equilibrium phases:**

- Using **CTMC** and **Bethe-Peierls** approx. (**cavity method**). **Phase diagram** and **critical properties** of the 16V model.
- Theory vs. experiments in 'a-thermal' Artificial spin ice: **Edwards' measure** vs. Canonical.

- **Stochastic dynamics:**

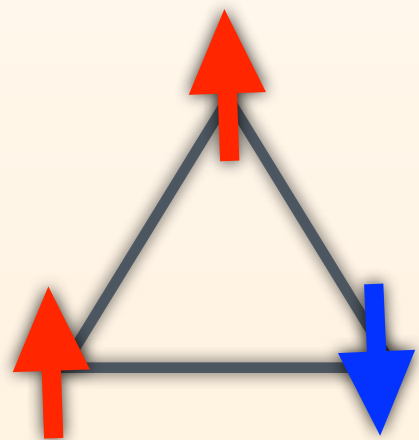
- Evolution after a **quench** into the PM, FM and AF phases.
- **Dynamical arrest**, mechanisms leading the evolution and **topological defects**.

- **Conclusion & perspectives**

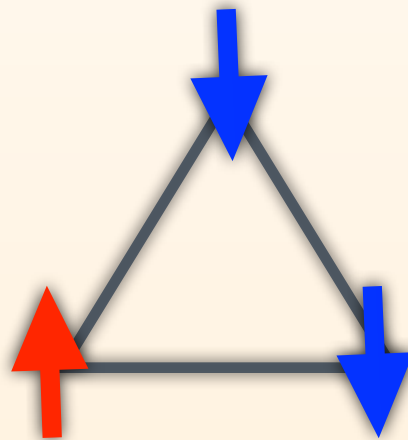
Geometrical frustration

Prototypical example: Ising **AF** on a **triangular** lattice

$$H = J \sum_{\langle i,j \rangle} S_i S_j \quad S_i = \pm 1 \quad \forall i \quad J > 0$$



$\equiv$



Ground state:

All configurations such that $\sum_{i=1}^3 S_i = \pm 1$

→ Macroscopic degeneracy $\Omega_0 \sim \exp(N)$

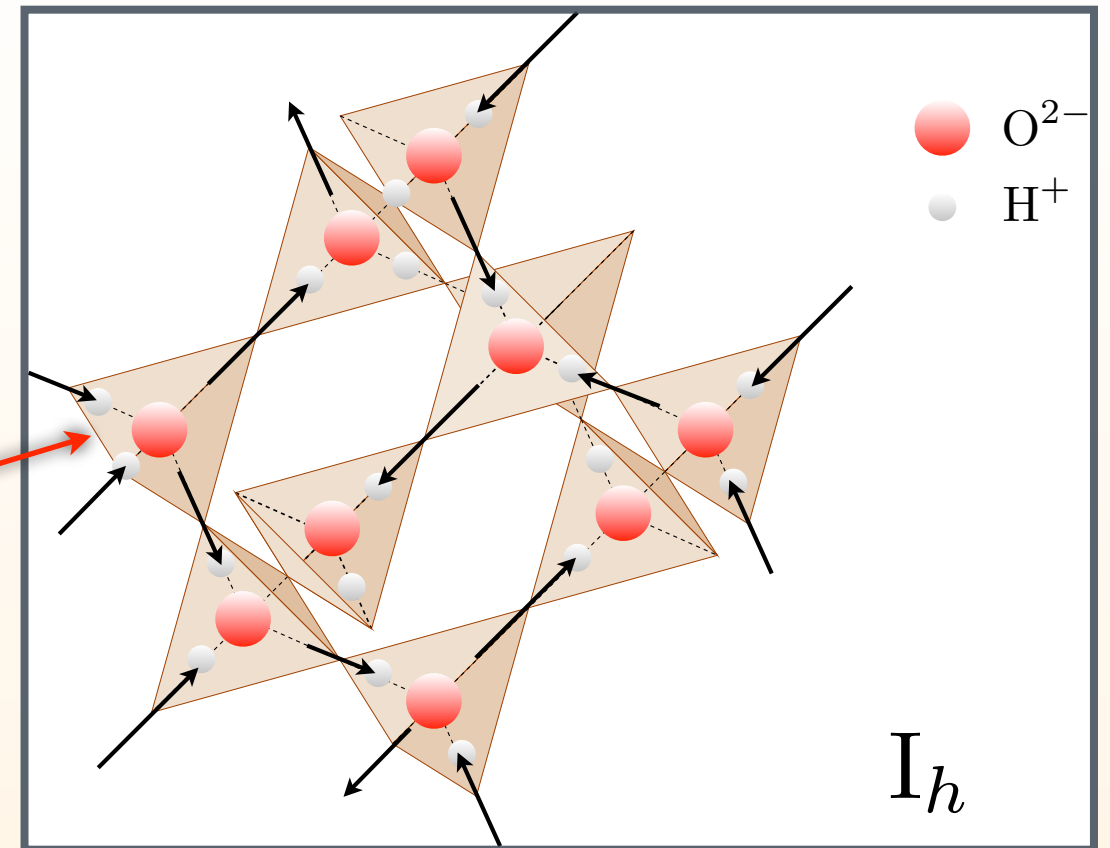
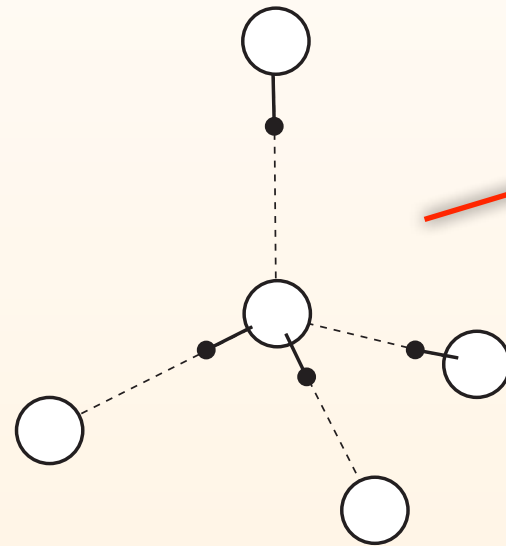
→ Extensive zero-point entropy $S_0 = \ln \Omega_0$

Frustrated because of the **geometry** of the lattice and the **antiferromagnetic** nature of the interactions.

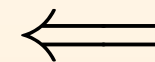
Geometrical frustration

Crucial example: **Water Ice**

Single unit:



Experimental evidence of an **extensive entropy at $T=0$**
Giauque & Stout 1936



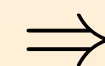
Predicted by **Pauling's model**
Pauling 1935



each bond carries a dipolar moment $\vec{\mu}$
verifying the **ice-rules**



at each **vertex** (oxygen atoms)
two in - two out



SIX vertices

Ground state : Ice-rule vertices are favoured $\Rightarrow$ **Geometrically frustrated**

Geometrical frustration

Harris, Bramwell, McMorro, Zeiske & Godfrey 1997

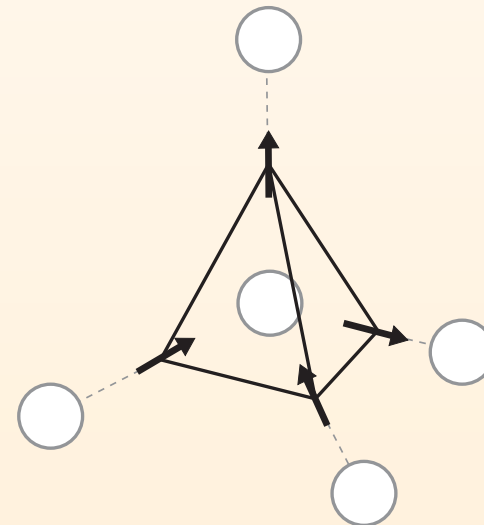
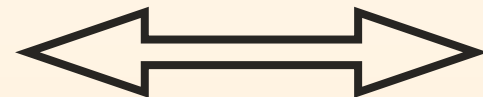
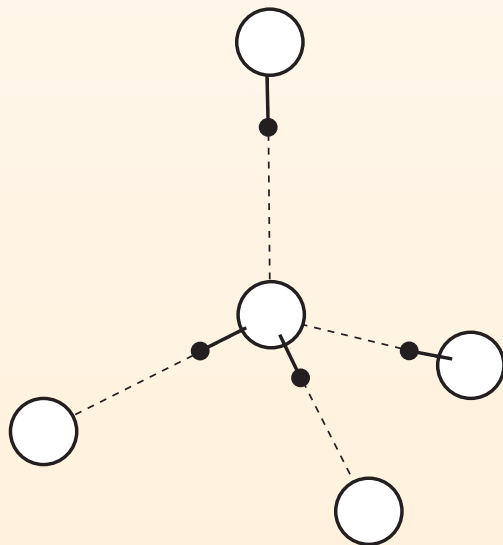
Water Ice



Spin Ice

electric dipoles

magnetic moments



$$S_w \approx 0.41R$$

$$S_{si} \approx 0.46R$$

zero point entropy
measured in $\text{Dy}_2\text{Ti}_2\text{O}_7$

Ramirez, Hayashi, Cava, Siddharthan & Shastry 1999

Geometrical frustration

Harris, Bramwell, McMorro, Zeiske & Godfrey 1997

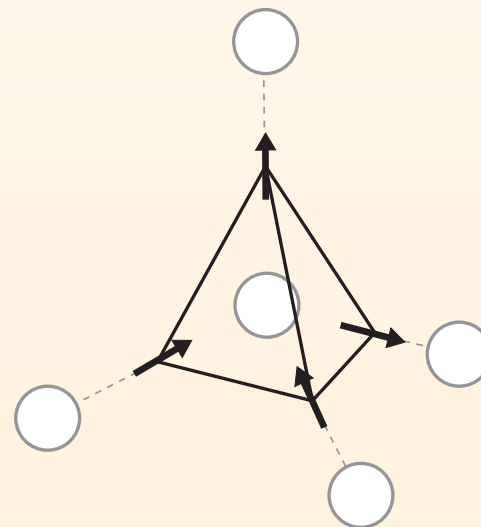
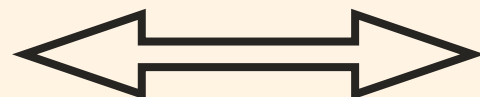
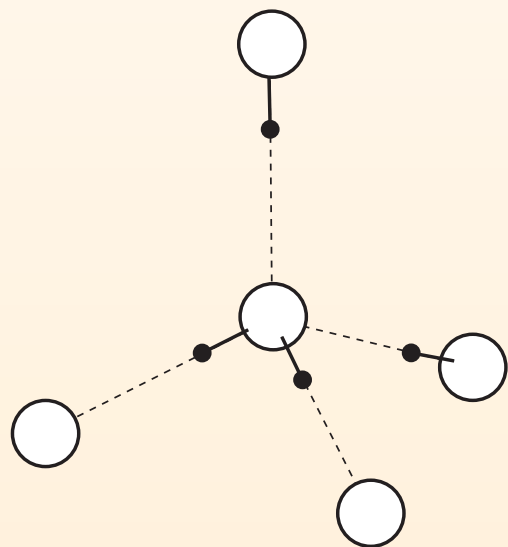
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Spin Ice is geometrically frustrated according to the ice rules

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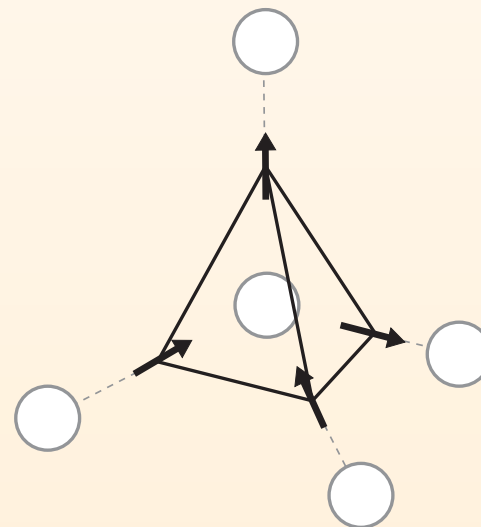
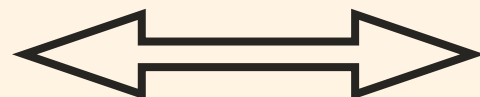
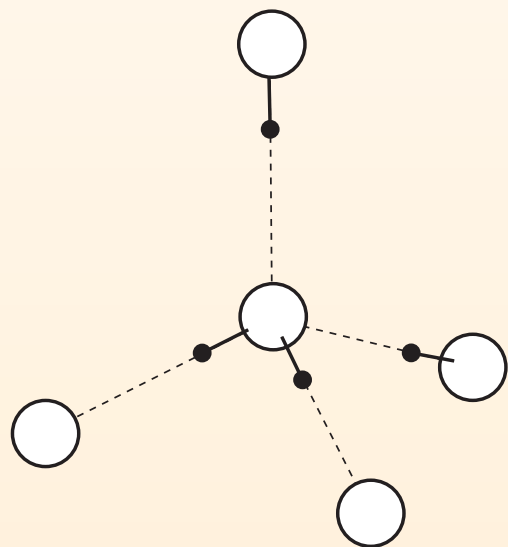
Water Ice



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Why??

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$$S_{si} \approx 0.46R$$

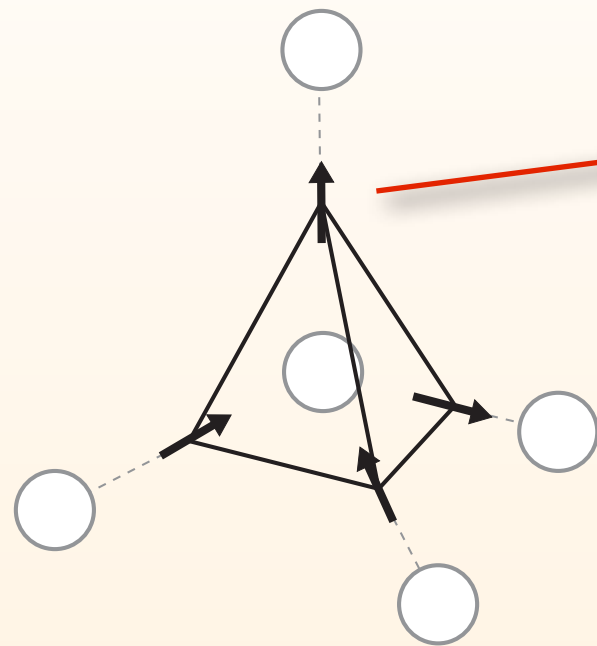
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Geometrical frustration

in spin ice

Harris, Bramwell, McMorro, Zeiske & Godfrey 1997



classical **Ising** spins

DSI: nn **FM** + *dipolar* interactions

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + Da^3 \sum_{i < j} \frac{\vec{S}_i \cdot \vec{S}_j}{r_{ij}^3} - 3 \frac{(\vec{S}_i \cdot \vec{r}_{ij})(\vec{S}_j \cdot \vec{r}_{ij})}{r_{ij}^5}$$

NN contribution: $H \approx \frac{J + 5D}{3} \sum_{\langle i,j \rangle} \sigma_i \sigma_j$ with: $\sigma_i = \pm 1$

AF

GS: **2 in-2 out** (ice-rules)
 $\Rightarrow$ Geometrically frustrated
Ferromagnet

Experiments 3D

$$S_w \approx 0.41R$$

$$S_{si} \approx 0.46R$$

$\simeq$

Exact 2D

$$S_{2D} = 3/2 \ln(4/3)$$

$$\approx 0.43R$$

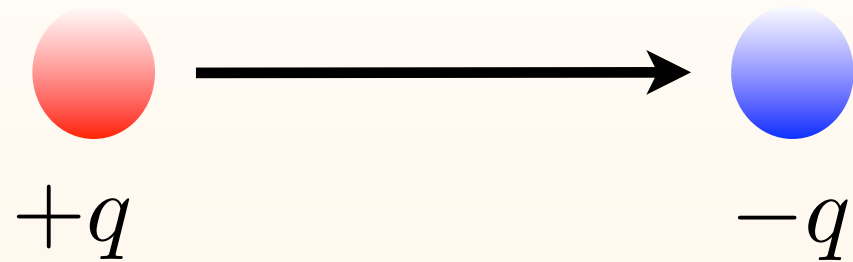
Lieb 1967

$\simeq$

Approx.

$$S_{\infty} \approx 0.40R$$

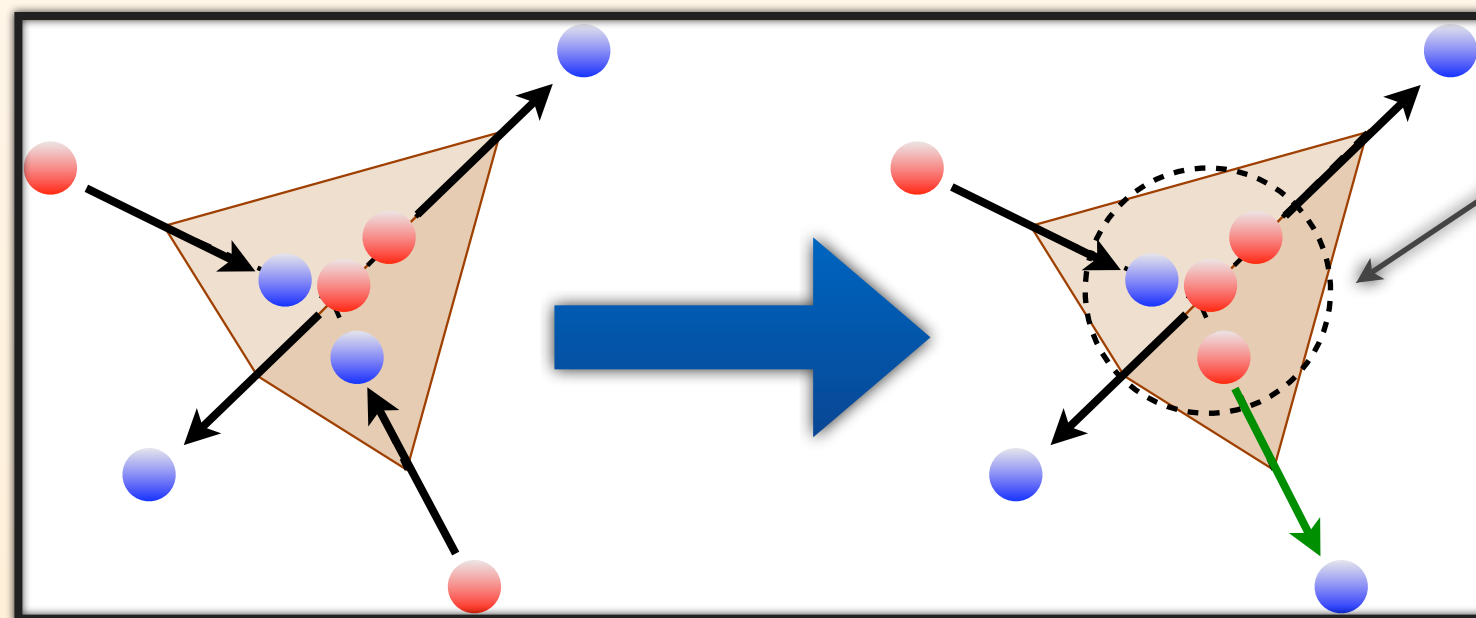
Thermal excitations in spin-ice



“Dumbbell picture”

$\Rightarrow$ Ice configurations $\equiv \{q_\alpha = 0\}$

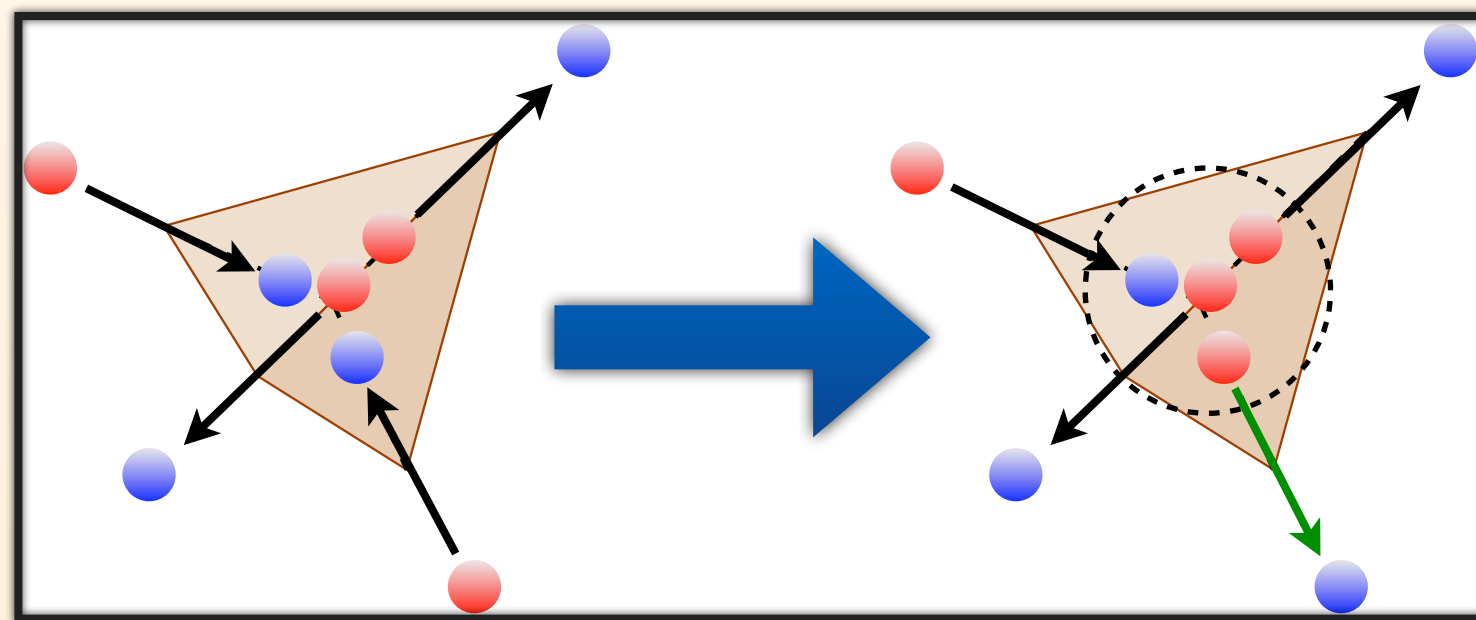
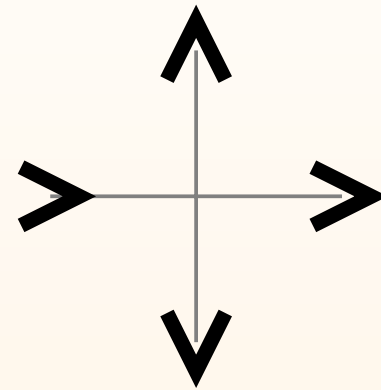
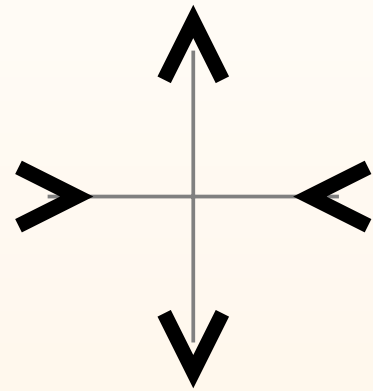
Thermal excitations
violating the ice rules =



magnetic monopoles

Thermal excitations in spin-ice

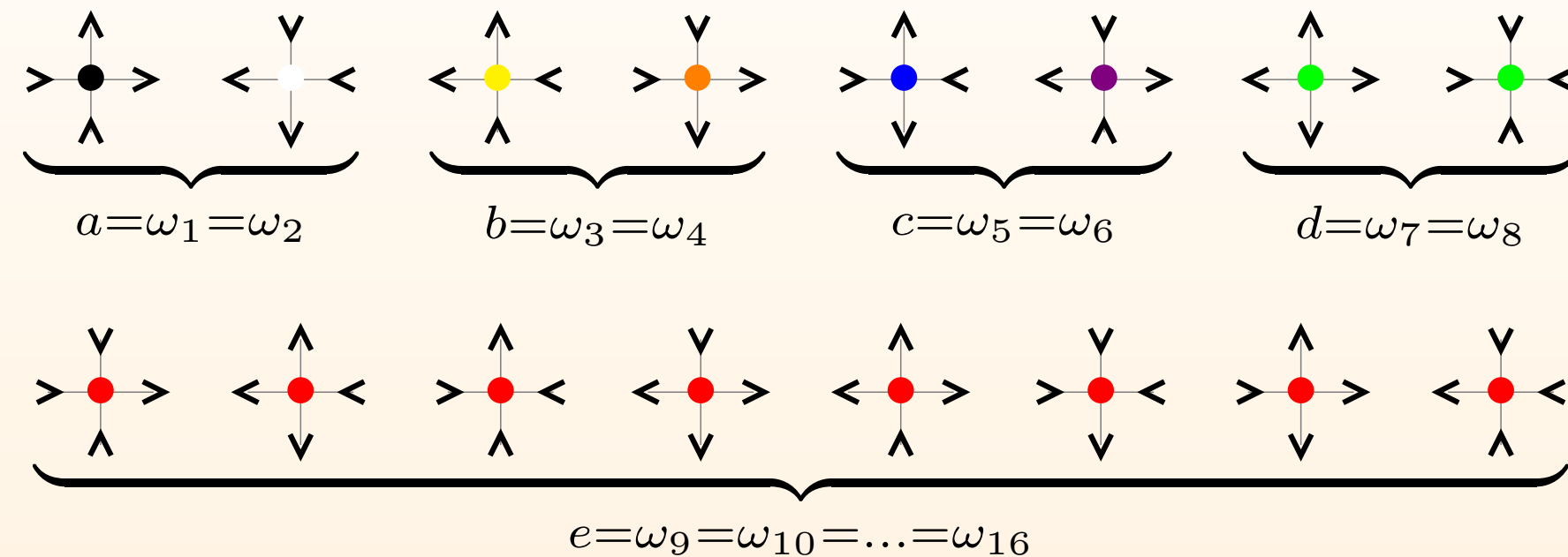
2D projection



$\Rightarrow 2^4 = 16$ - vertex model

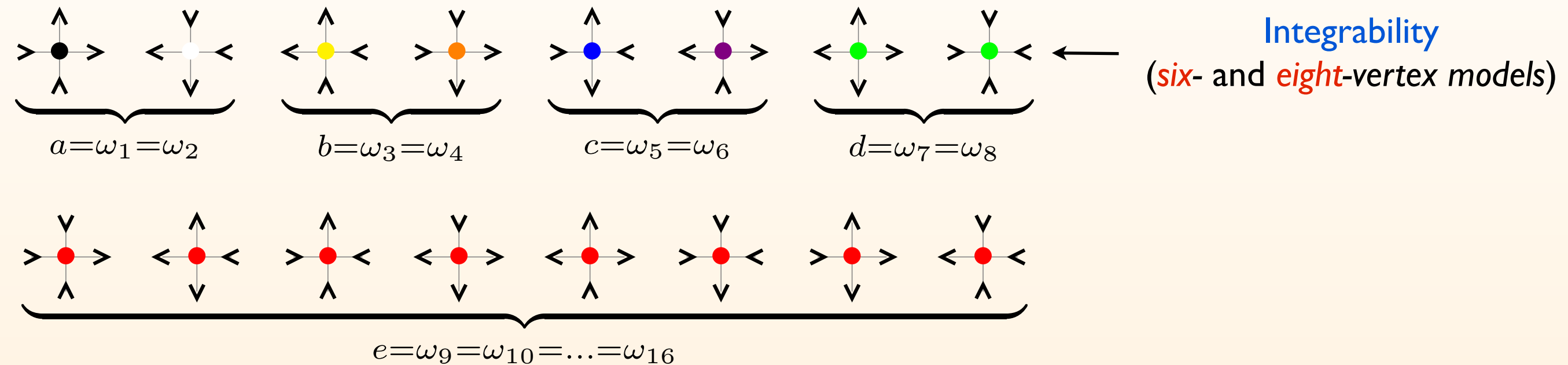
2D Spin-Ice theory: the sixteen-vertex model

Fix the Boltzmann weight of each vertex: $\omega_k = e^{-\beta \epsilon_k}$



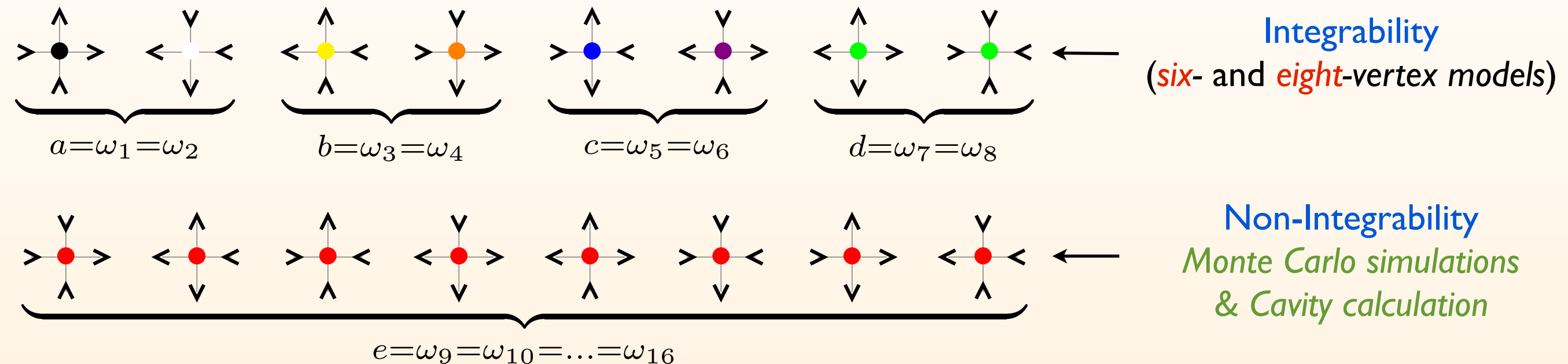
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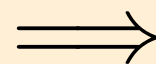
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Thermal excitations:

Vertices breaking the ice-rule are allowed but un-favoured = *defects*

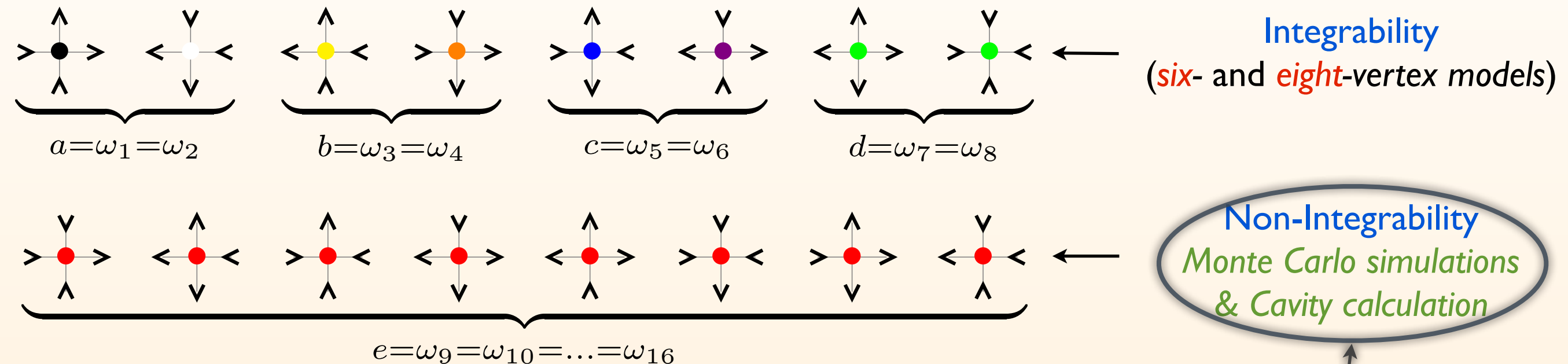
Dynamics



Stochastic extension of a general
integrable model

2D Spin-Ice theory: the sixteen-vertex model

Fix the Boltzmann weight of each vertex: $\omega_k = e^{-\beta \epsilon_k}$



Integrability
(*six*- and *eight*-vertex models)

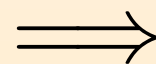
Non-Integrability
Monte Carlo simulations
& Cavity calculation

Equilibrium phases of the
general model ?

Thermal excitations:

Vertices breaking the ice-rule are allowed but un-favoured = *defects*

Dynamics

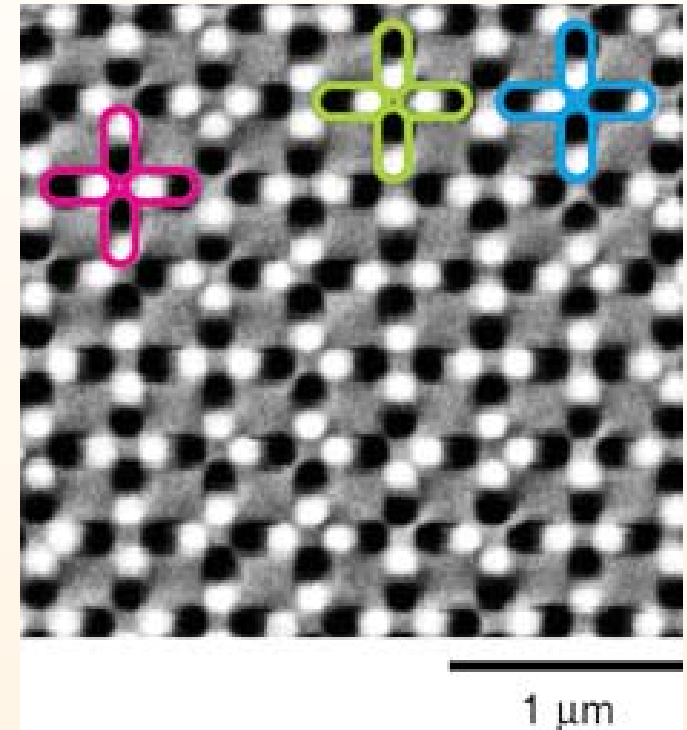


Stochastic extension of a general
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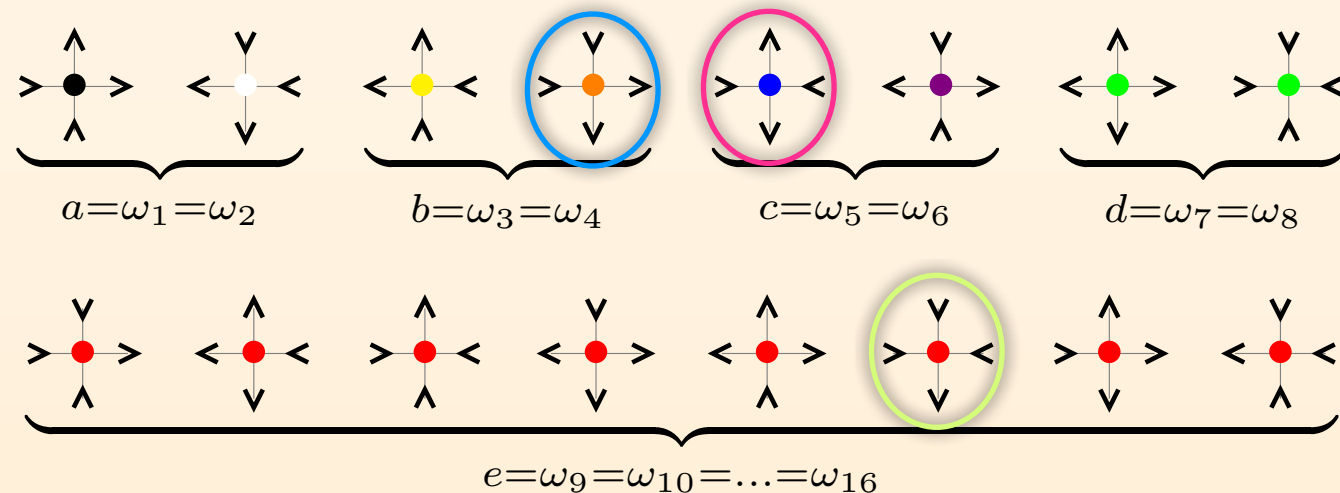
2D experiments: Artificial Spin-Ice

1. Array of elongated ferromagnetic islands behave as classical Ising spins.
2. Dipolar interactions $\rightarrow c > a = b$
3. Direct visualisation of **defects'** dynamics

Ladak, Read, Perkins, Cohen, Branford 2010 ;
Mengotti, Heyderman, Rodríguez, Nolting, Hügli, Braun 2011.



from Wang et al., Nature 2008

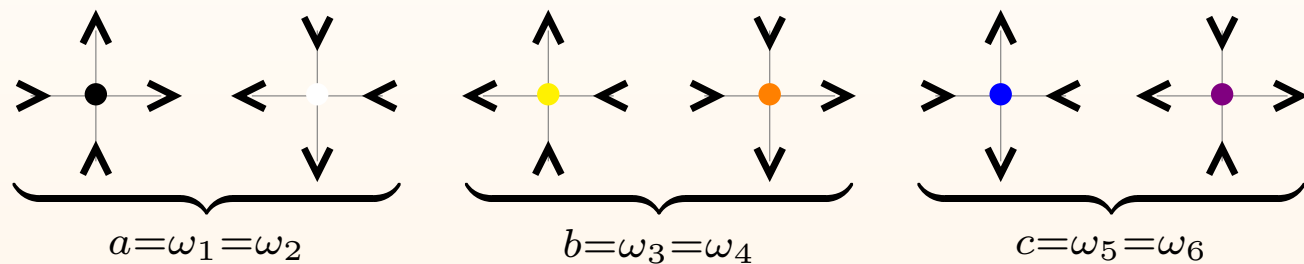


Wang, Nisoli, Freitas, Li, McConville, Cooley, Lund, Samarth, Leighton, Crespi, Schiffer 2006.

Equilibrium.

Six-vertex model (exact results)

Ice-rules $\Rightarrow d = e = 0$



Equilibrium phases:

$$\Delta_6 = \frac{a^2 + b^2 - c^2}{2ab}$$

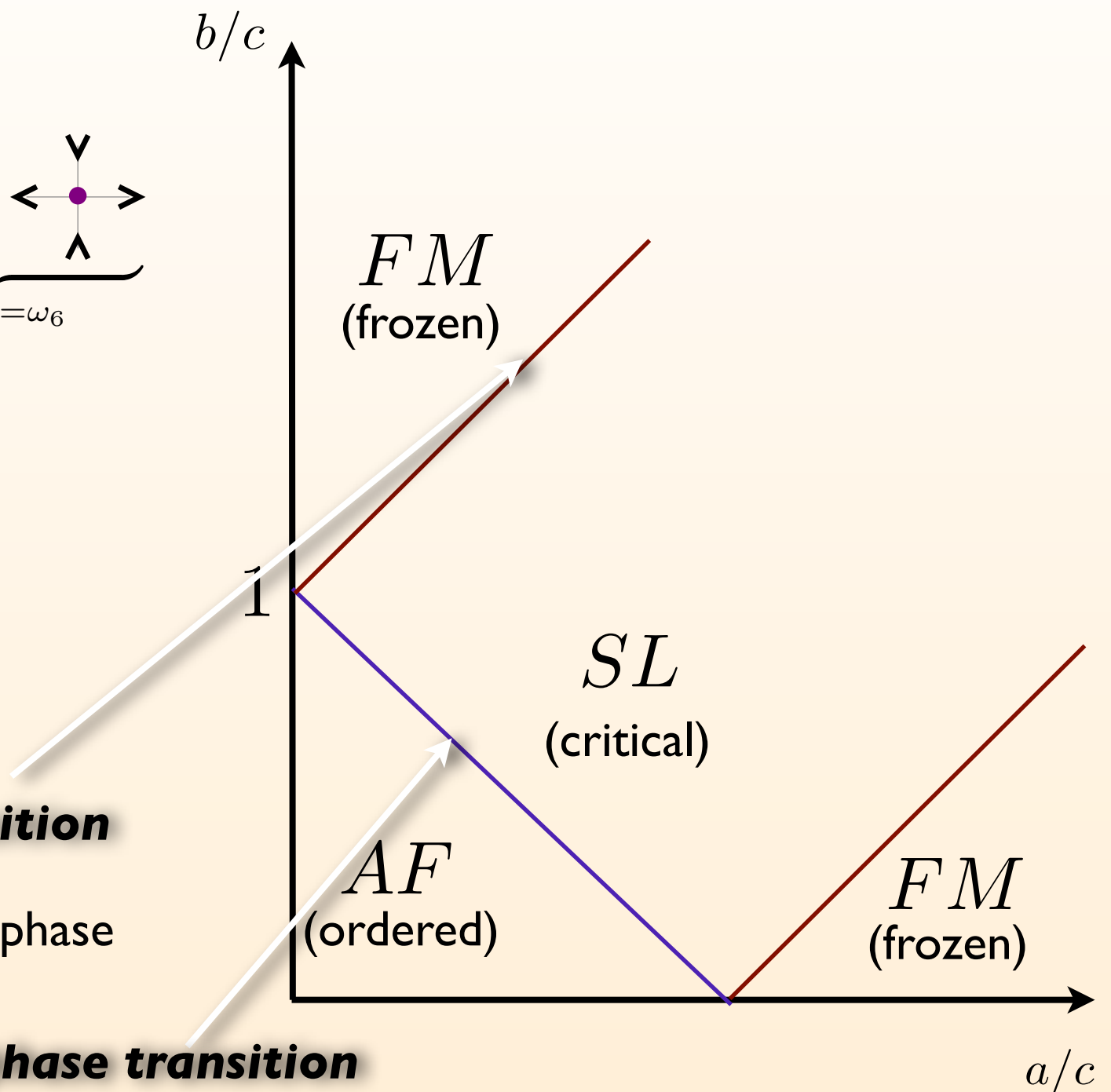
$\Delta_6 > 1$ frozen FM phase

'Frozen-to-critical' phase transition

$1 > \Delta_6 > -1$ quasi long-range ordered SL phase

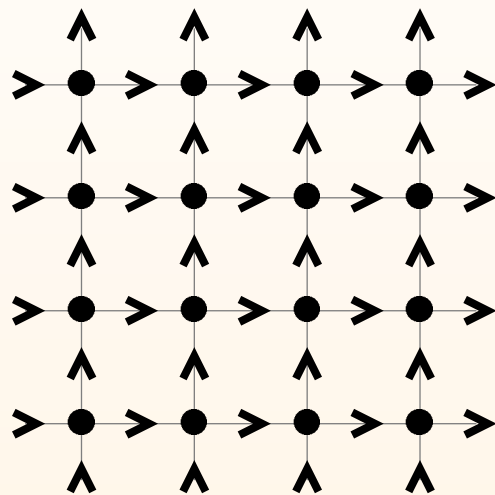
Kosterlitz-Thouless phase transition

$\Delta_6 < -1$ ordered AF phase with low energy excitations



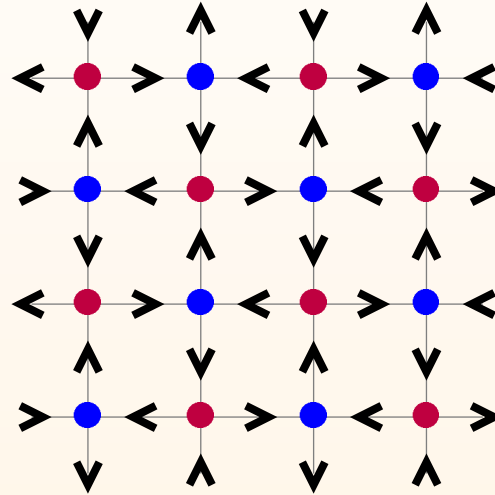
Equilibrium.

Six-vertex model (exact results)



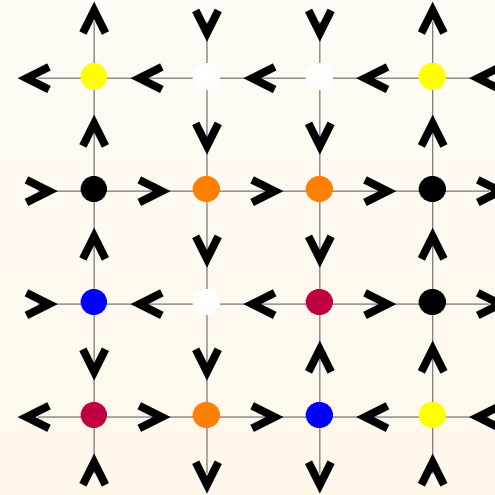
FM
(frozen)

a or b



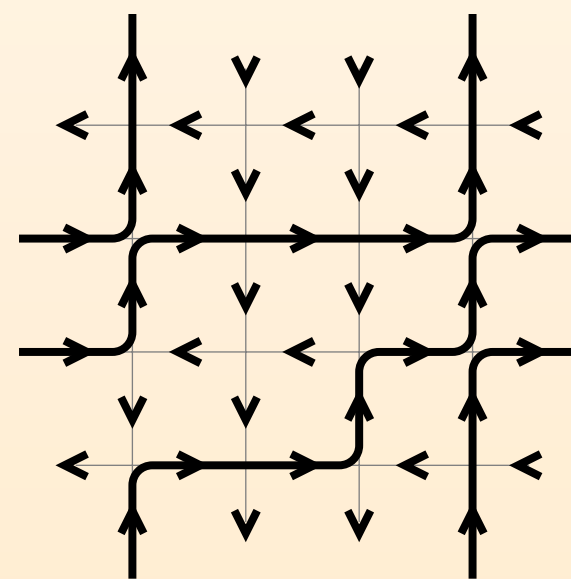
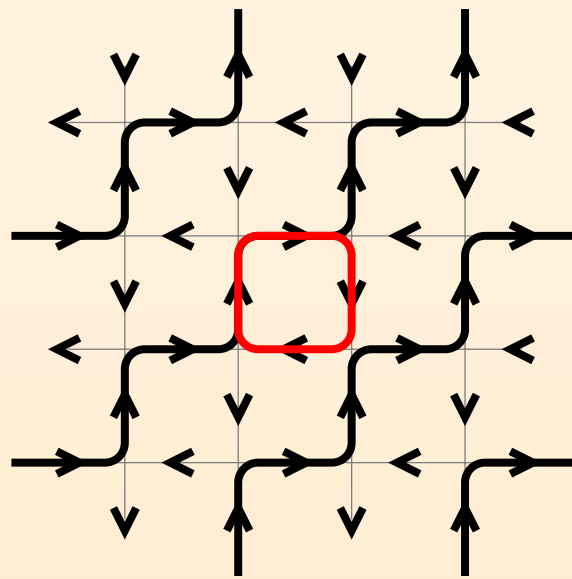
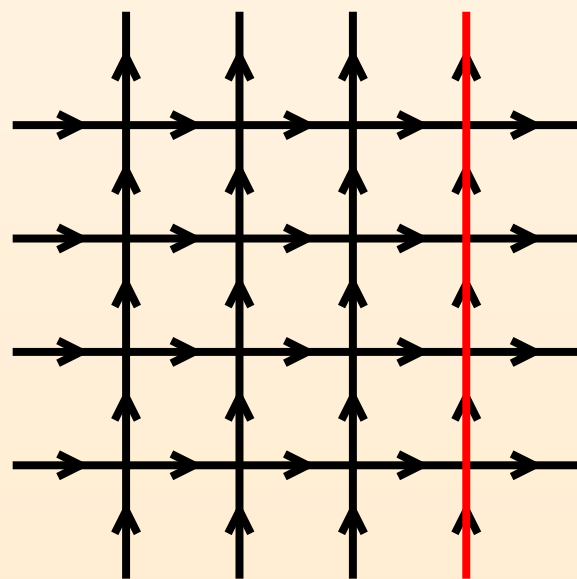
AF
(ordered)

c



SL
(critical)

a b c



Sixteen-vertex model (numerics)

Allow defects $\Rightarrow d = e \neq 0$

Conjecture: (numerics)

$$\Delta_{16} = \frac{a^2 + b^2 - c^2 - (3e + d)^2}{2(ab + c(3e + d))} \quad \xrightarrow{e=0} \quad \Delta_8 = \frac{a^2 + b^2 - c^2 - d^2}{2(ab + cd)}$$

1. All the transitions become **continuous**
2. The PM phase is **not critical**, the FM phase is **not frozen**.
3. Finite size scaling: **Critical exponents** depend on the value of the parameters: a, b, c, d, e .
4. Phase diagram characterised by a generalised '**anisotropy parameter**'.

$\Rightarrow$ consistent with the **exact** results on the **eight-vertex model** **Baxter** 1971, 1982
and (the very few) the **sixteen-vertex model** **Wu** 1969

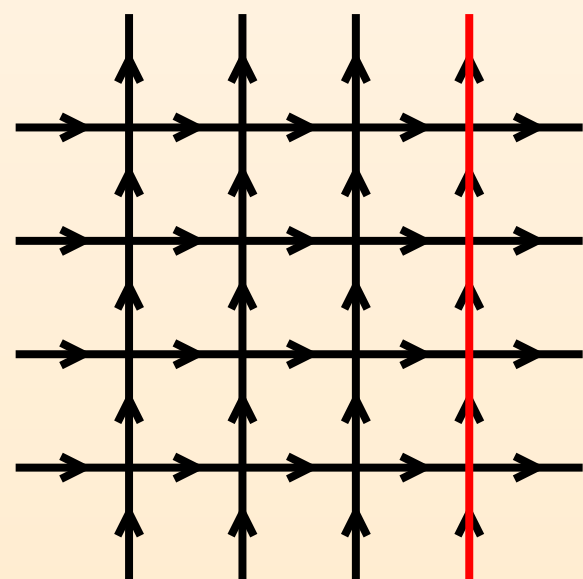
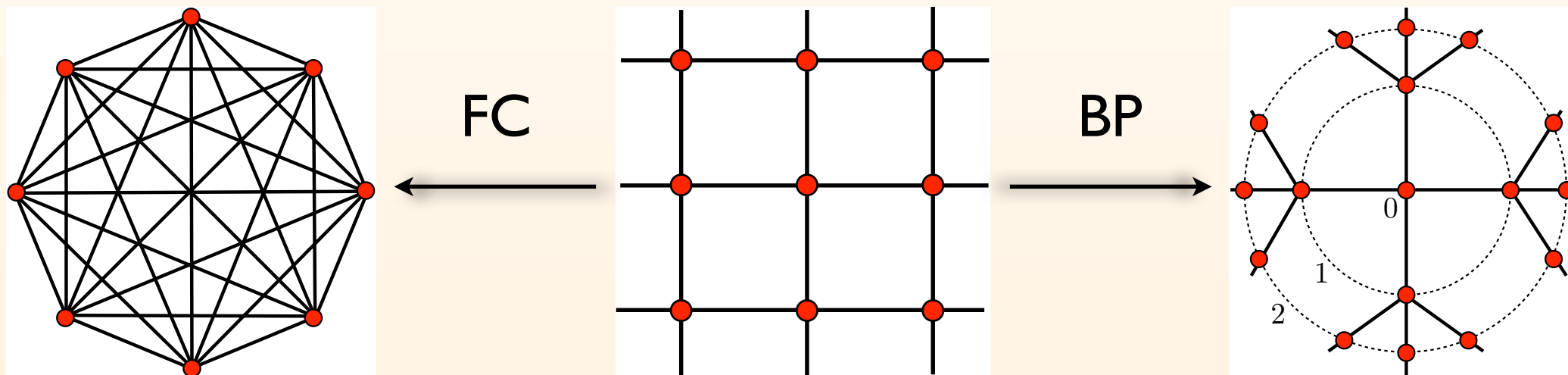
Levis & Cugliandolo 2011
Foini, Levis, Tarzia & Cugliandolo 2012

Spin-ice on a tree graph (cavity method)

Bethe-Peierls approximation:

In the absence of a given site, the neighbours are de-correlated.

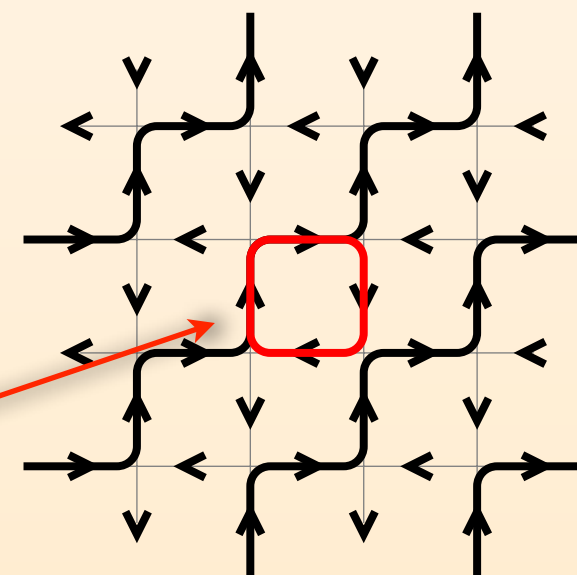
- The **connectivity** of the original model is preserved BUT **no loops**
- Allows for a **recursive** treatment to be solved **self-consistently**



⇒ Good approximation
for FM order

No loops

AF order ?
Defects ?



Loop
fluctuations

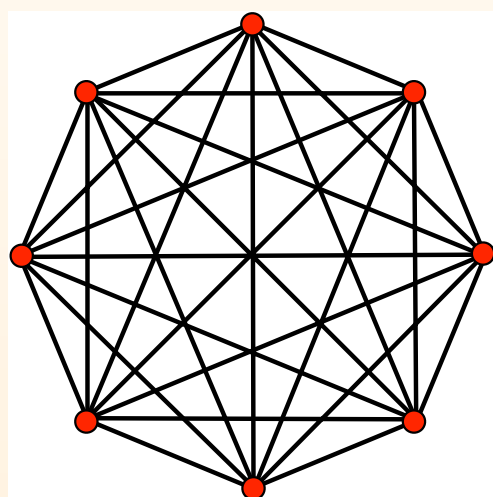
Spin-ice on a tree graph (cavity method)

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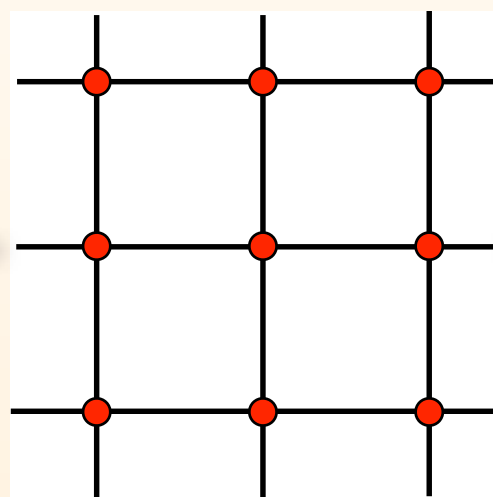
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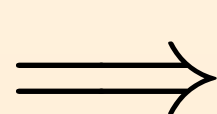
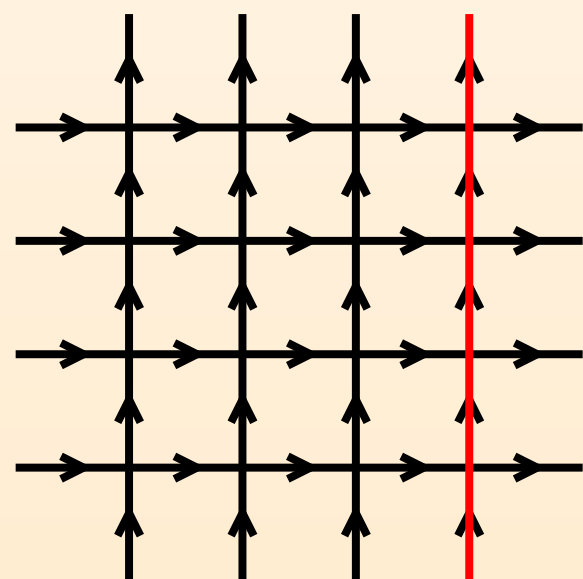
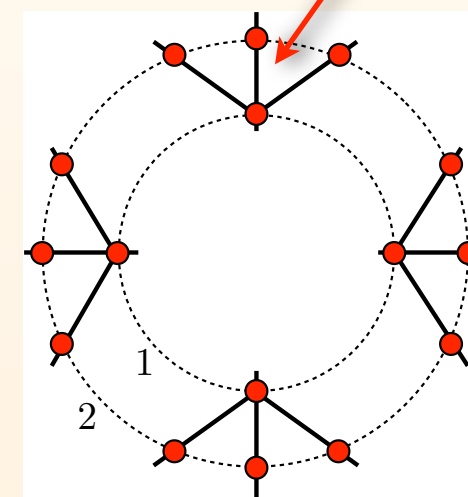
4 disconnected
rooted trees



FC



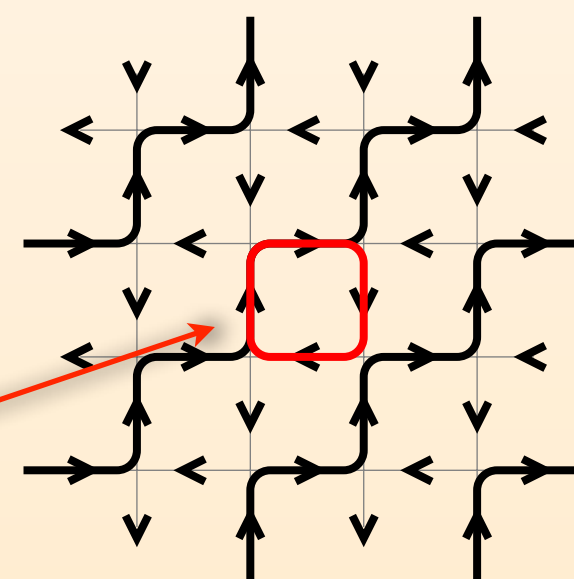
BP



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Loop
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Spin-ice on a tree graph (cavity method)

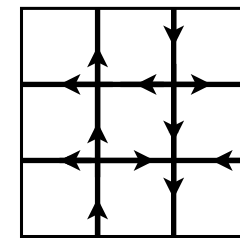
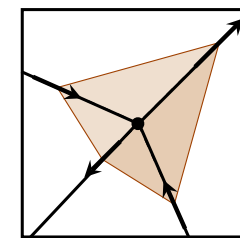
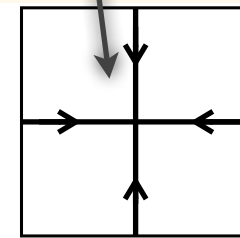
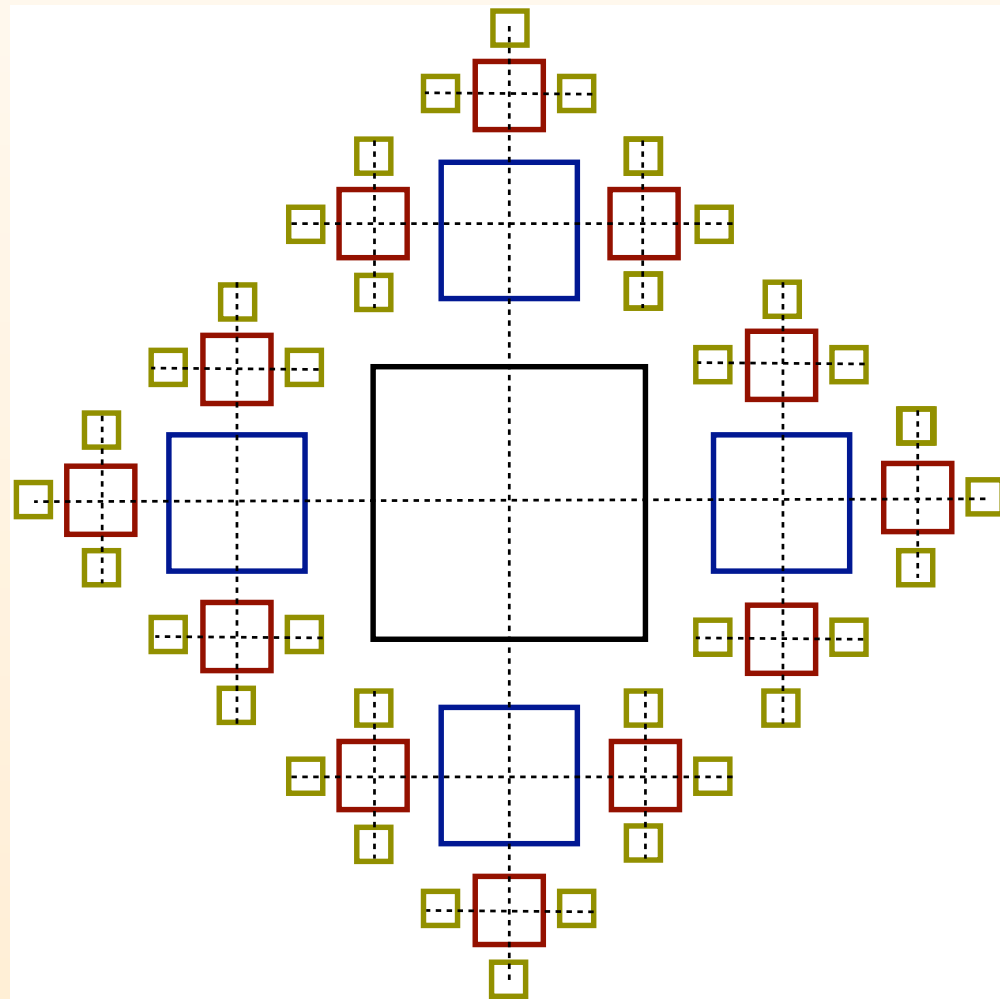
Two models:

1. An **oriented tree** of vertices 'single vertex tree'

No loop fluctuations

2. A **tree of plaquettes** made of four vertices 'plaquette tree'

Include elementary loop fluctuations



Spin-ice on a tree graph (cavity method)

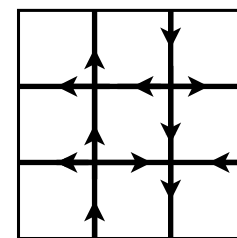
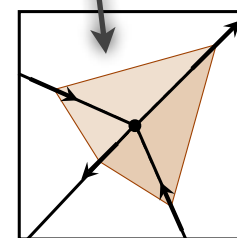
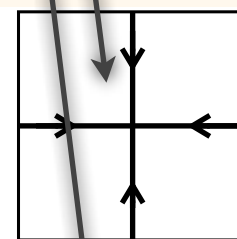
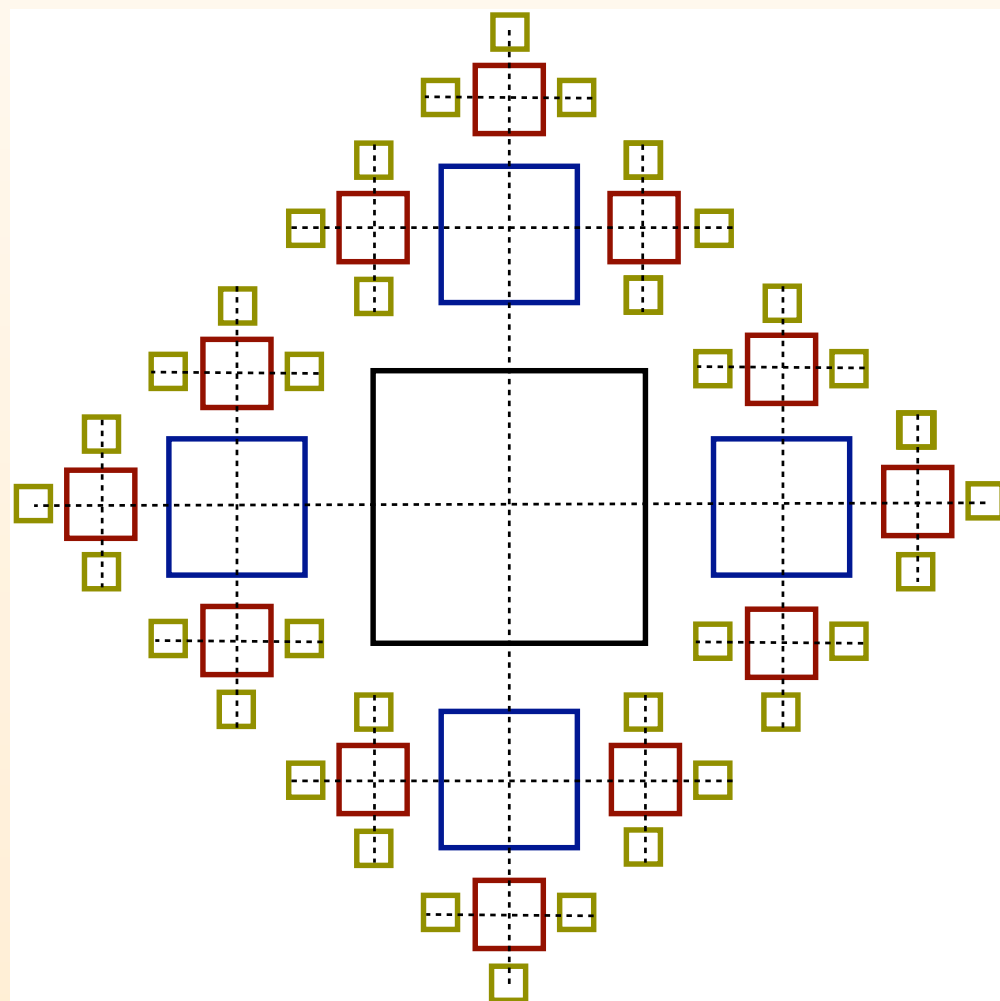
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**Jaubert, Chalker,
Holdsworth &
Moessner 2008**

Spin-ice on a tree graph (cavity method)

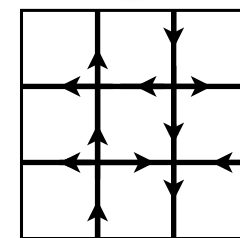
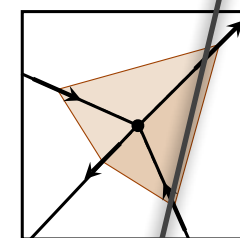
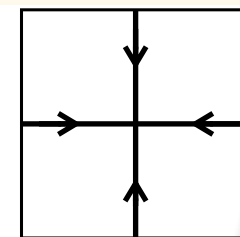
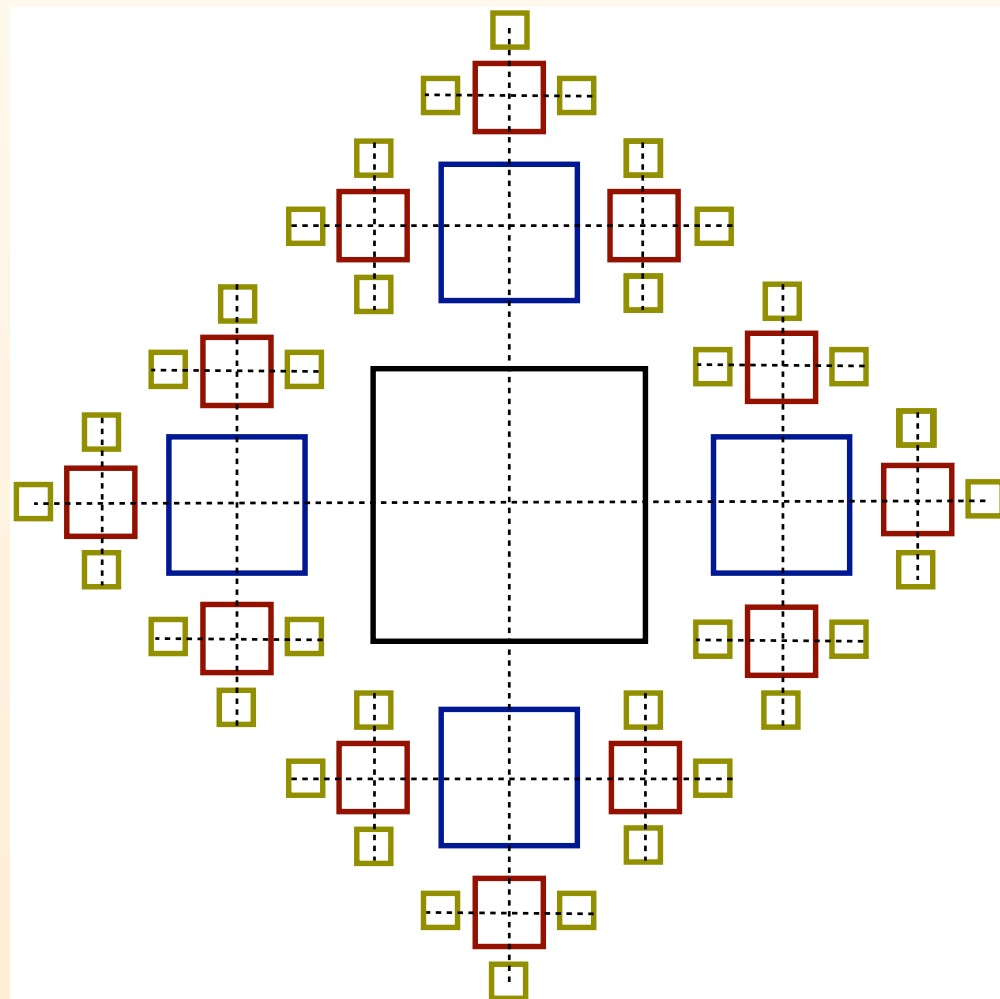
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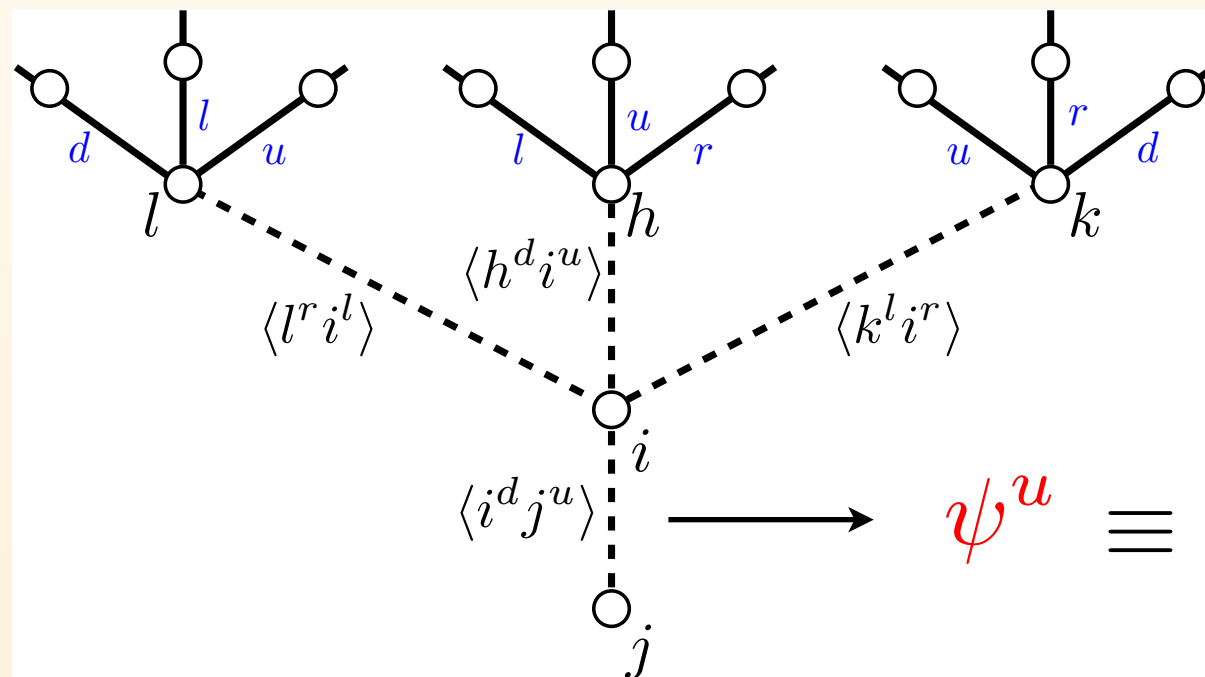
2. A **tree of plaquettes** made of four vertices '**plaquette tree**'

Include elementary loop fluctuations



Spin-ice on a tree graph (cavity method)

- Strategy:**
1. Define an **oriented tree** (up, left, down, right) where vertices can be identified.
 2. Write the **self-consistent equations** satisfied by the '**cavity probabilities**': n -th shell as a function of the $(n+1)$ th shell.



probability that the spin in the missing edge $\langle i^d j^u \rangle$ points towards i (up).

up-rooted tree from
merging a right, up and
left rooted tree

Spin-ice on a tree graph (cavity method)

- Strategy:
1. Define an **oriented tree** (up, left, down, right) where vertices can be identified.
 2. Write the **self-consistent equations** satisfied by the ‘**cavity probabilities**’: n -th shell as a function of the $(n+1)$ th shell.

The simplest example: eight-vertex model in the single vertex tree

$$\psi^u = \frac{1}{z^u} \left[a\psi^l\psi^u\psi^r + b(1 - \psi^l)\psi^u(1 - \psi^r) \right. \\ \left. + c(1 - \psi^u)(1 - \psi^l)\psi^r + d\psi^l(1 - \psi^u)(1 - \psi^r) \right] \quad \times 4 : \psi^{l,d,r}$$

$$\psi^\alpha = \hat{\Psi}^\alpha[a, b, c, d, e, \psi^u, \psi^d, \psi^l, \psi^r]$$

Self-consistent equations

$$\alpha = u, l, d, r$$

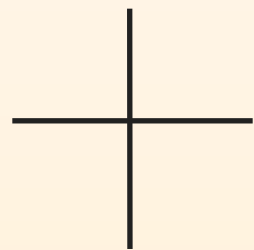
Spin-ice on a tree graph (cavity method)

- Strategy:**
1. Define an **oriented tree** (up, left, down, right) where vertices can be identified.
 2. Write the **self-consistent equations** satisfied by the ‘**cavity probabilities**’: n -th shell as a function of the $(n+1)$ th shell.

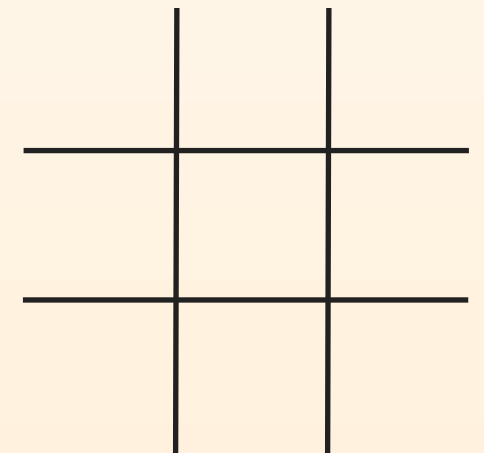
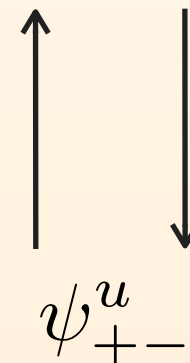
$$\psi^\alpha = \hat{\Psi}^\alpha[a, b, c, d, e, \psi^u, \psi^d, \psi^l, \psi^r]$$

Self-consistent equations

$$\alpha = u, l, d, r$$



**Plaquette
model**



$$\psi_{s_1 s_2}^\alpha = \hat{\Psi}_{s_1 s_2}^\alpha[a, b, c, d, e, \psi^u, \psi^d, \psi^l, \psi^r]$$

$$4 \times 4$$

Spin-ice on a tree graph (cavity method)

Strategy: 1. Define an **oriented tree** (up, left, down, right) where vertices can be identified.

2. Write the **self-consistent equations** satisfied by the ‘**cavity probabilities**’: n -th shell as a function of the $(n+1)$ th shell.

3. Find the **fixed points** of the self-consistent equations.

—————→ Equilibrium phases

4. Compute **thermodynamic observables**: free energy, magnetisation, etc.

5. Study the **stability** of the solutions

$M_{\alpha,\beta} = \left. \frac{d\hat{\Psi}^\alpha}{d\psi^\beta} \right|_{fp}$ —————→ Phase **transitions** and nature of the **phases**.

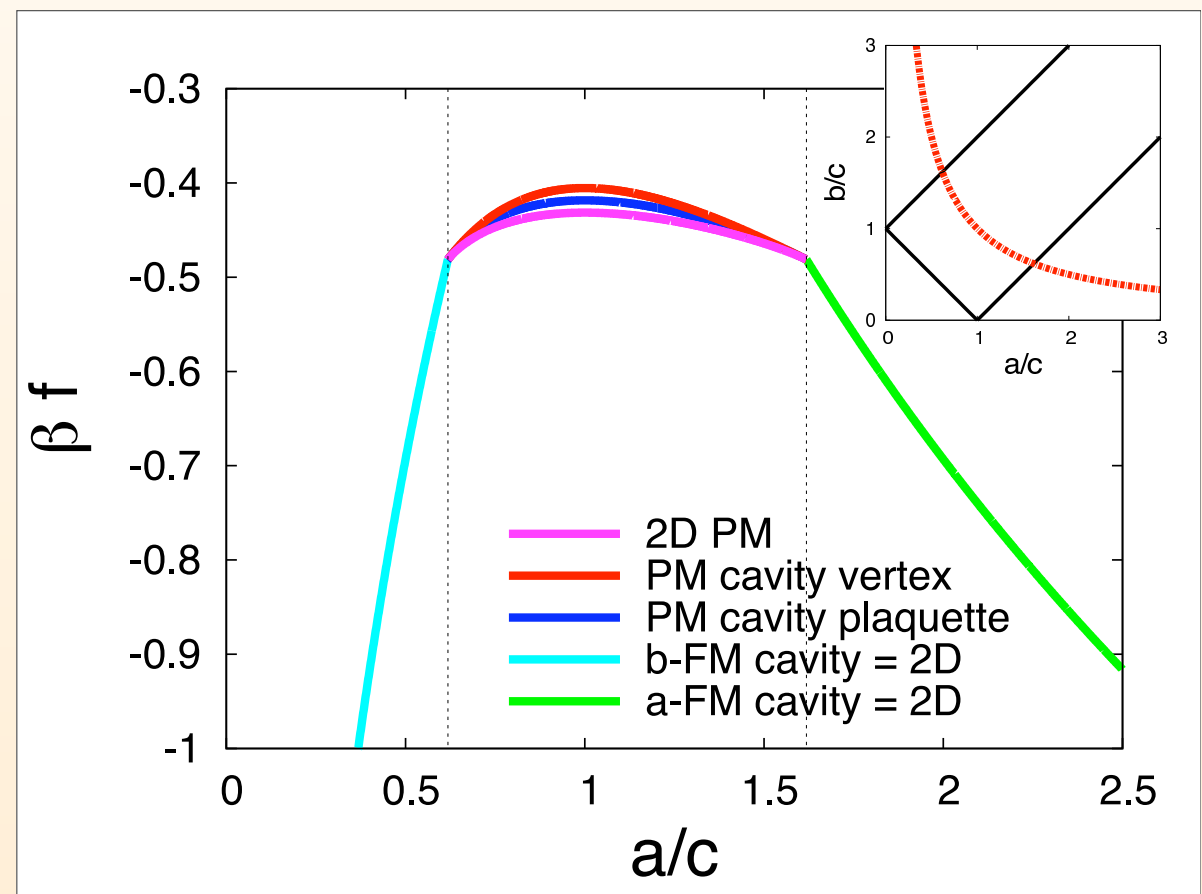
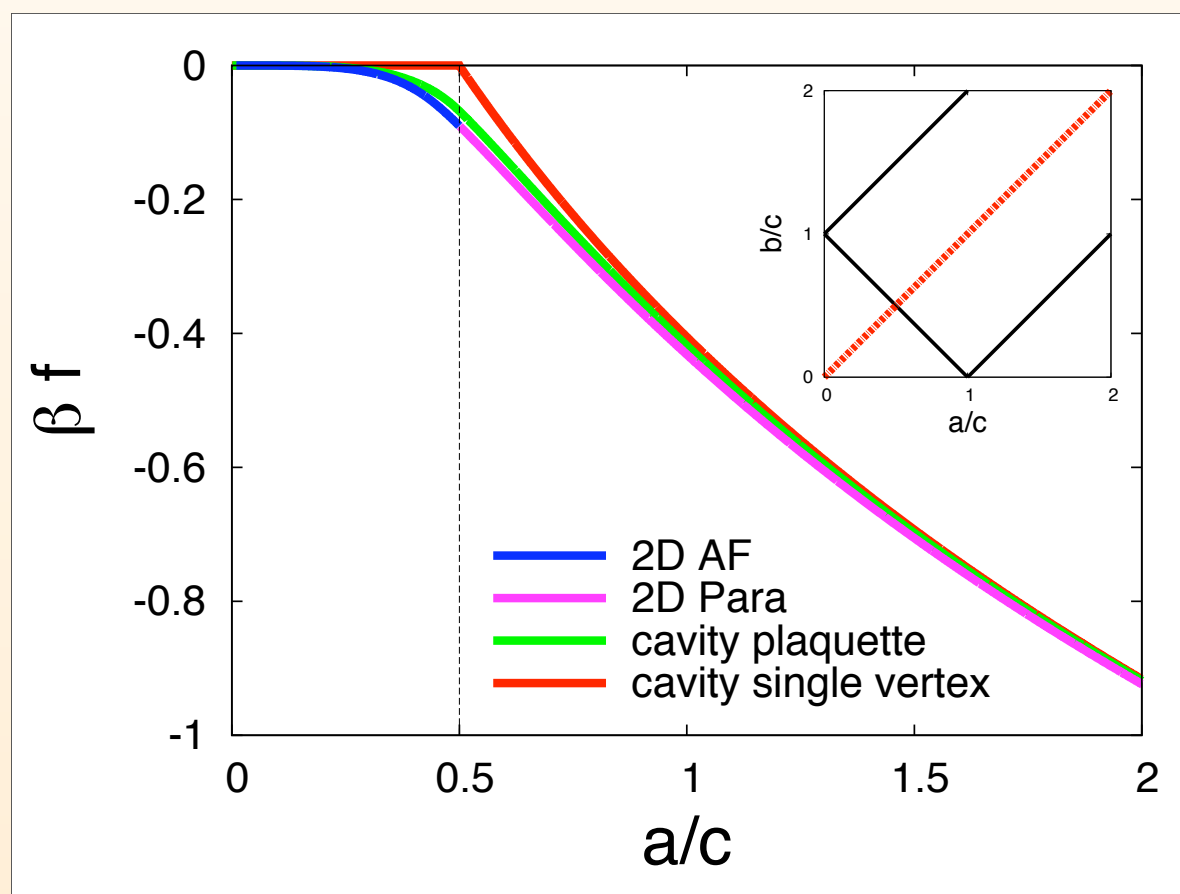
Eigenvalues: $E_1, E_2, \dots$

—————→ Try to find an **anisotropy parameter** $\Delta(E_1, E_2, \dots)$ which characterises the phase diagram

Spin-ice on a tree graph (cavity method)

Results for the six-vertex model:

1. **Exact** location of the transition lines with both the single vertex and the plaquette model.
2. Thermodynamic quantities in remarkable agreement with the 2D results.



Free energy of the 6V model on trees vs.
exact results in 2D.

Spin-ice on a tree graph (cavity method)

Results for the six-vertex model:

1. **Exact** location of the transition lines with both the single vertex and the plaquette model.
2. Thermodynamic quantities in remarkable agreement with the 2D results.
3. Nature of the phase transitions is qualitatively improved by making use of the tree of plaquettes.

	6V single vertices	6V plaquettes	6V 2D
PM-FMs	Frozen-to-PC	Frozen-to-PC	Frozen-to-crit
PM-AFs	Frozen-to-PC	Cont.-to-PC	KT

Spin-ice on a tree graph (cavity method)

Results for the six-vertex model:

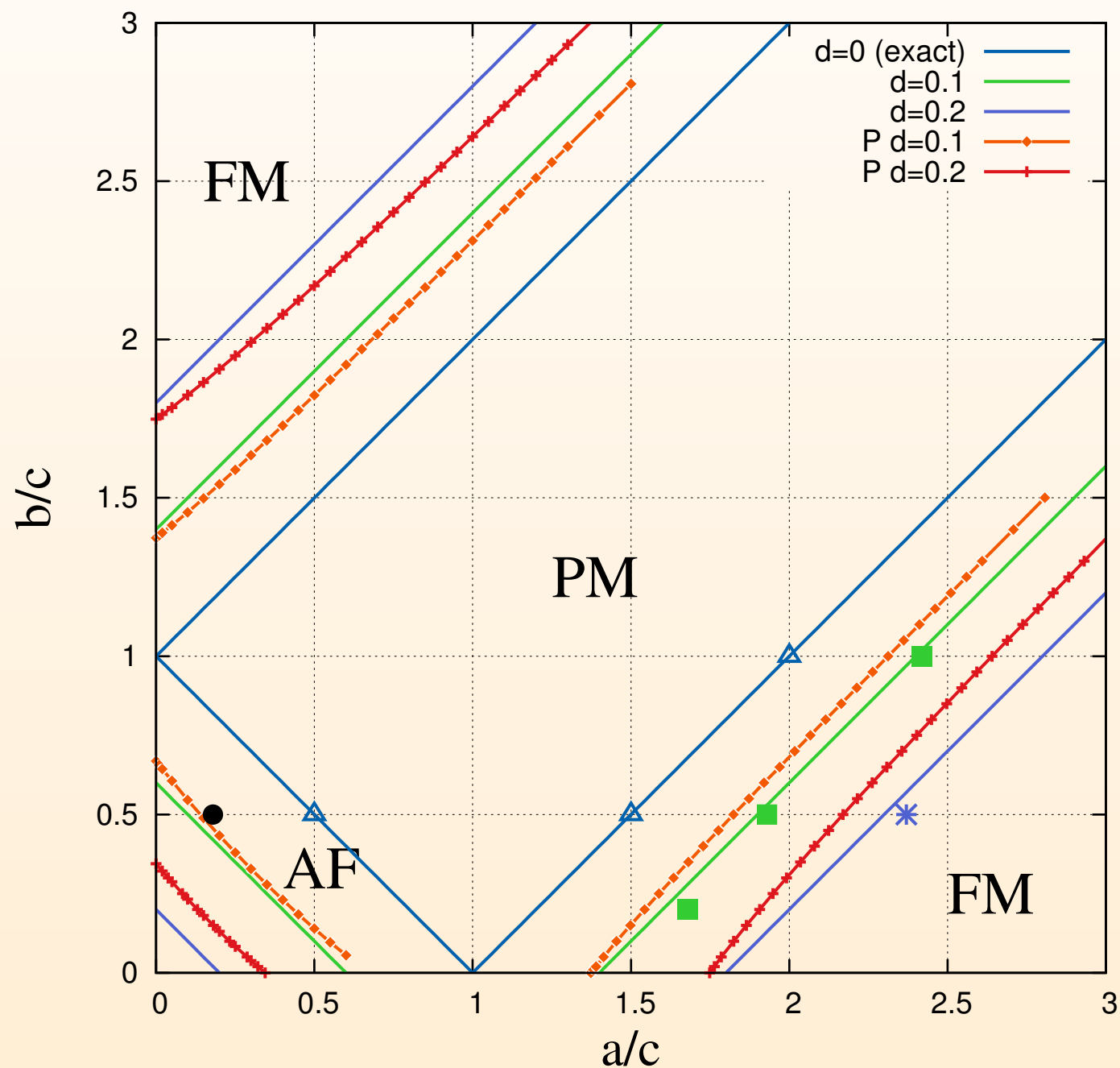
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PM-FMs	Frozen-to-PC	Frozen-to-PC	Frozen-to-crit
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→ goes in the good direction

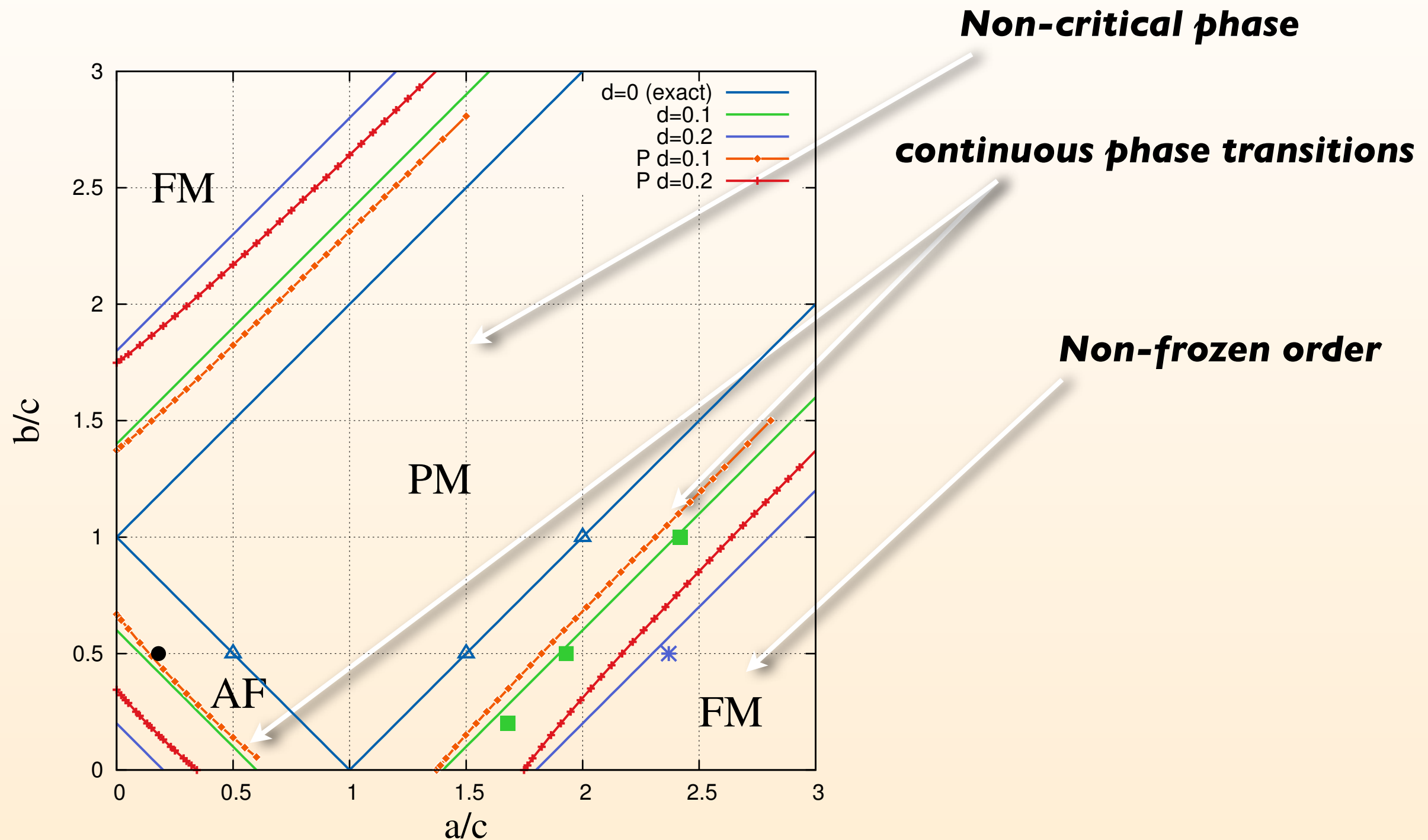
Spin-ice on a tree graph & CTMC

Results for the sixteen-vertex model:



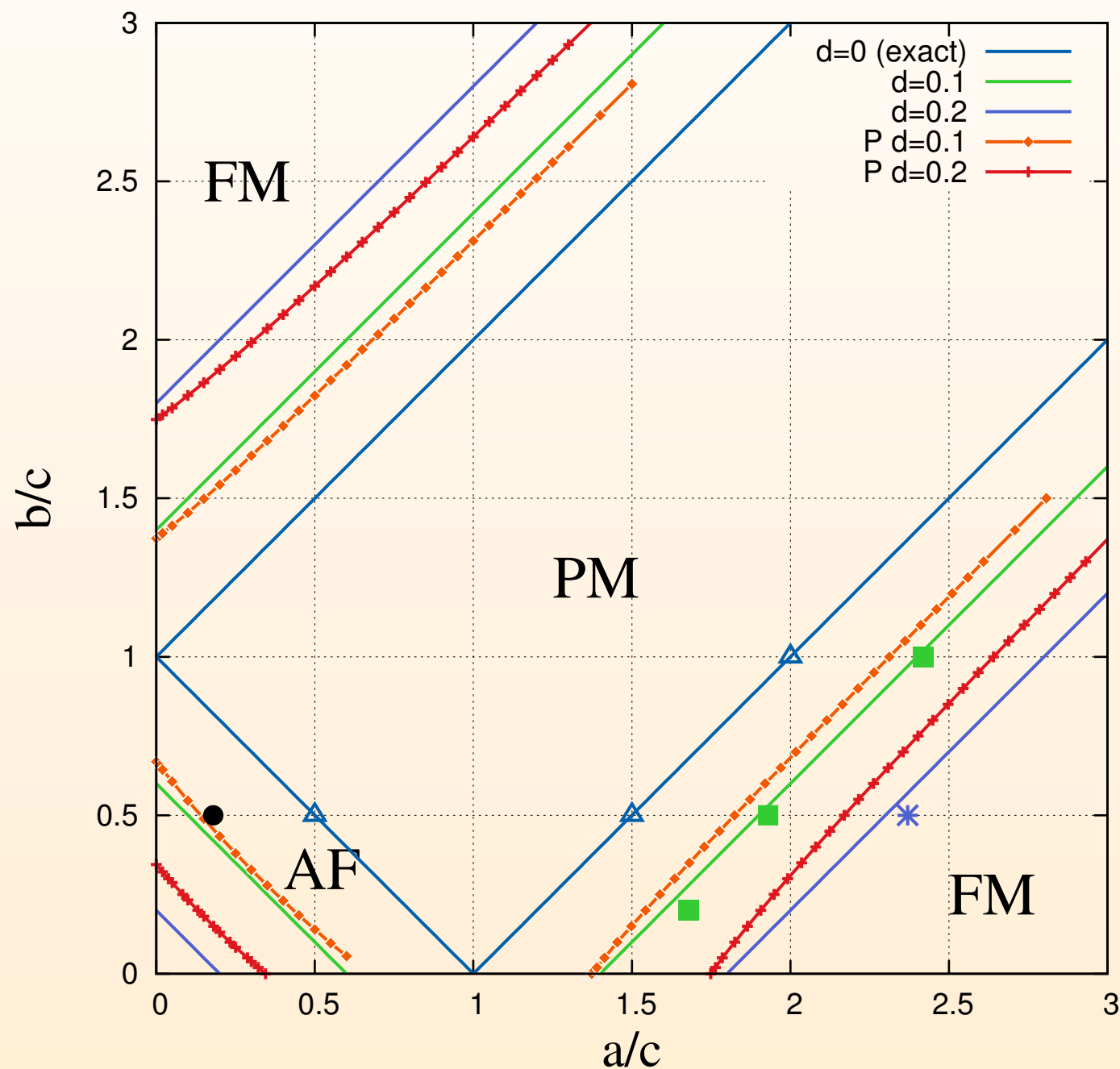
Spin-ice on a tree graph & CTMC

Results for the sixteen-vertex model:



Spin-ice on a tree graph & CTMC

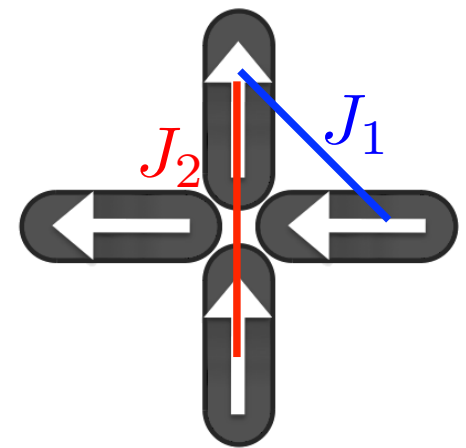
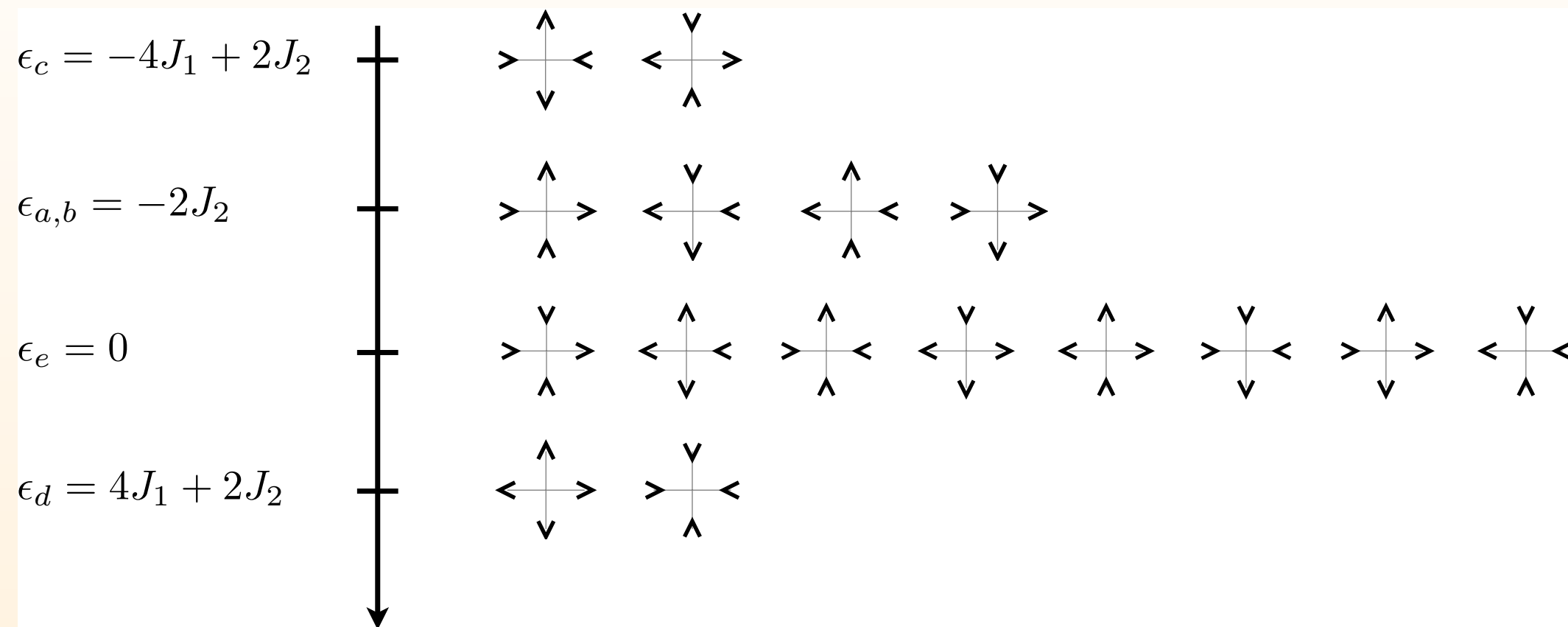
Results for the sixteen-vertex model:



**Apply this general picture to
concrete experimental
realisations**

Artificial spin ice

Fix the energy levels:



$$J_1 > J_2$$

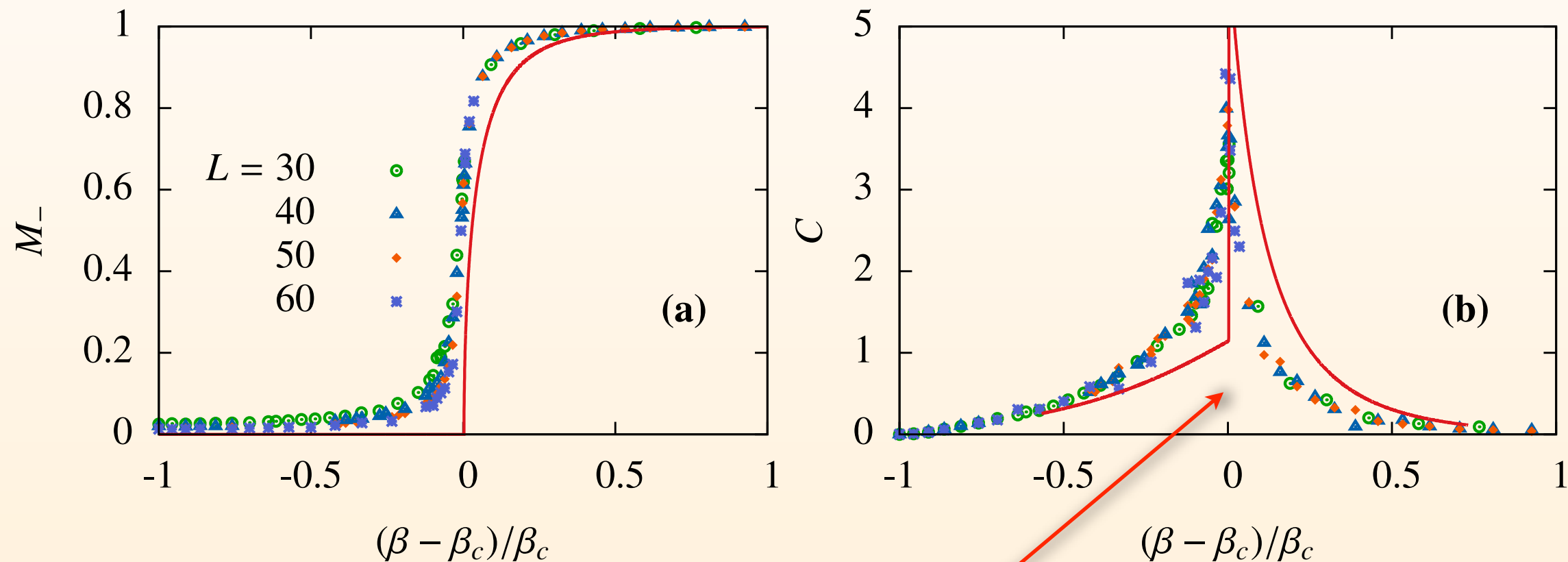
Dipolar interactions in the square lattice

$\implies$ 2 in - 2 out vertices are not equivalent.

One external parameter, the canonical temperature: $\beta = -\frac{\ln a}{\epsilon_a}$

'Thermal' Artificial spin ice

Numerics vs. Cavity calculation



Second order phase transition at $\beta_c \approx 2.65$

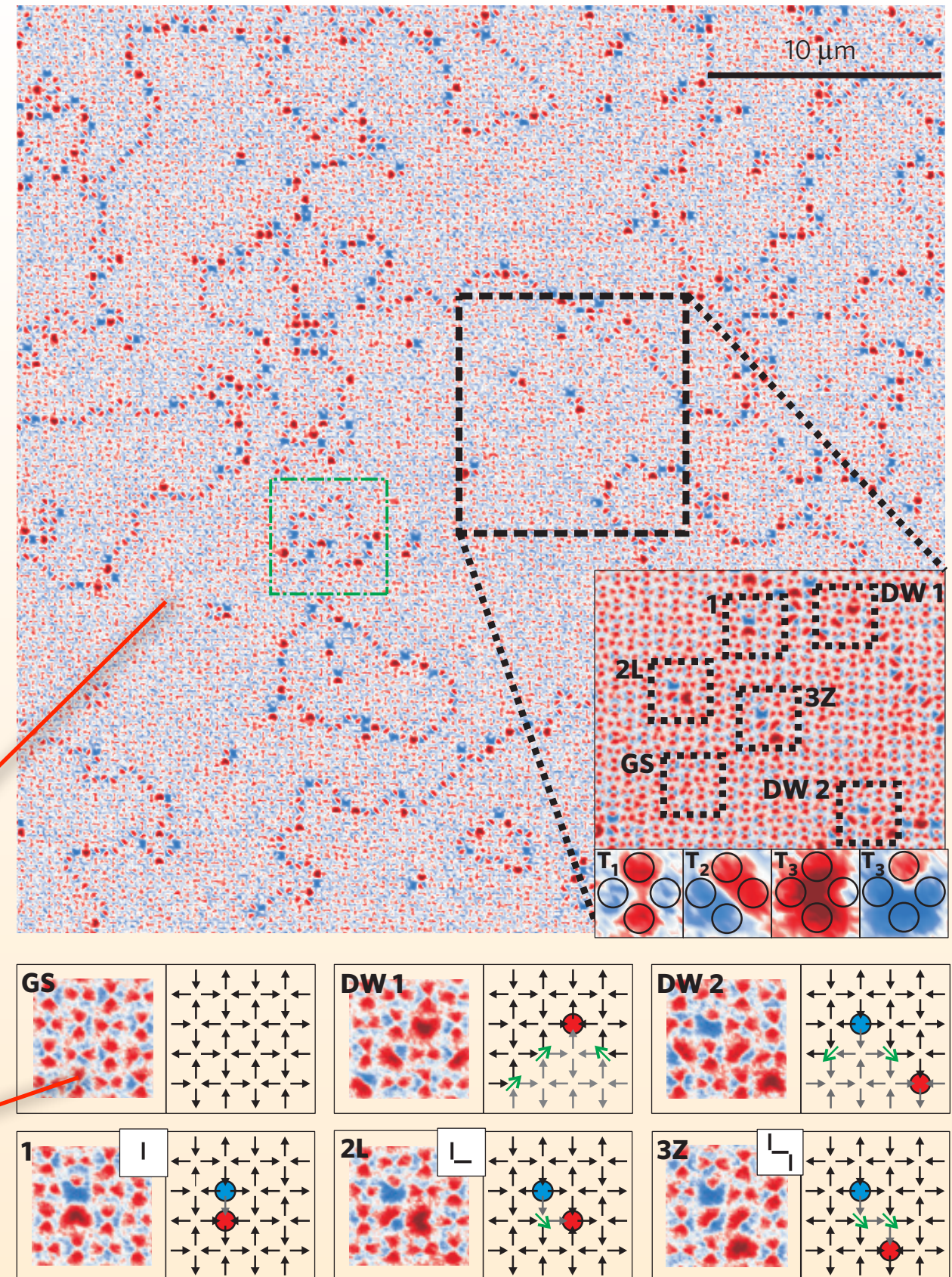
→ Compare with experiments

'Thermal' Artificial spin ice

1. **Thermal annealing** during deposition.
2. Nano-islands feel **thermal fluctuations** during the growth process.
3. After the growing process the islands **freeze**.

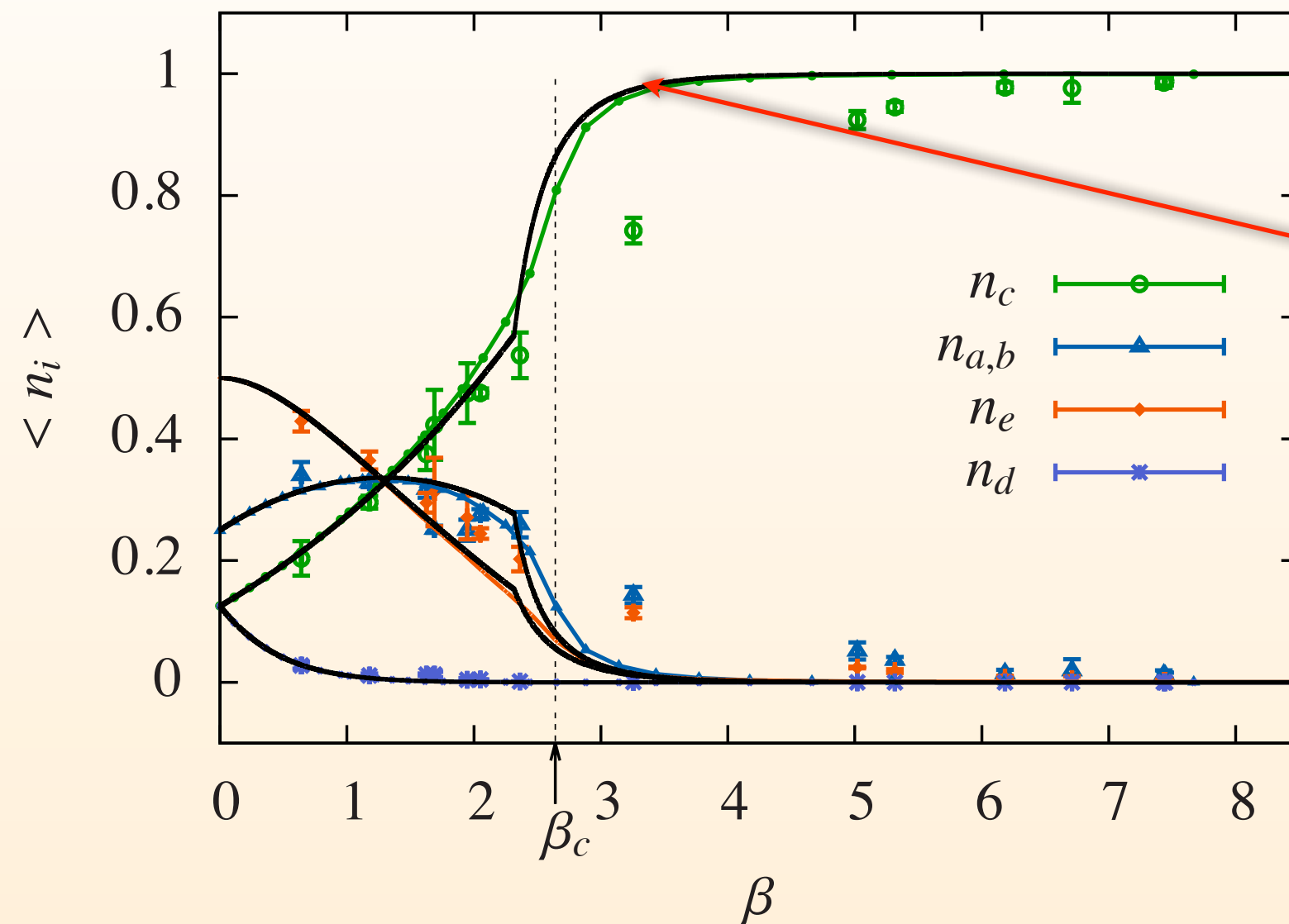
Very close to the expected
ground state

Excitations and **defects** can be
visualised



'Thermal' Artificial spin ice

Unpublished data from Morgan *et al.* 2012 ←

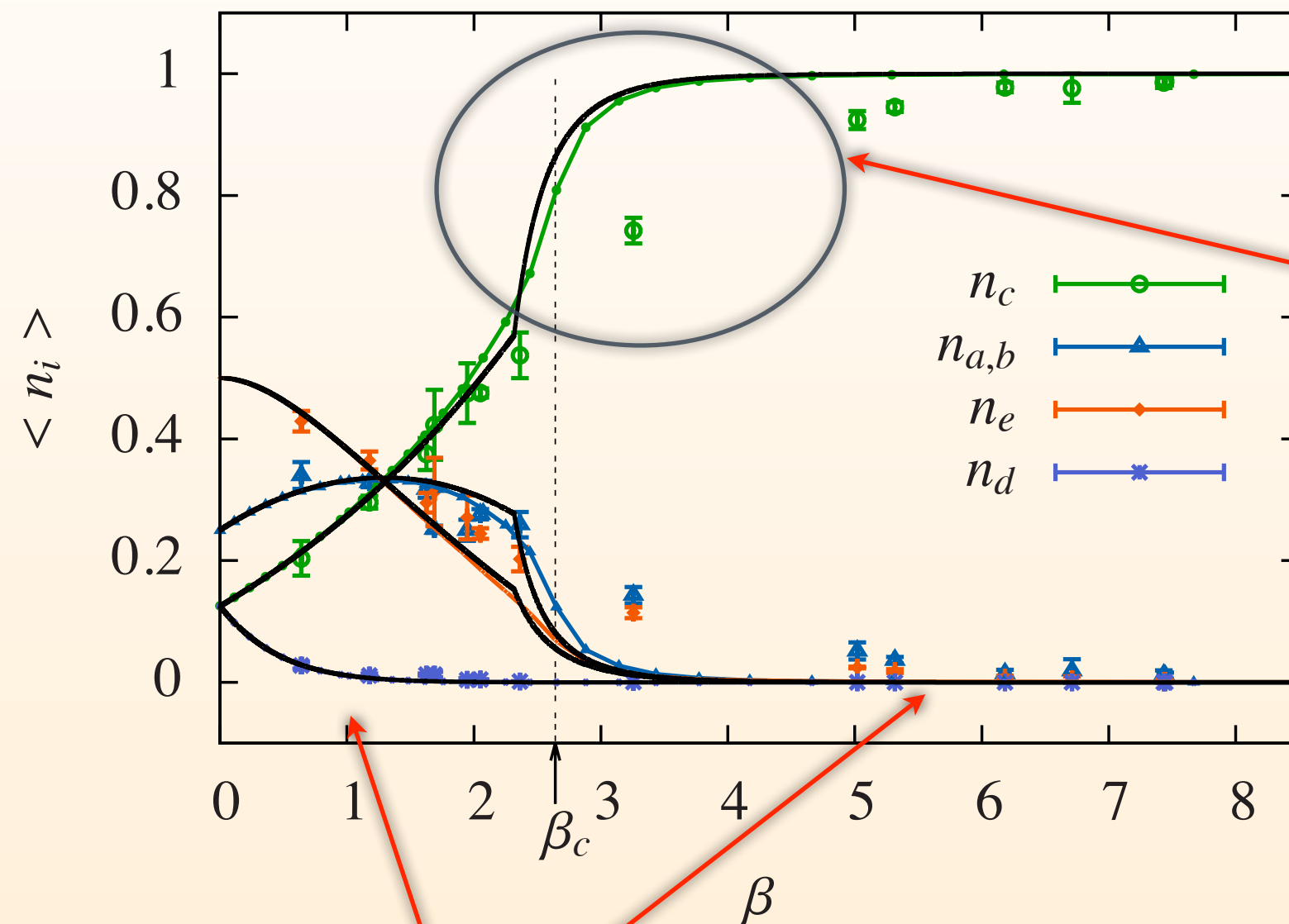


Numerics and analytics in agreement

Experimental data: $\beta_E = \ln \left(\frac{4n_c}{n_e} \right) (\epsilon_e - \epsilon_c)^{-1}$ vs. Canonical temperature

'Thermal' Artificial spin ice

Unpublished data from Morgan *et al.* 2012 ←



Critical slowing down
Equilibrium is not reached close to the critical point

$\beta \neq \beta_E$
Why ??

Our model reproduces quantitatively the experimental data

Conclusions equilibrium.

1. **Phase diagram** of the sixteen-vertex model.
The inclusion of **defects** modifies dramatically the thermodynamics.
2. **Continuously varying critical exponents** verify 'weak universality'.
3. Approximating the system by a **tree of square plaquettes** leads to **good agreement with 2D** results.
4. The model **reproduces experimental data** away from the critical point
→ Relationship between **configurational temperature** and **canonical temperature in ASI?**
→ Out-of-equilibrium phenomena ?

Out-of-equilibrium.

Phase ordering dynamics after a quench.

Evolution of the system across a phase transition.

- Give updating rules: **Non-conserved** order parameter (single spin flips)

coupled to a thermal bath

Stochastic dynamics

- Prepare the system in a **disordered** equilibrium state and **quench** it into a known equilibrium **ordered symmetry broken** phase



Competition between opposite orders

Slow dynamics $L(t) \sim t^z$



Apply this procedure to the sixteen-vertex model

Out-of-equilibrium.

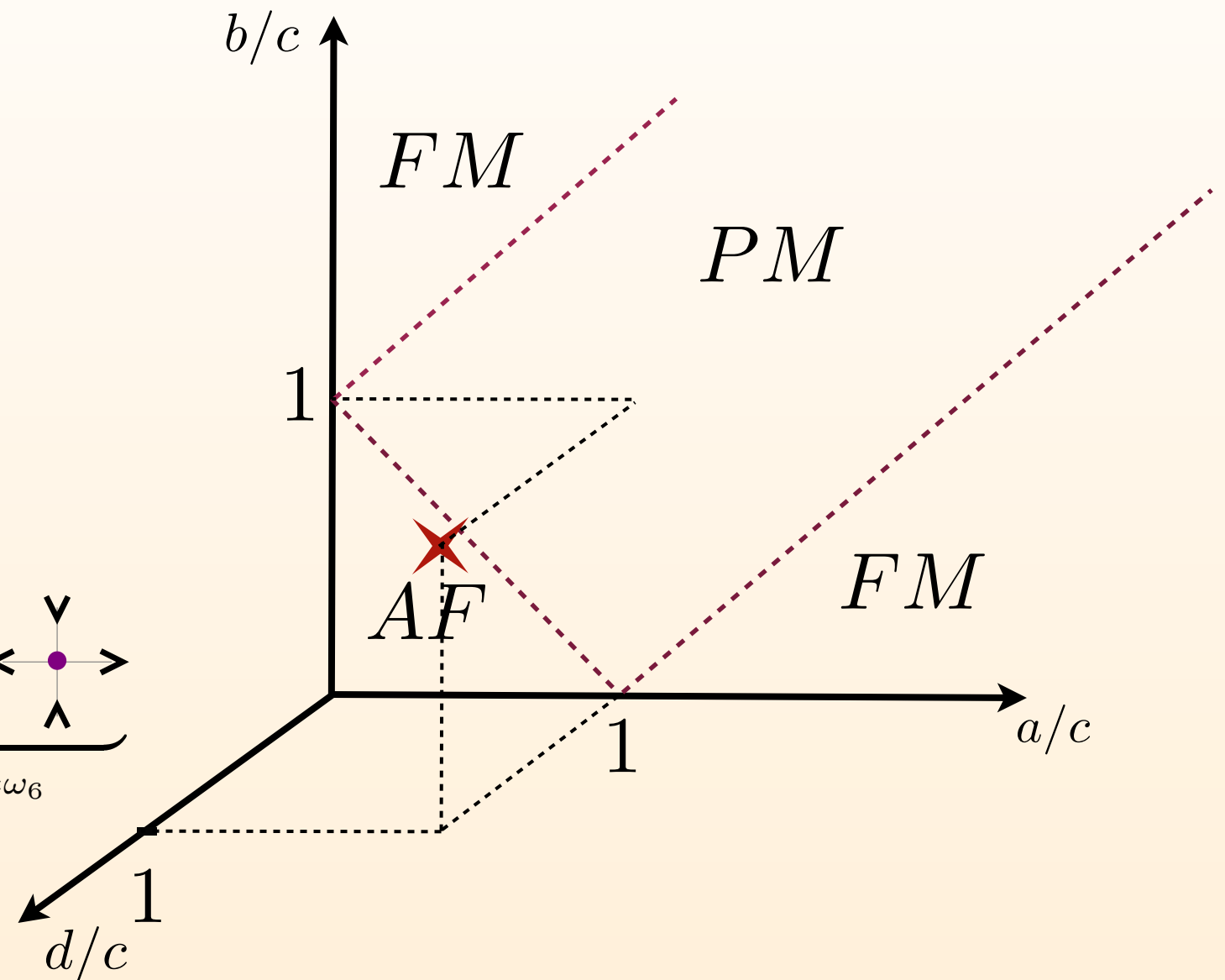
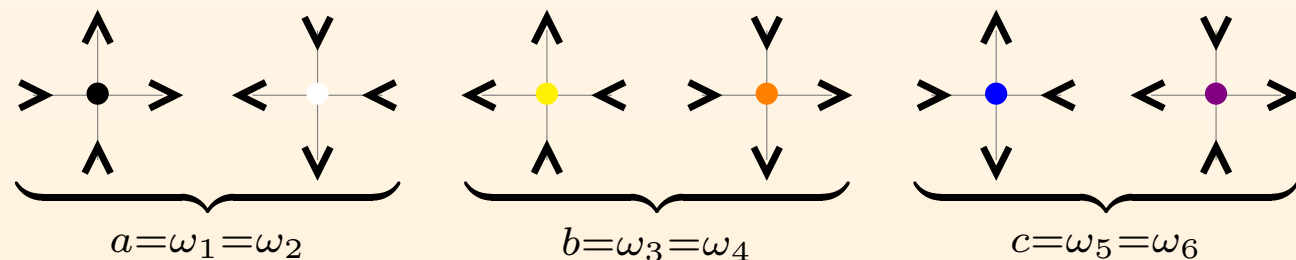
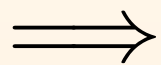
Quench into the PM phase.

initial configuration:

$$a = b = c = d = e = 1 \quad (T = \infty)$$

at $t=0$ (instantaneous)

$$a = b = c \gg d, e$$



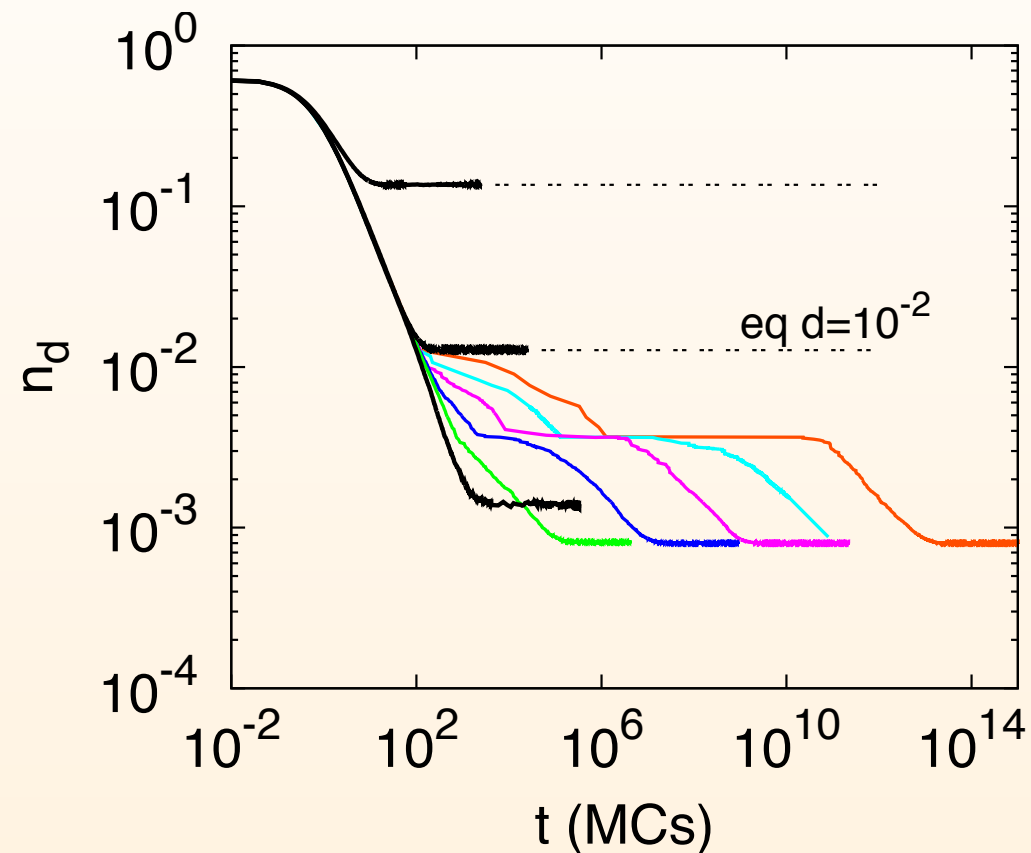
Magnetisation = 0 BUT 'close' to a QLRO phase $\Rightarrow$

No order parameter to describe the relaxation process

Out-of-equilibrium.

Quench into the PM phase.

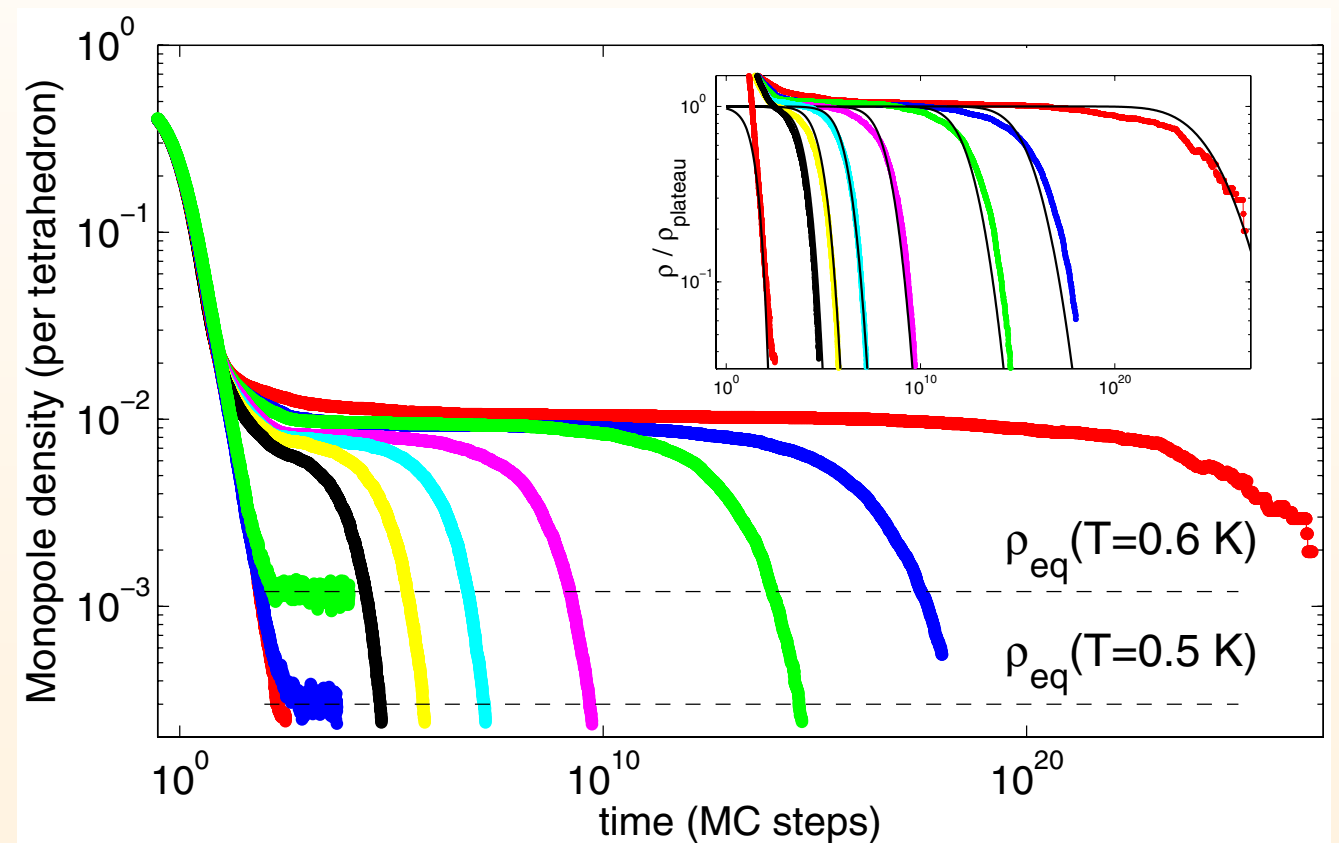
Density of defects



2D vertex model

$$d = e = 10^{-1}, \dots, 10^{-4}, \dots, 10^{-8}$$
$$N = 2L^2 = 5000$$

Levis & Cugliandolo 2011



3D pyrochlore spin ice with dipolar interactions

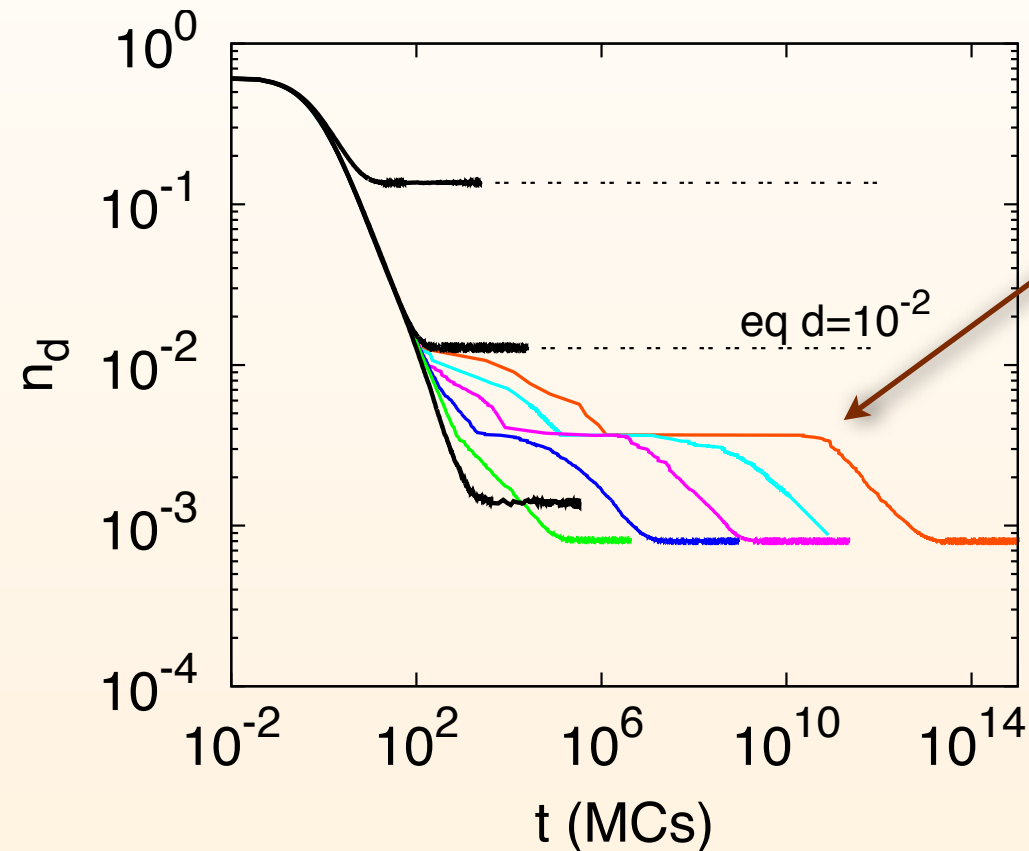
$$T = 0.6 \text{ K}, \dots, 0.025 \text{ K}$$
$$N = 8192$$

Castelnovo, Moessner & Sondhi 2012

Out-of-equilibrium.

Quench into the PM phase.

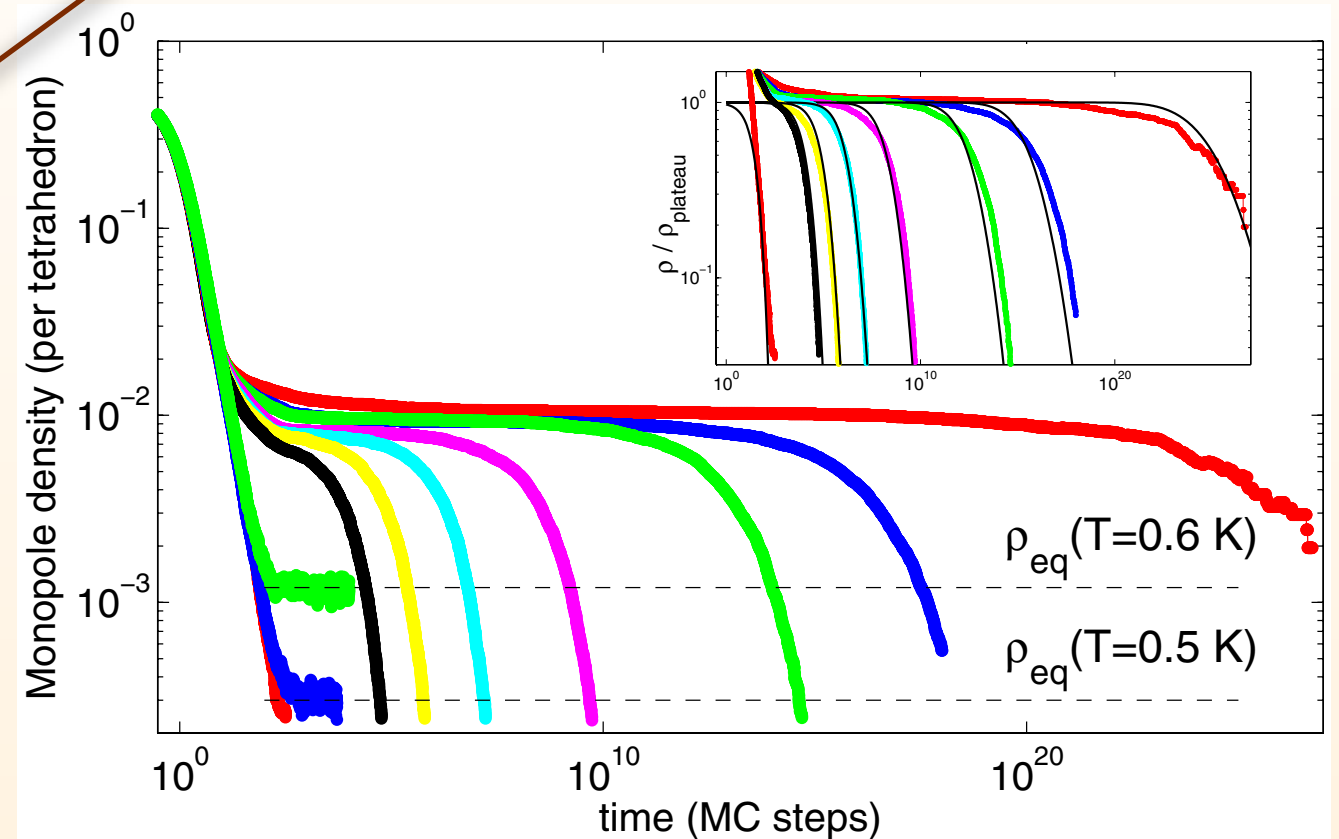
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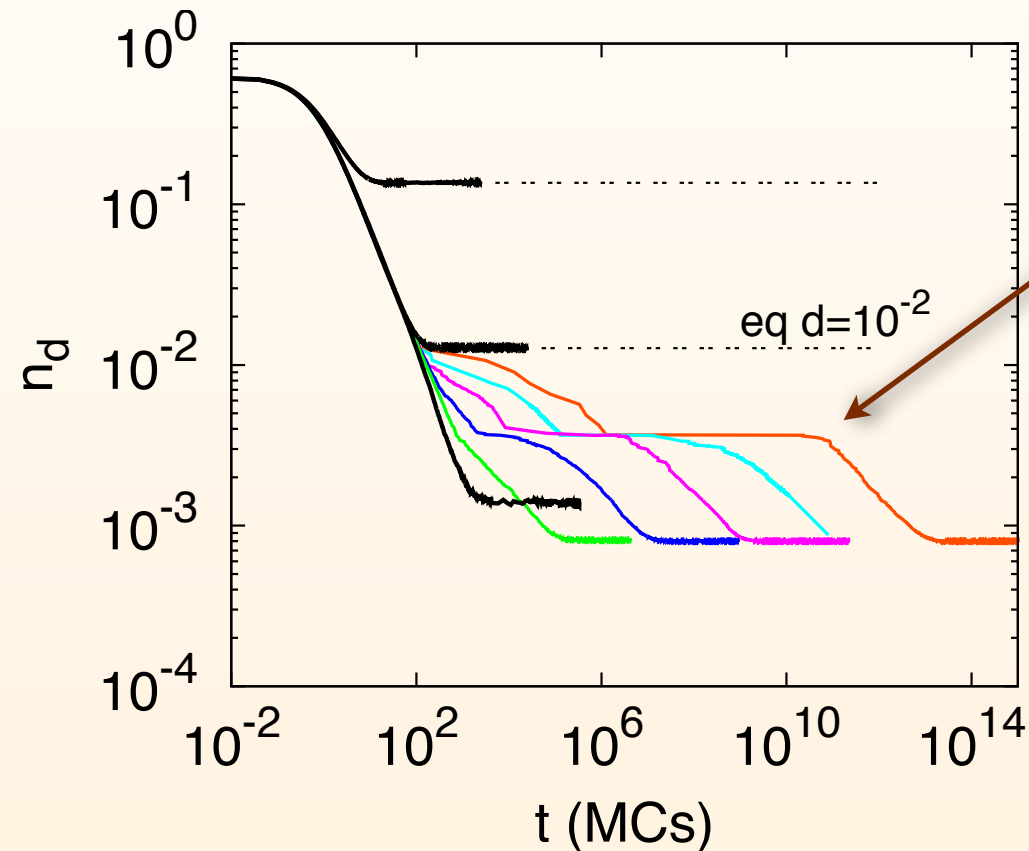
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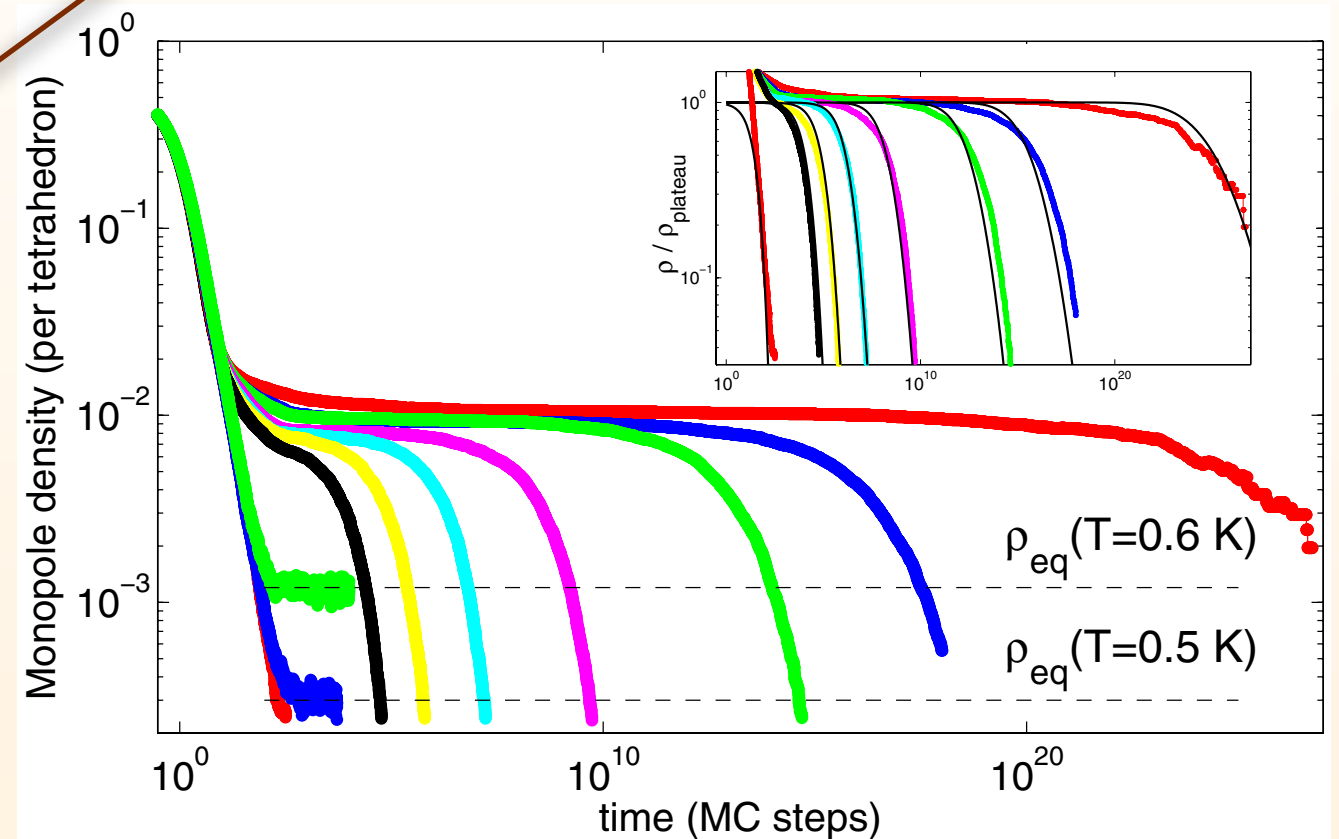
2D vertex model

$$d = e = 10^{-1}, \dots, 10^{-4}, \dots, 10^{-8}$$
$$N = 2L^2 = 5000$$

Levis & Cugliandolo 2011

$\Rightarrow$ Due to finite size ? $d = e$? are long range interactions needed ?

Dynamical arrest for
 $d < 10^{-4}$



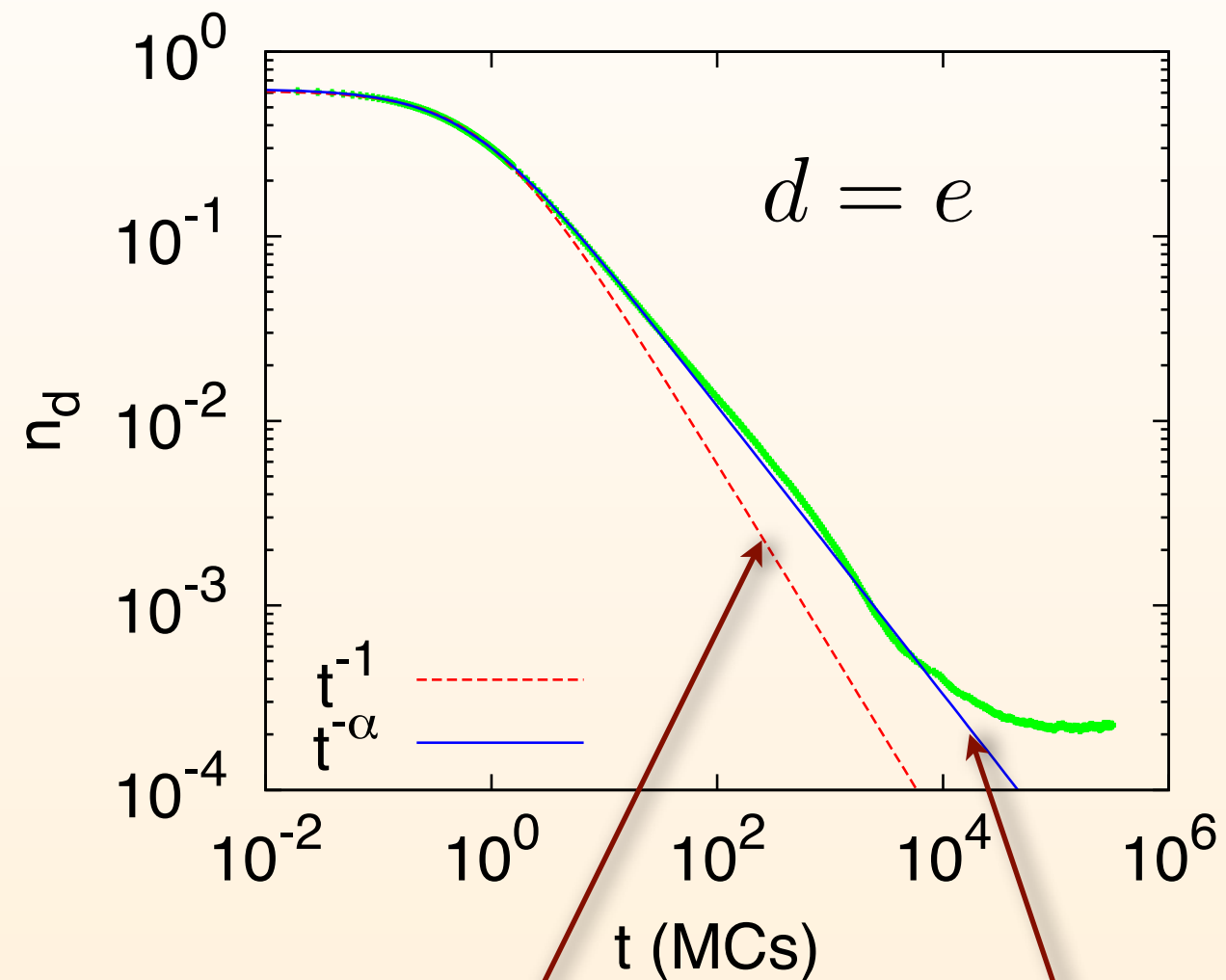
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Quench into the PM phase.



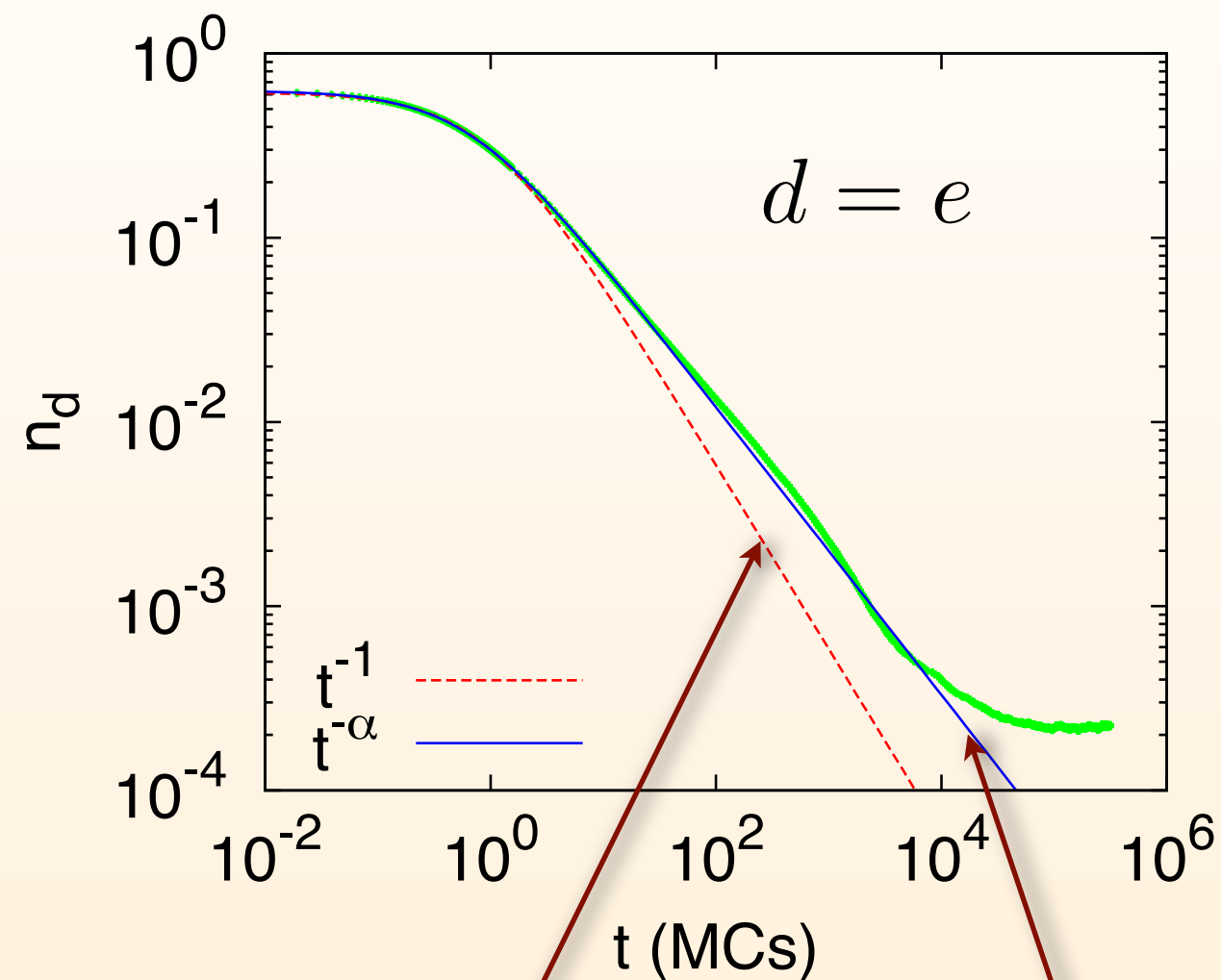
$$\alpha \approx 0.78$$

NN spin ice model described
by a mean field reaction-
diffusion model

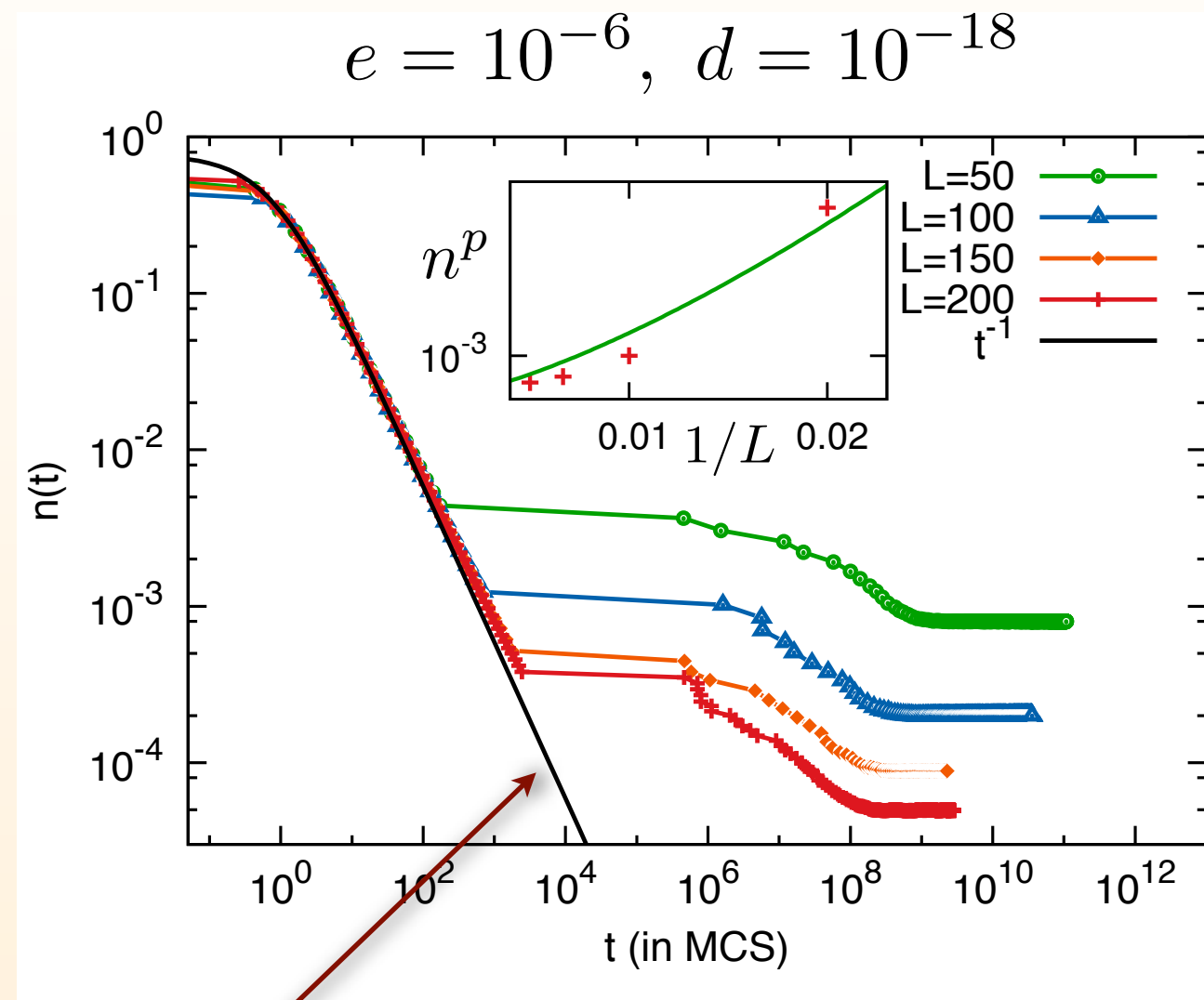
$$n(t) = \frac{\rho_0}{(1 + \Omega t)^\alpha}$$

Out-of-equilibrium.

Quench into the PM phase.



$$\alpha \approx 0.78$$



$$\alpha \approx 1$$

$$d < e^2$$

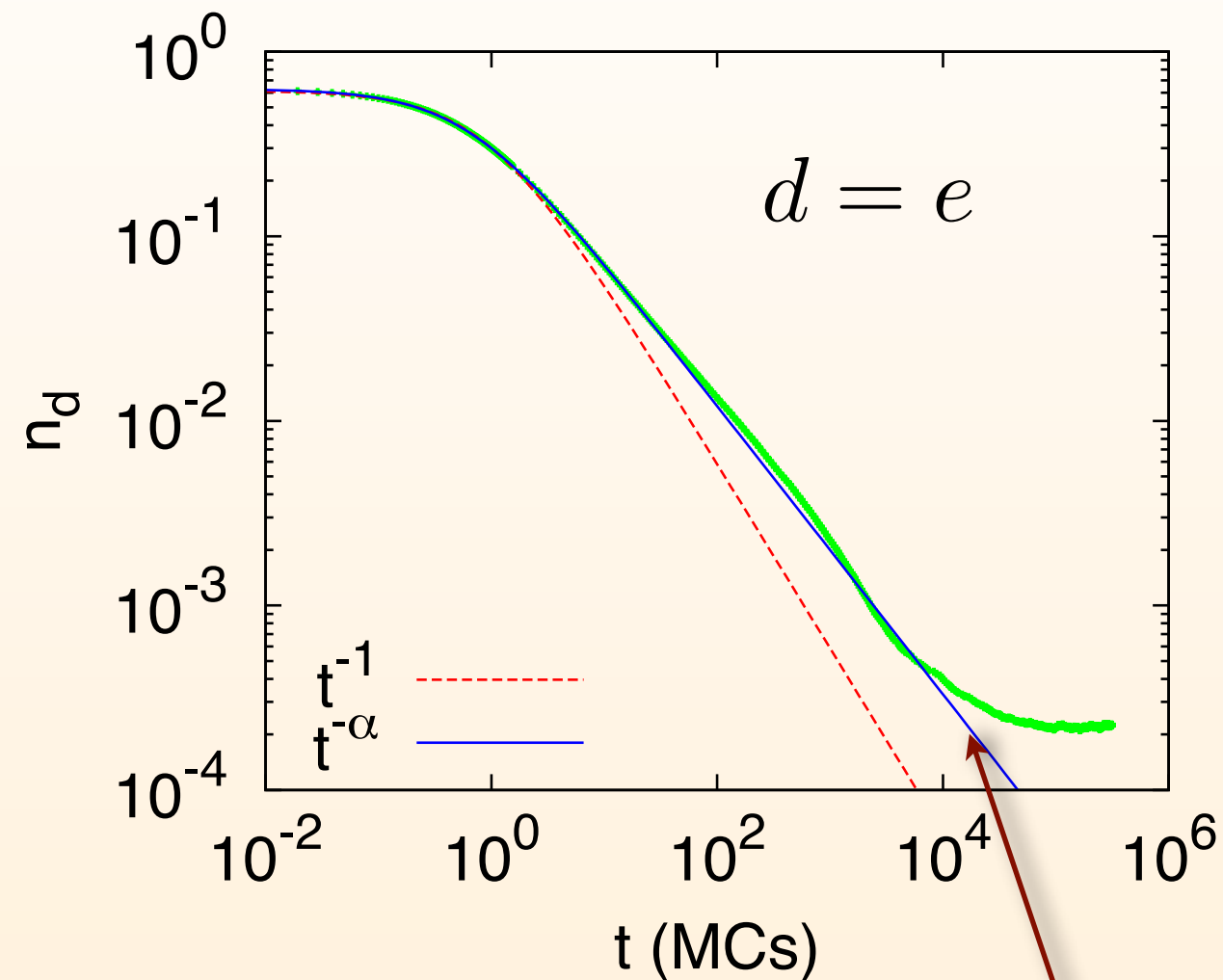
$\Rightarrow (2q) \rightarrow (q) + (q)$
spontaneously.

NN spin ice model described
by a mean field reaction-
diffusion model

$$n(t) = \frac{\rho_0}{(1 + \Omega t)^\alpha}$$

Out-of-equilibrium.

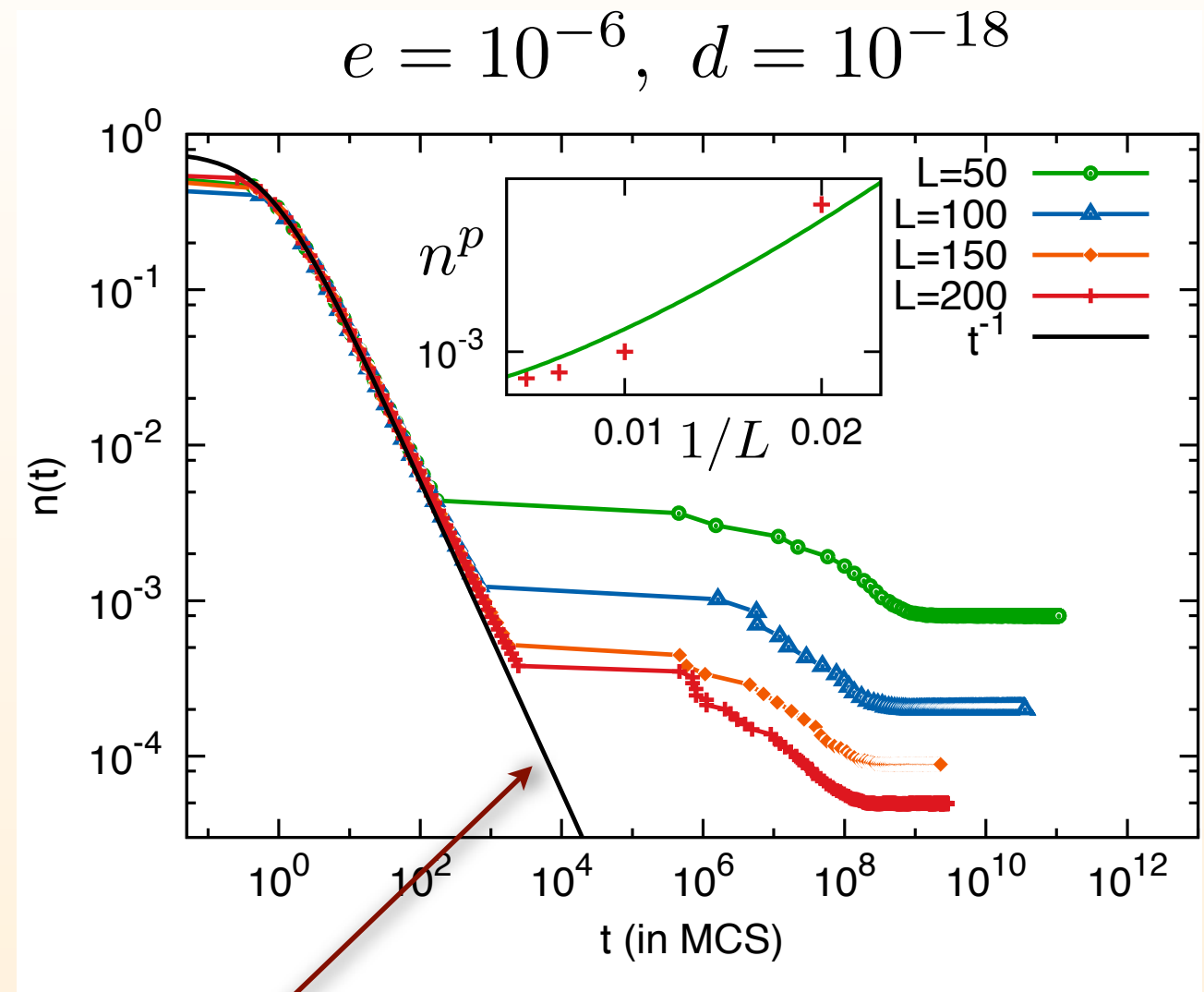
Quench into the PM phase.



$$\alpha \approx 0.78$$

Same power law as in **3D spin-ice**.

The decay **power** depends on the value of the parameters.



$$\alpha \approx 1$$

$$d < e^2$$

$\Rightarrow (2q) \rightarrow (q) + (q)$
spontaneously.

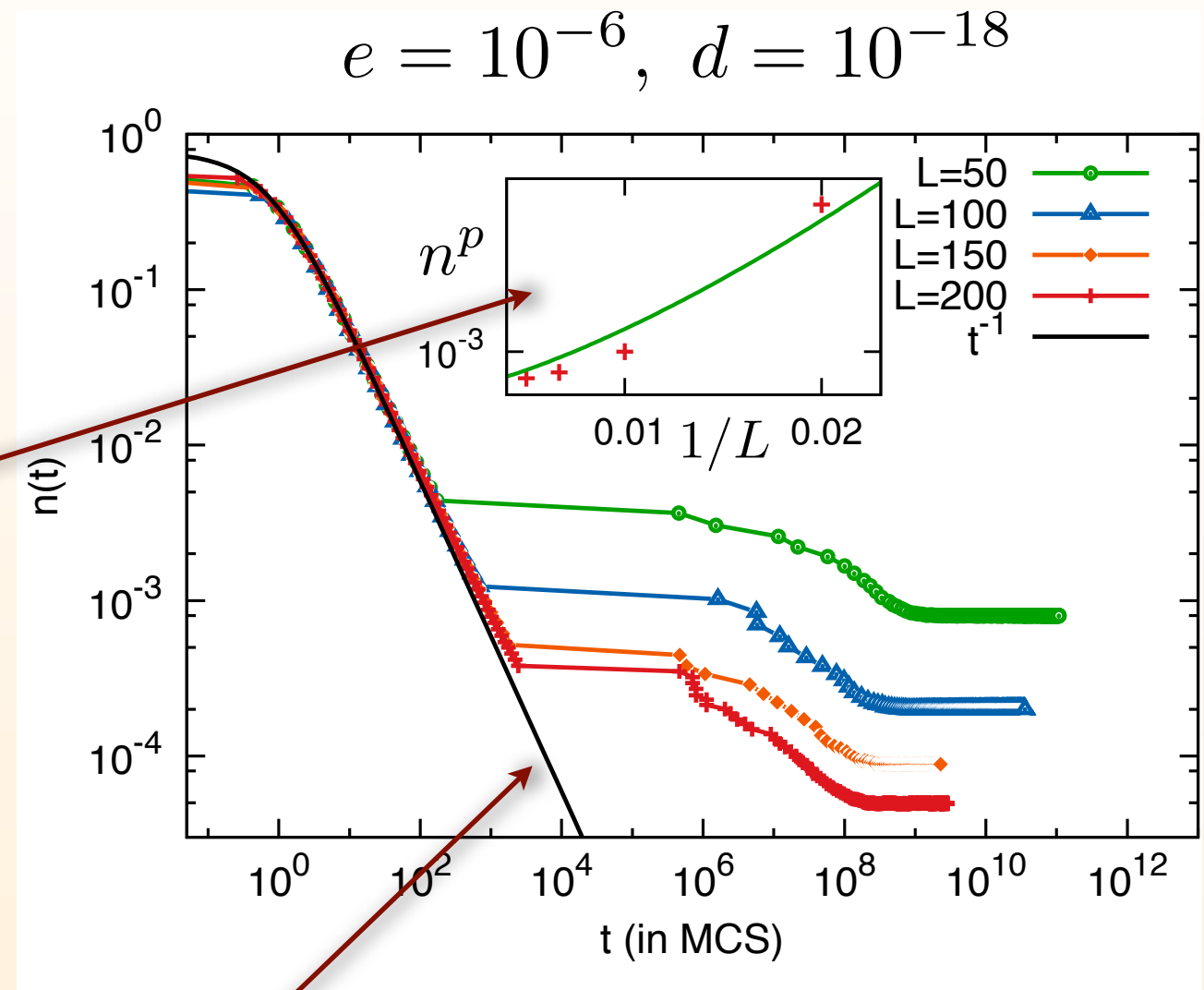
Quench into the PM phase.

Size dependence

The dynamical arrest is **size dependent**:

the **height** and the **time spend** in the plateau decrease for larger systems.

At the **thermodynamic limit** ?



$$\alpha \approx 1$$

$$d < e^2$$

$$\Rightarrow (2q) \rightarrow (q) + (q)$$

spontaneously.

Out-of-equilibrium.

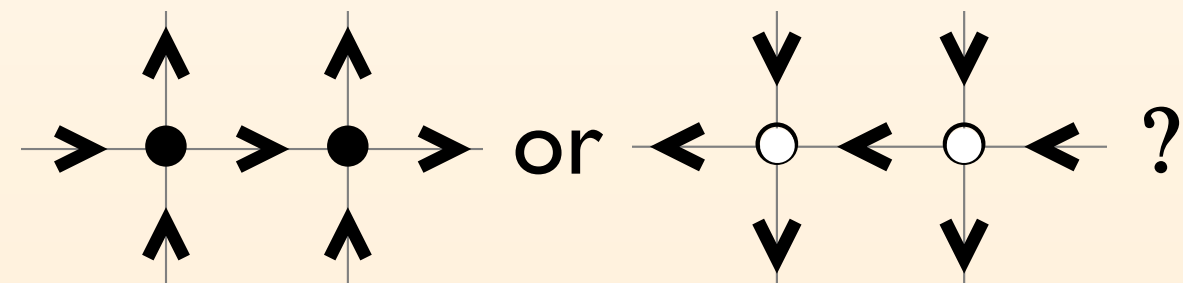
Quench into the FM phase.

initial configuration:

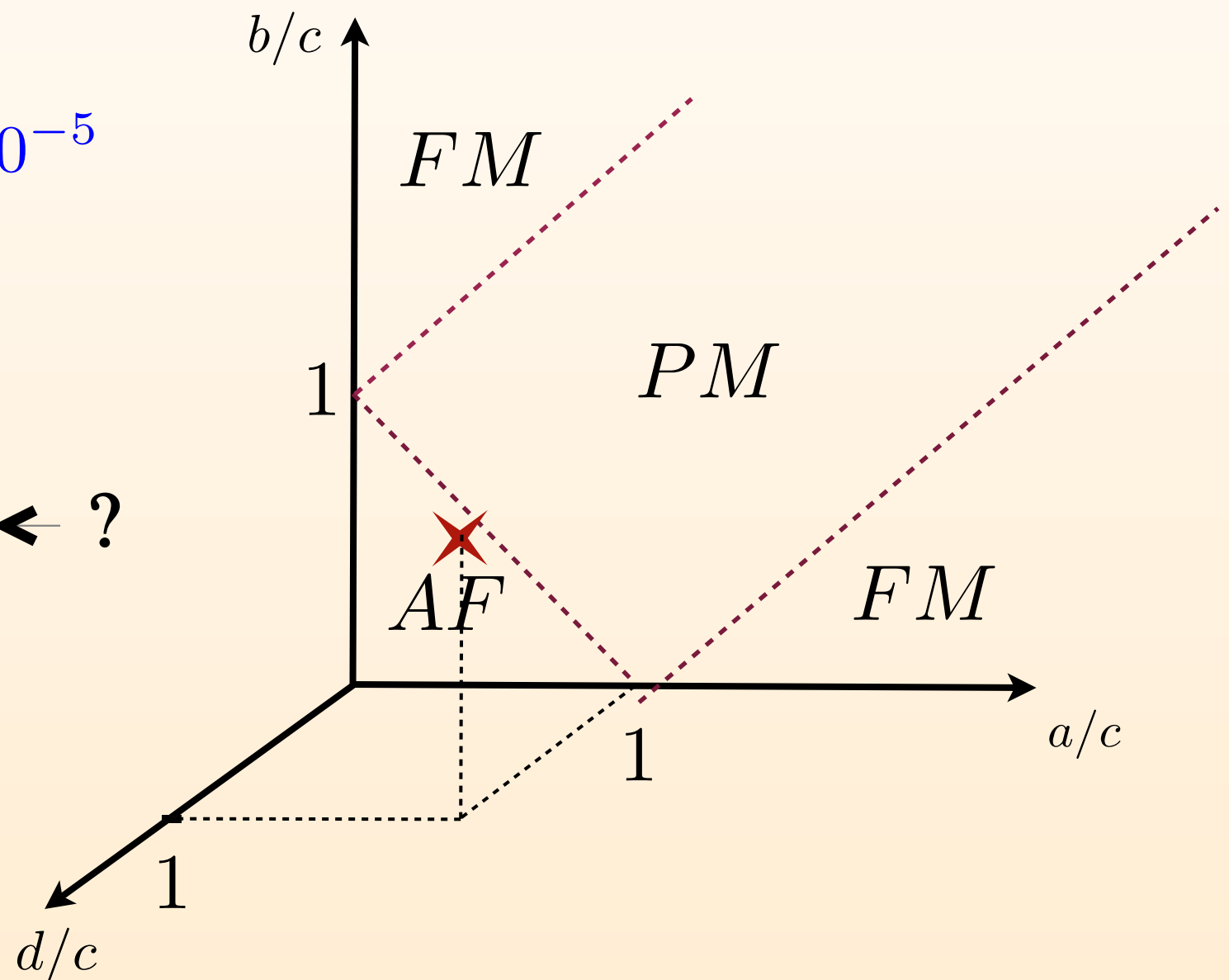
$$a = b = c = d = e = 1 \quad (T = \infty)$$

at $t=0$ (instantaneously)

$$a = 5, \quad b = c = 1, \quad d = e = 10^{-5} \quad (T < T_c)$$

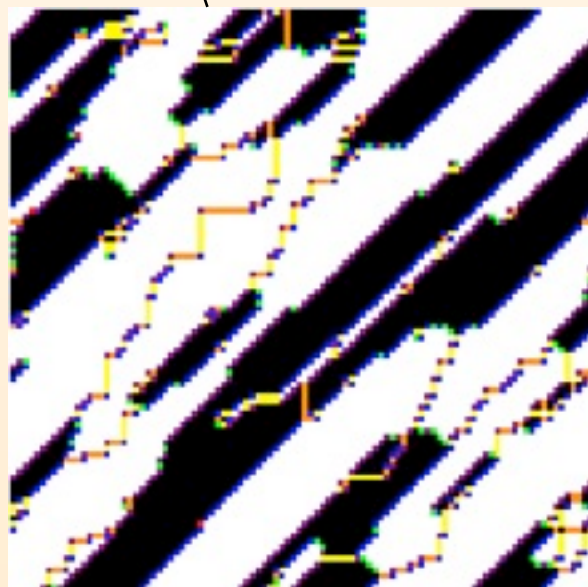
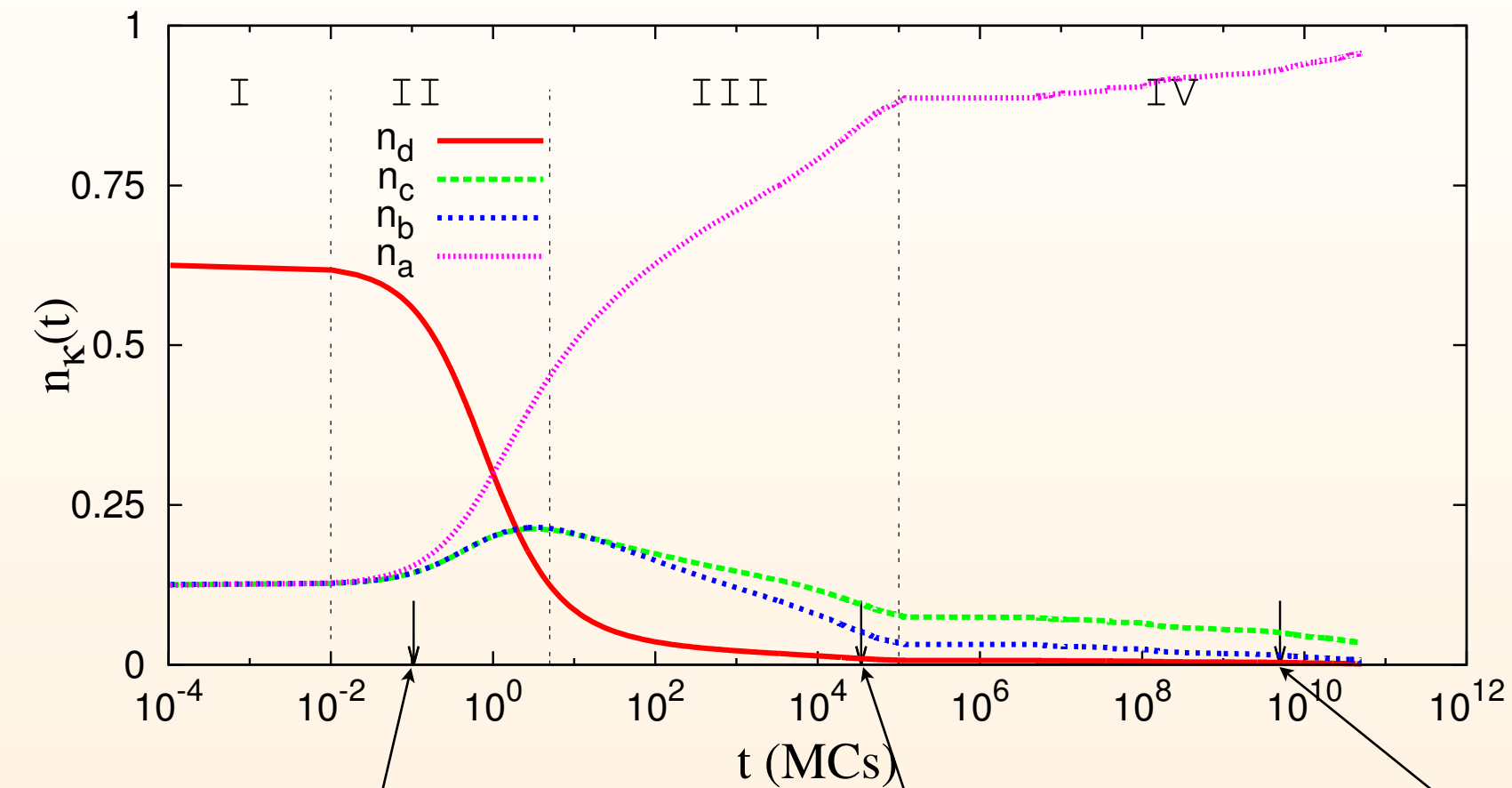


→ *slow relaxation*



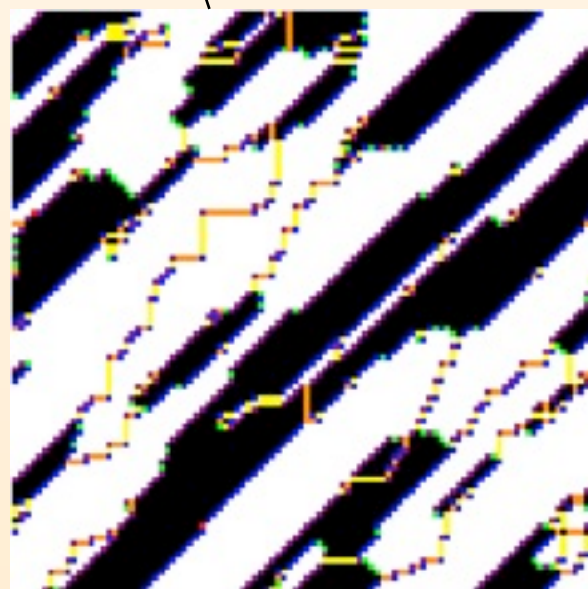
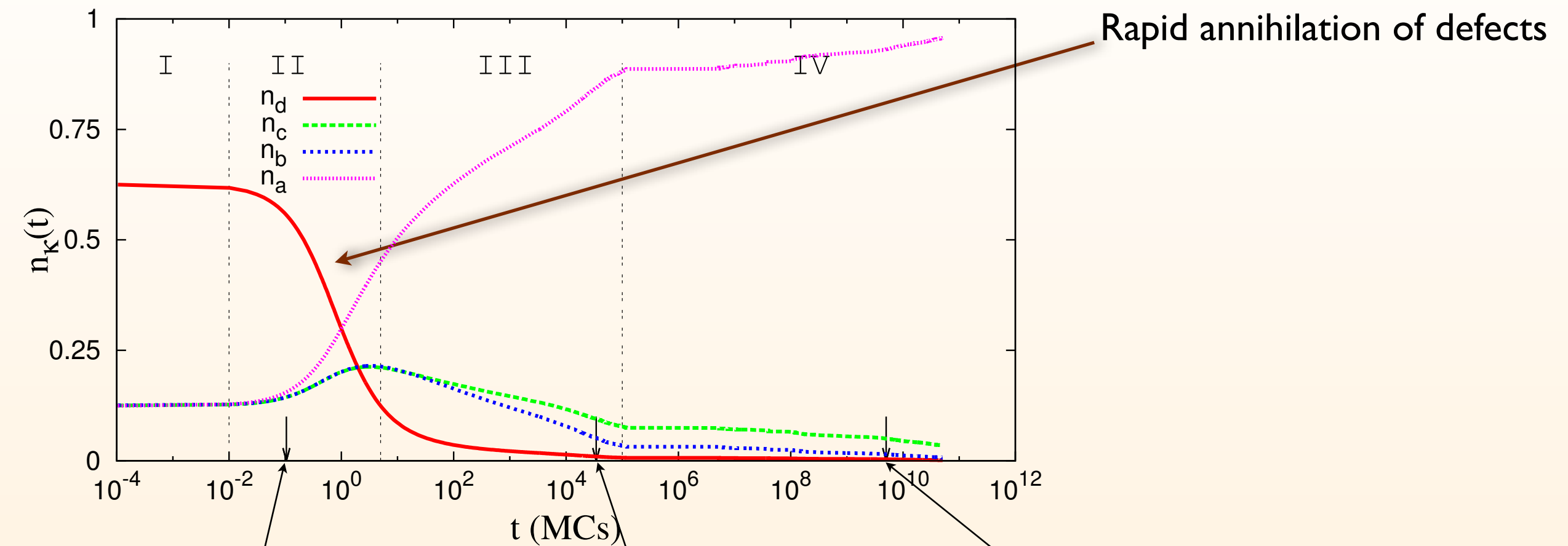
Out-of-equilibrium.

Quench into the FM phase.



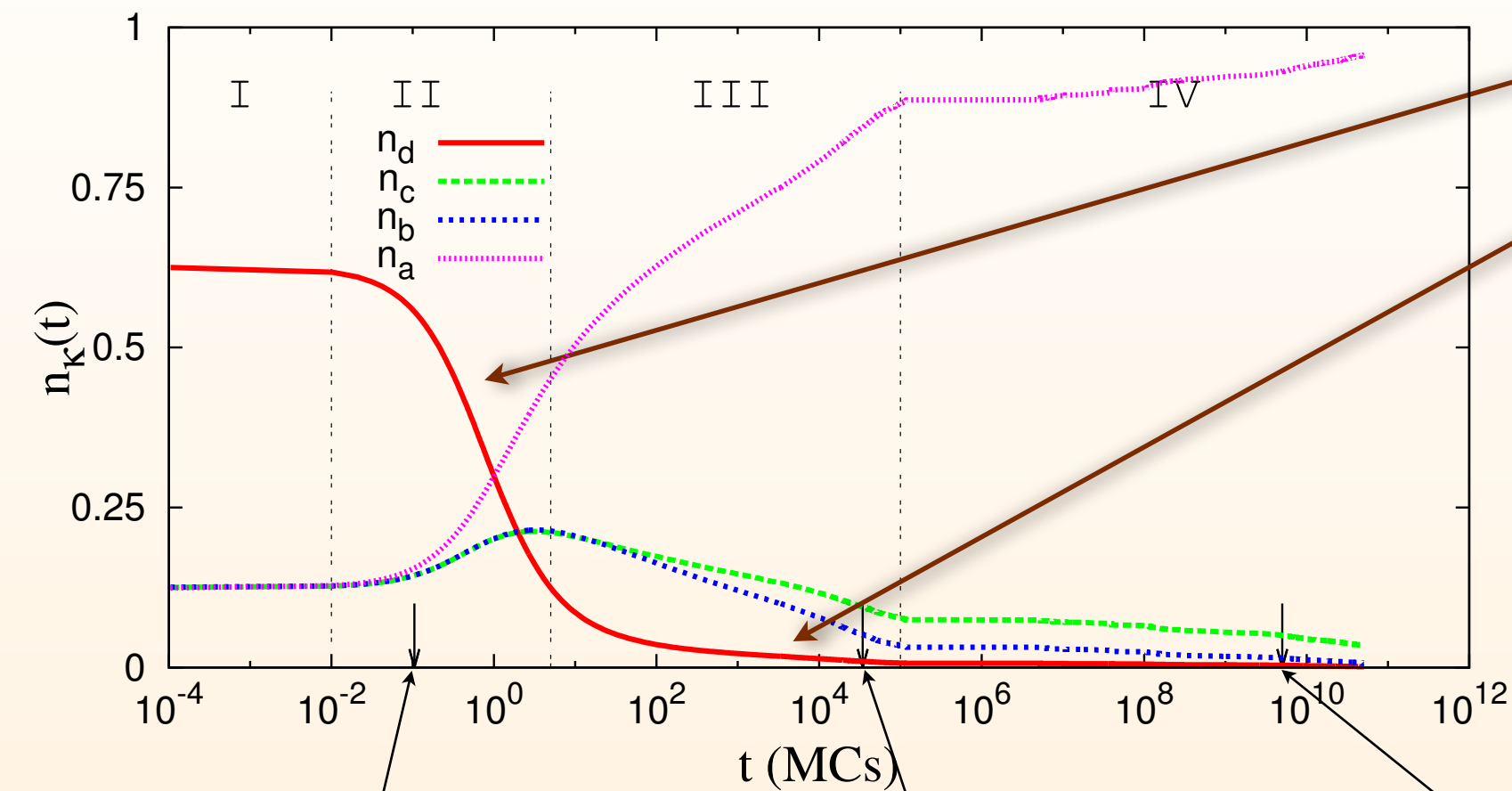
Out-of-equilibrium.

Quench into the FM phase.



Out-of-equilibrium.

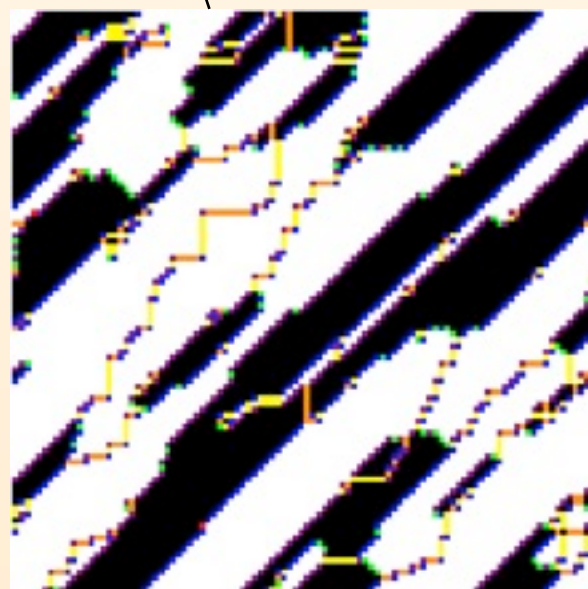
Quench into the FM phase.



Rapid annihilation of defects

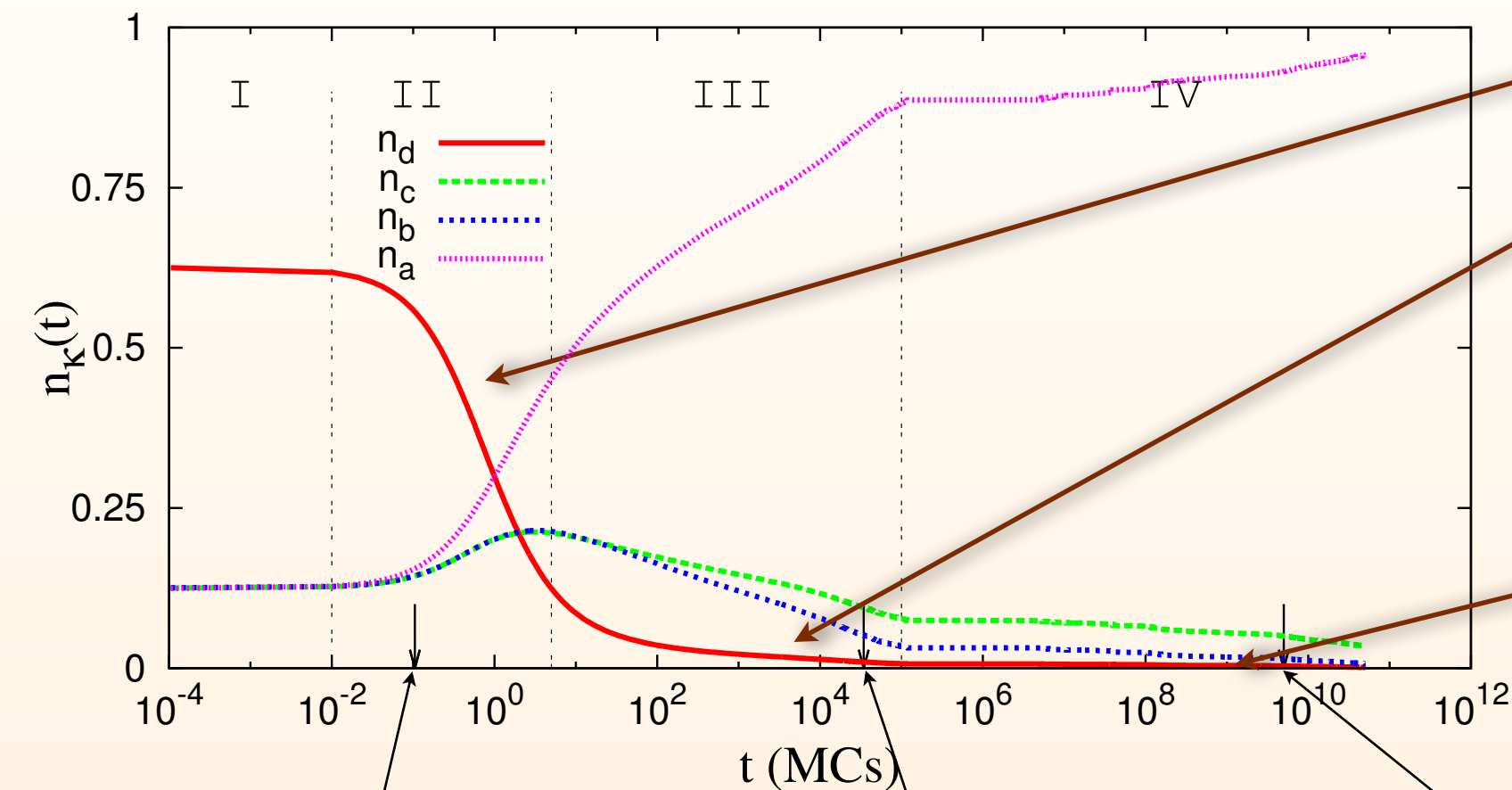
Growth of FM **domains** with walls made of c-vertices and linked by **strings**.

Defects far from each other, difficult to annihilate: **slow dynamics**.



Out-of-equilibrium.

Quench into the FM phase.

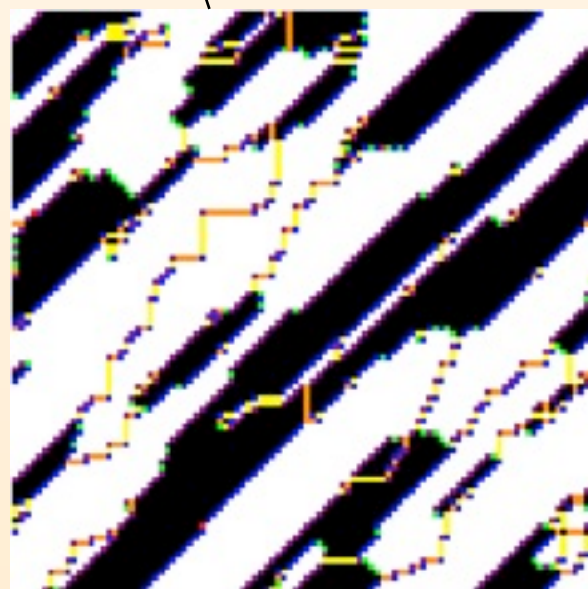


Rapid annihilation of defects

Growth of FM **domains** with walls made of c-vertices and linked by **strings**.

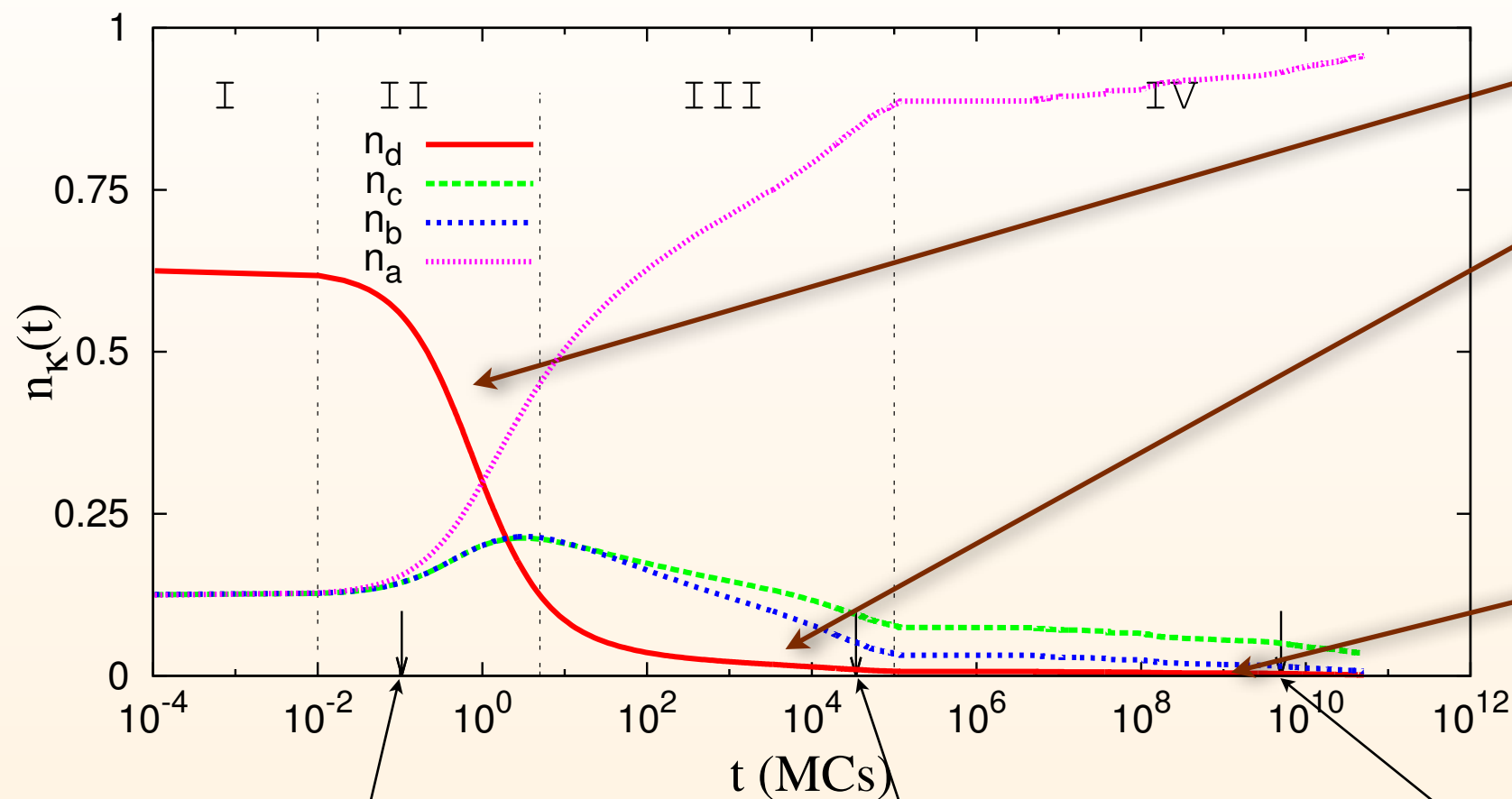
Defects far from each other, difficult to annihilate: **slow dynamics**.

Very stable domains = **Parallel bands**



Out-of-equilibrium.

Quench into the FM phase.

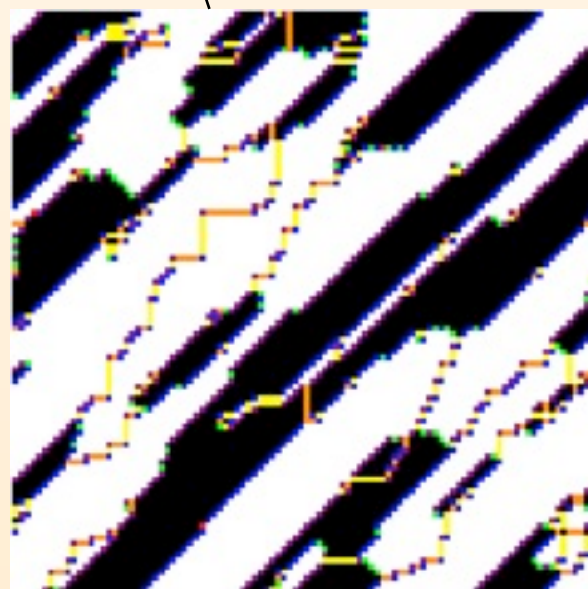


Rapid annihilation of defects

Growth of FM **domains** with walls made of c-vertices and linked by **strings**.

Defects far from each other, difficult to annihilate: **slow dynamics**.

Very stable domains = **Parallel bands**



$$L_{\parallel} \sim t^{1/2}$$

$$L_{\perp}?$$

Out-of-equilibrium.

Quench into the AF phase.

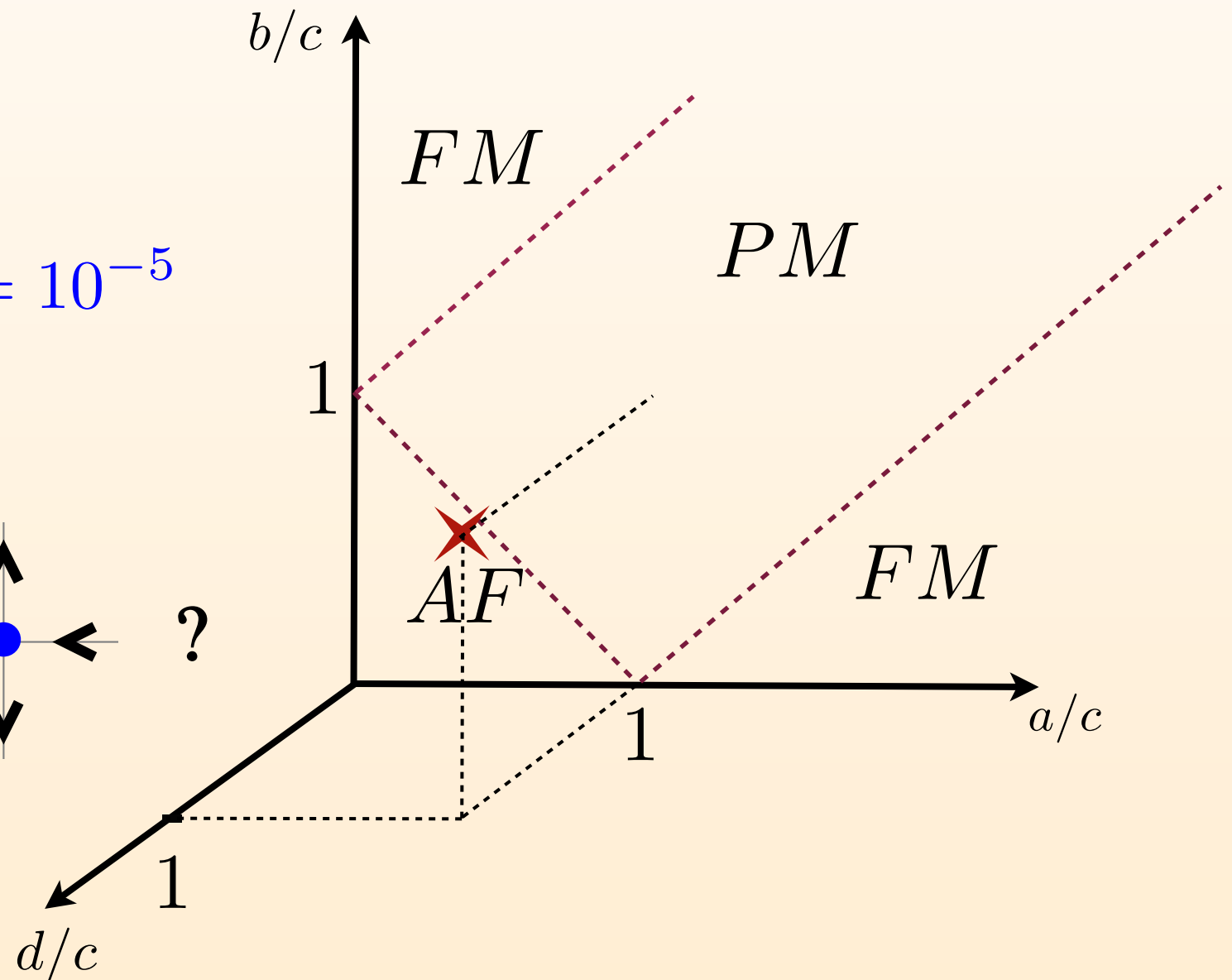
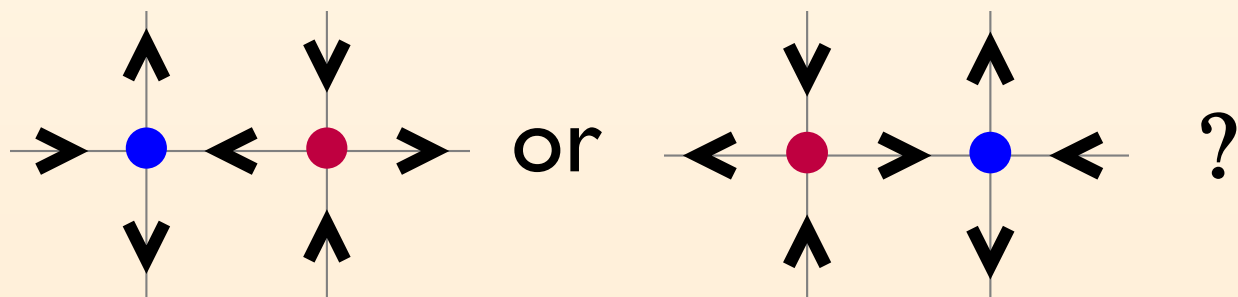
Same procedure

initial configuration:

$$a = b = c = d = e = 1 \quad (T = \infty)$$

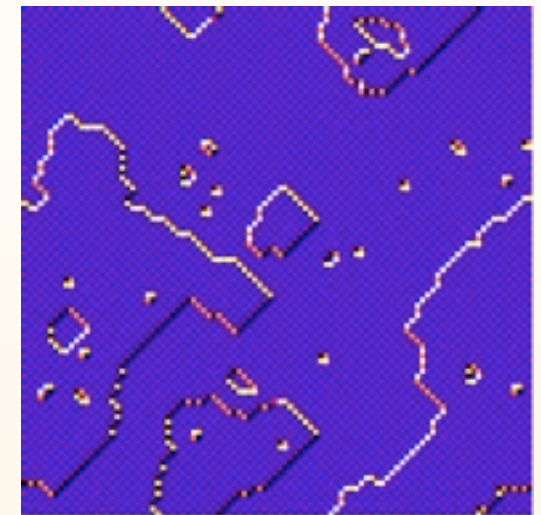
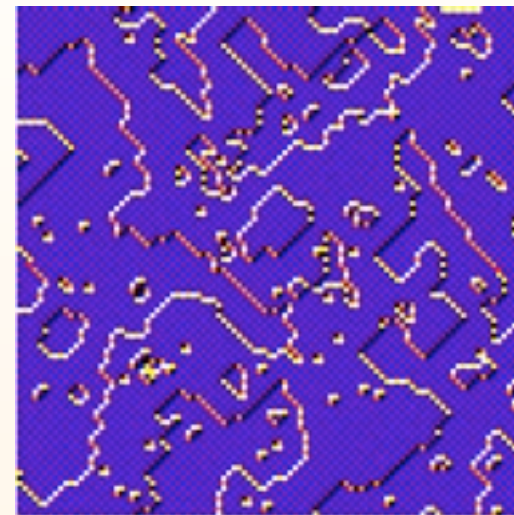
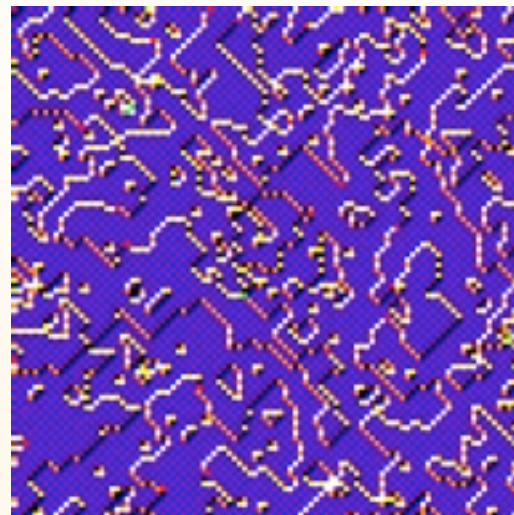
at $t=0$ (instantaneously)

$$a = b = 0.1; \quad c = 1, \quad d = e = 10^{-5} \quad (T < T_c)$$

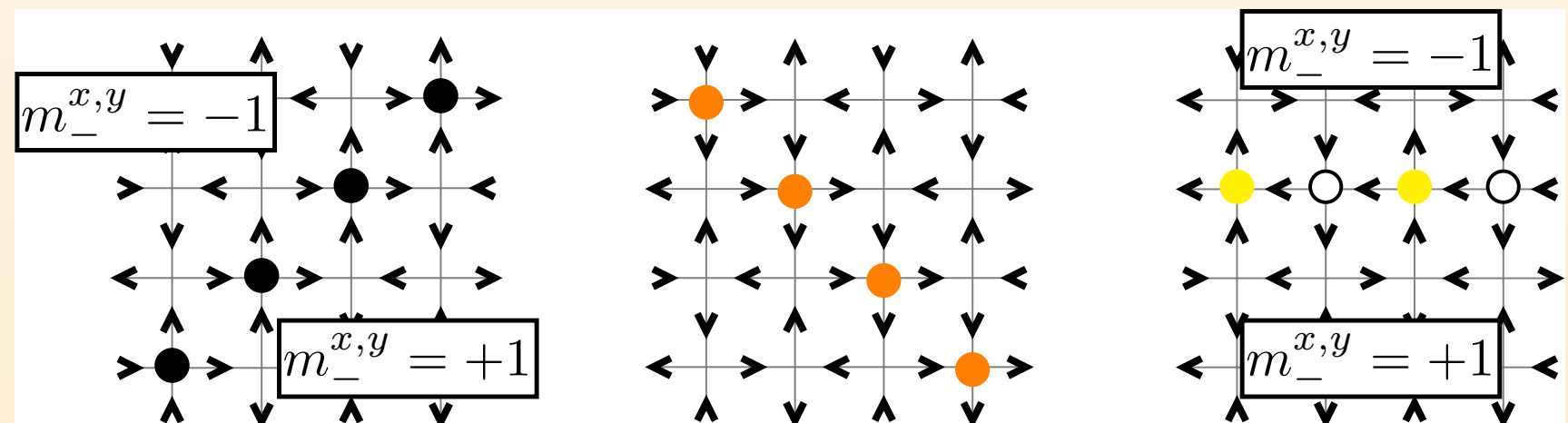


Out-of-equilibrium.

Quench into the AF phase.

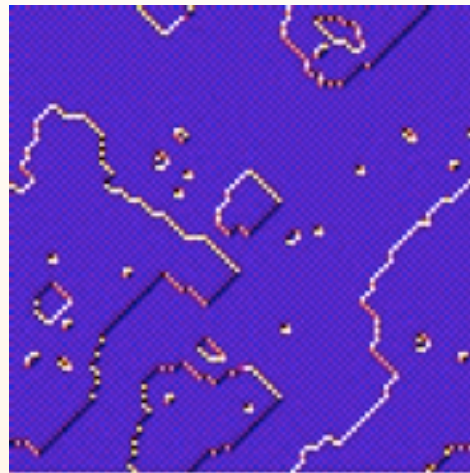
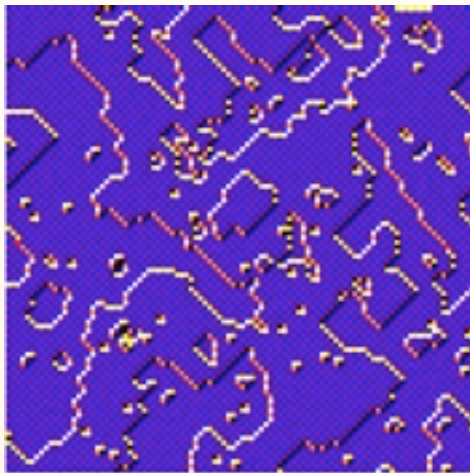


Growth of AF **domains** with walls
made of FM-vertices (a- b-type).
Defects on domain walls,
far from each other,
difficult to annihilate: **slow dynamics**.

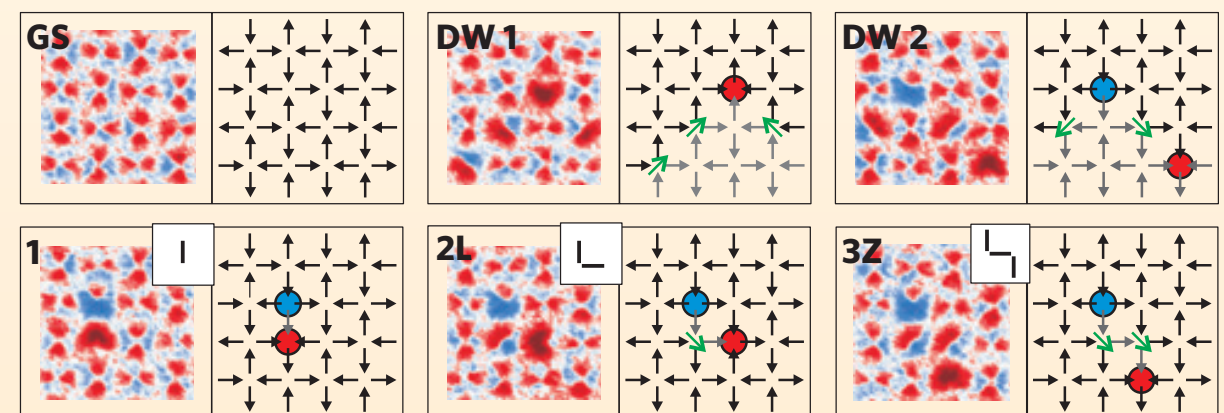
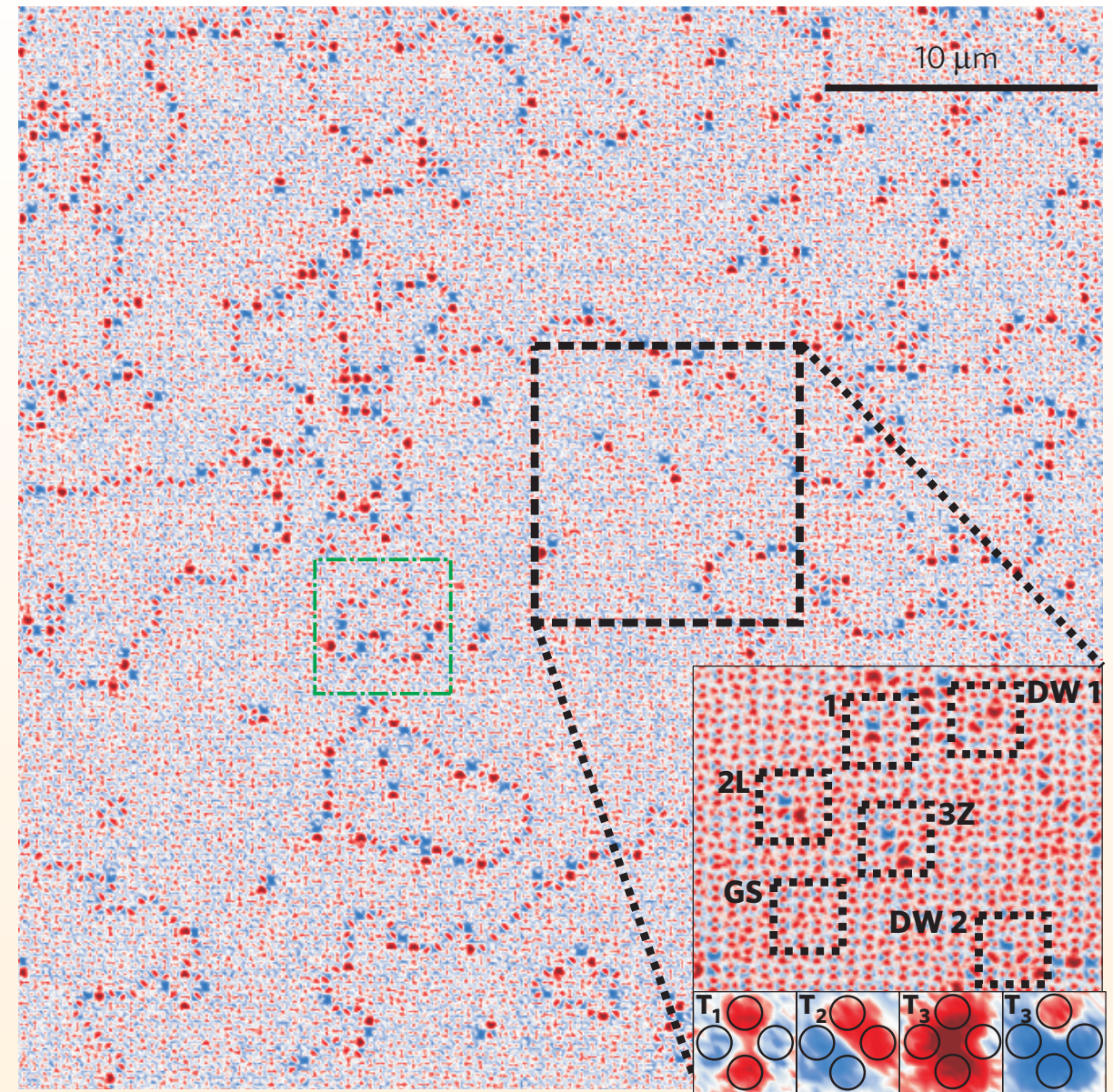
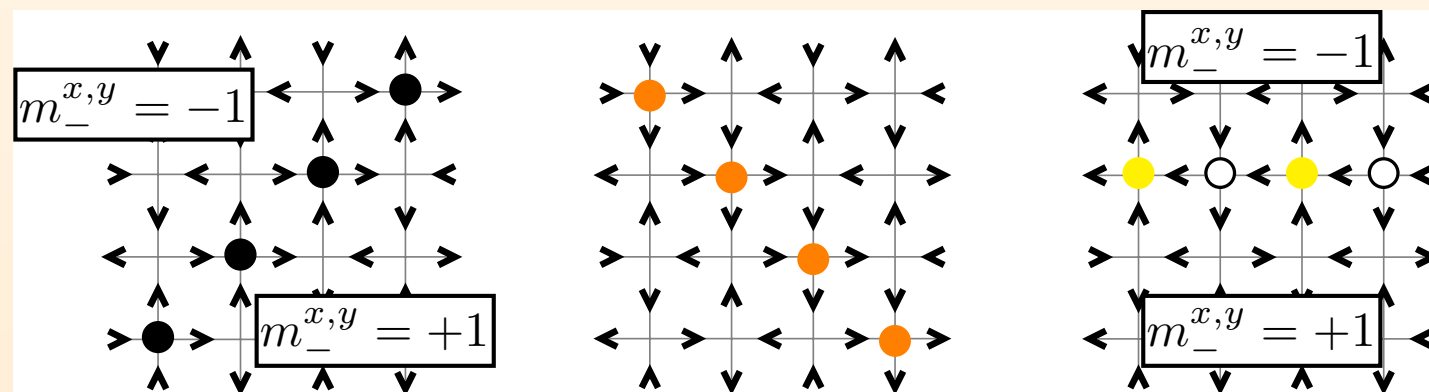


Out-of-equilibrium.

Quench into the AF phase.



Same kind of domain walls
observed in as-grown ASI
samples.



From **Morgan** *et al.*, Nature Phys. 7 2011.

Conclusion out-of-equilibrium.

1. **Dynamical arrest** appears for all type of quenches for $e < 10^{-4}$.

Why ?

i) presence of 4in 4out vertices ? **NO**

ii) presence of winding loops ? **NO**

iii) finite-size effects? **YES** ? Arrhenius barrier $\tau \sim e^{-2}$

2. The evolution of the density of defects follows a **power-law** $n_d(t) \sim t^{-\alpha}$.

The **exponent depends on the value of the parameters** (how?).

3. **Stripes** of competing FM order with two different growing lengths:
anisotropic coarsening.

Rich microscopic **dynamical mechanisms.**

4. Coarsening dynamics in the AF regime:

artificial spin-ice samples?

effective 'cooling rate' during deposition? vs. MC simulated annealing?

time-dependent correlations? geometric properties of the domain walls?

Conclusion & outlook.

Conclusion & outlook.

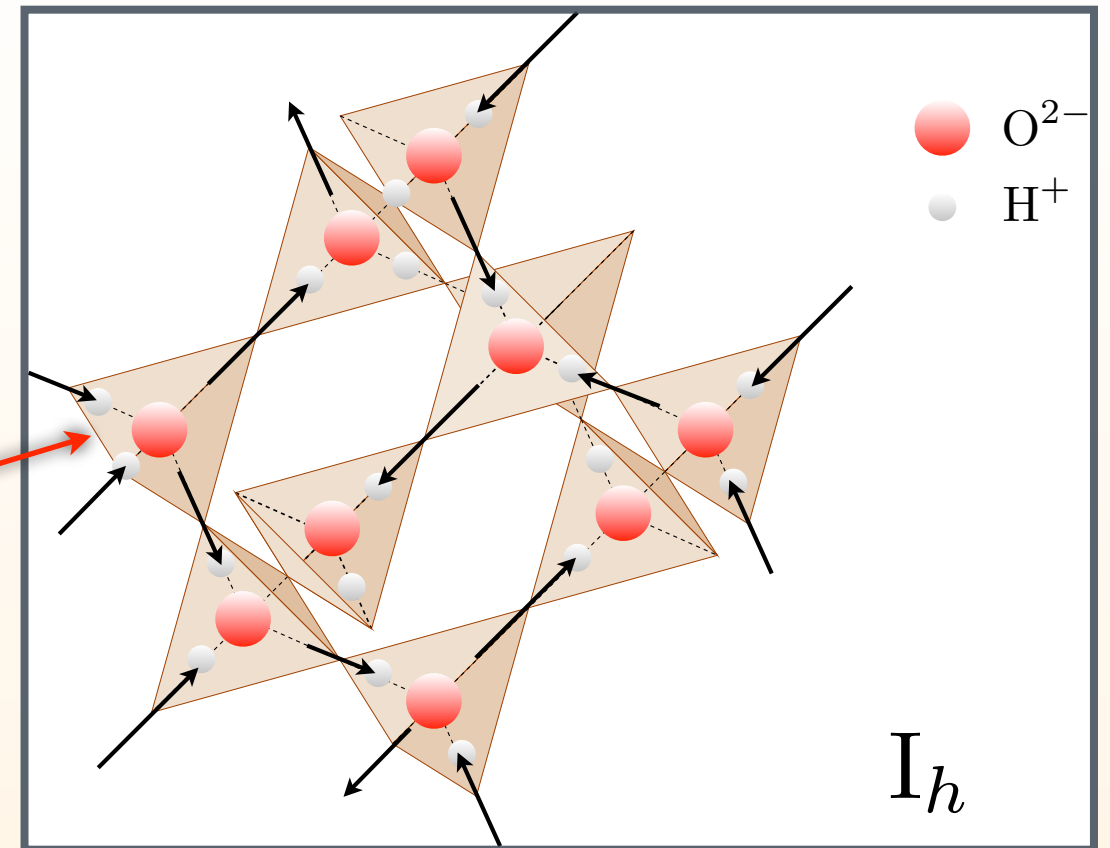
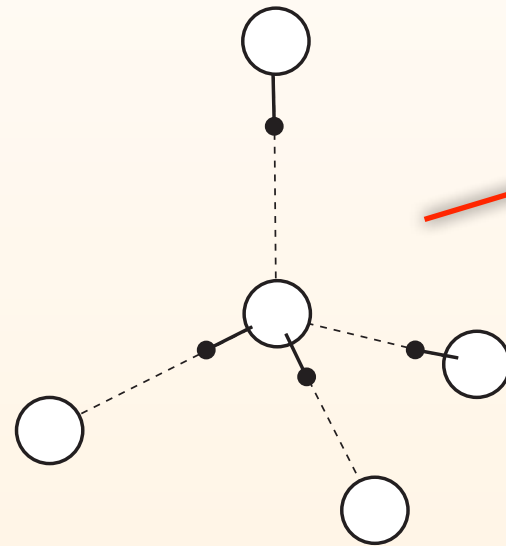
1. Investigate the variation of critical exponents in the 16V model by a real-space **Renormalisation Group** approach.
2. Extend the mappings between **integrable vertex models** (6V and 8V) into **quantum spin chains** (XXZ and XYZ resp.) to the unconstrained 16V model. Then, use our understanding on the classical model to predict the behaviour of the quantum system?
3. Link between **configurational temperatures** in ASI and the **canonical temperature**? In experiments:
 - properties of the domain walls?
 - thermal equilibration?
 - growth rate (link with a cooling rate)
4. **Defects' motion** in 2D (square or hexagonal).
5. Effect of **boundary conditions** on the dynamics of hardly constrained models. **Topological glass** ?

END OF EVERYTHING

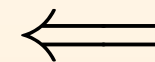
Geometrical frustration

Crucial example: **Water Ice**

Single unit:



Experimental evidence of an **extensive entropy at $T=0$**
Giauque & Stout 1936



Predicted by **Pauling's model**
Pauling 1935



each bond carries a dipolar moment $\vec{\mu}$
verifying the **ice-rules**



at each **vertex** (oxygen atoms)
two in - two out

$\Rightarrow$ **SIX** possible vertices

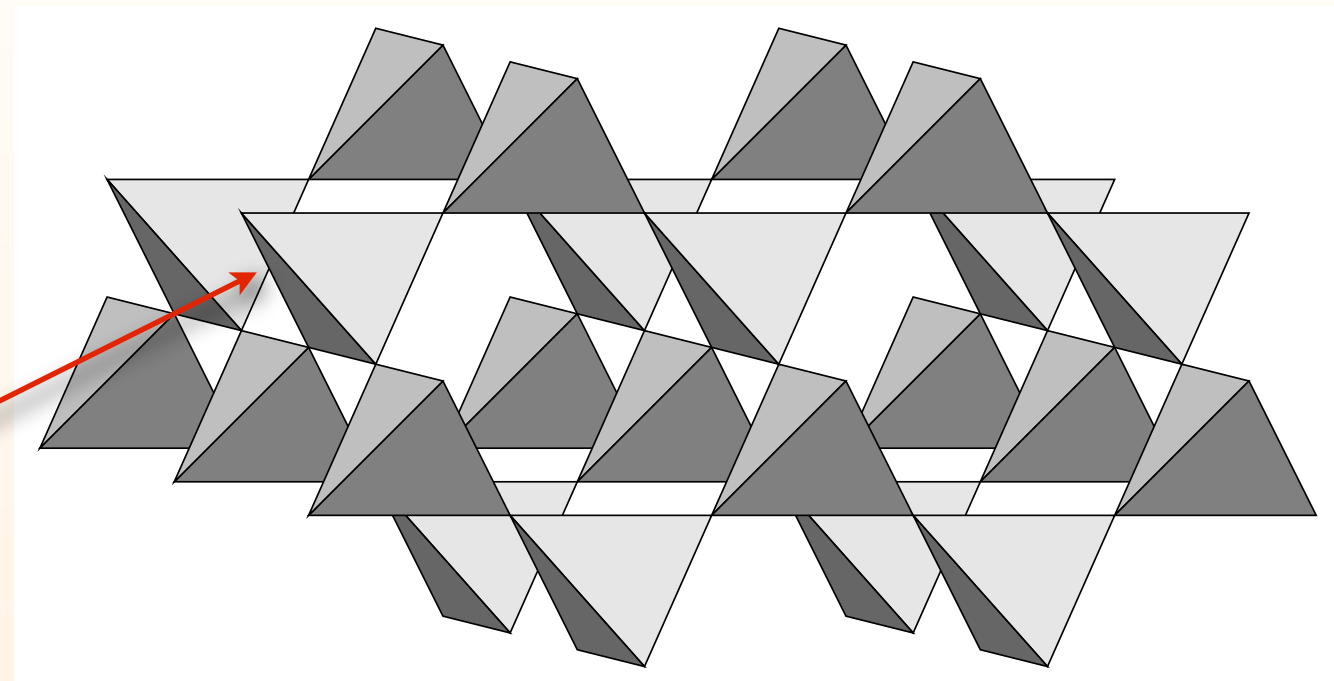
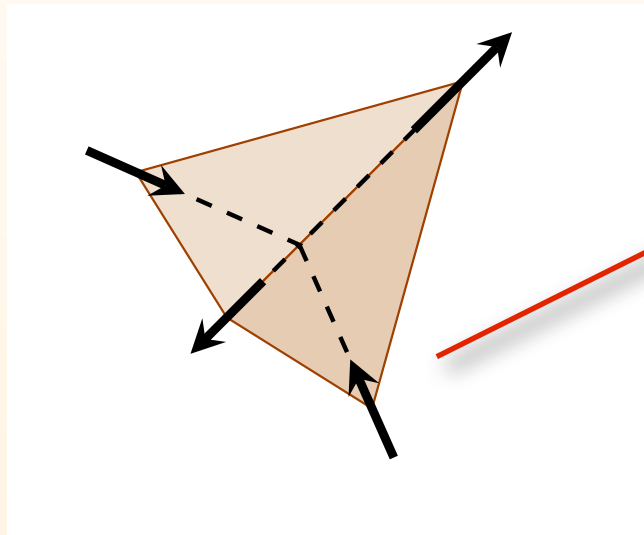
Ground state : $\vec{\nabla} \cdot \vec{\mu} = 0$ Ice-rule vertices are favoured $\Rightarrow$ **Geometrically frustrated**

Geometrical frustration

in spin ice

Harris, Bramwell, McMorro, Zeiske & Godfrey 1997

Pyrochlore lattice
+ magnetic moments



classical **Ising spins** pointing in the local direction connecting a site with the centre of its tetrahedron

DSI: nn **FM** + **dipolar** interactions

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + Da^3 \sum_{i < j} \frac{\vec{S}_i \cdot \vec{S}_j}{r_{ij}^3} - 3 \frac{(\vec{S}_i \cdot \vec{r}_{ij})(\vec{S}_j \cdot \vec{r}_{ij})}{r_{ij}^5}$$

NN contribution: $H \approx \frac{J + 5D}{3} \sum_{\langle i,j \rangle} \sigma_i \sigma_j$ with: $\sigma_i = \pm 1$

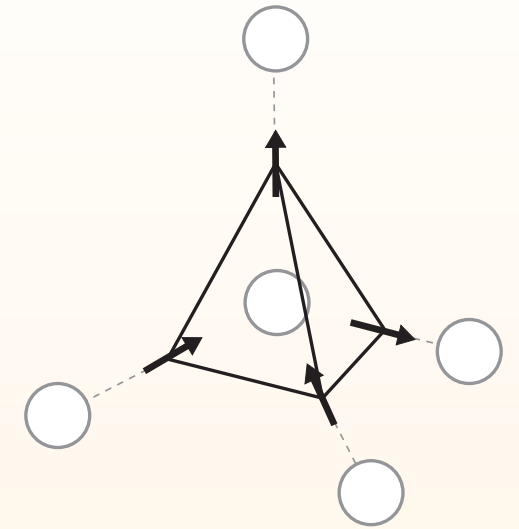
AF $\Rightarrow$ **GS: 2 in-2 out (ice-rules)**
Geometrically frustrated **Ferromagnet**
«in» or «out»

Zero-point entropy

Pauling's argument: N tetrahedra, $2N$ links (4 NN)

Pauling 1935 $\rightarrow \Omega_0 = 2^{2N}$ (without ice-rules)

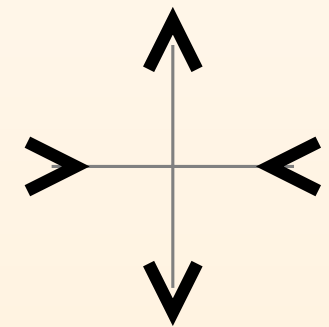
vertices indept. $\rightarrow \Omega_\infty = 2^{2N} (6/16)^N$
 $\rightarrow S_\infty \approx 0.40R$



2D Lieb's exact result (Bethe Ansatz):

Lieb 1967

$$S_{2D} = Nk_B \frac{3}{2} \ln \left(\frac{4}{3} \right) \approx 0.43R$$



3D Experiments (both Spin and Water **Ice**):

$$S_w \approx 0.41R$$

$$S_{si} \approx 0.46R$$

Giauque & Stout 1936

Ramirez, Hayashi, Cava, Siddharthan & Shastry 1999

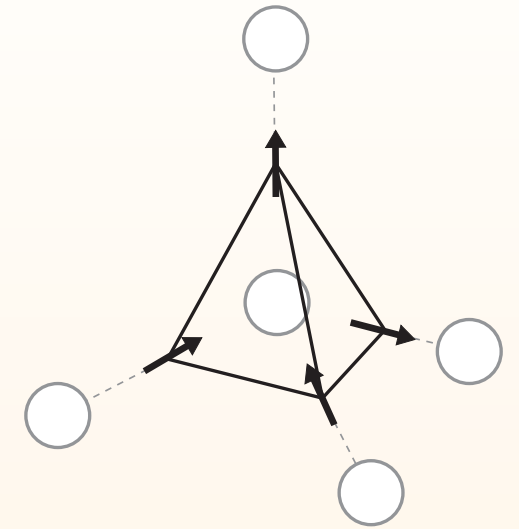
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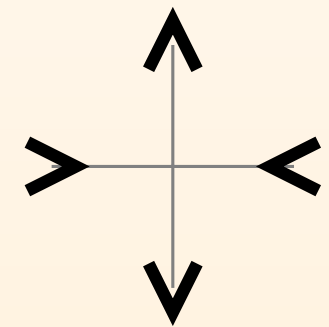
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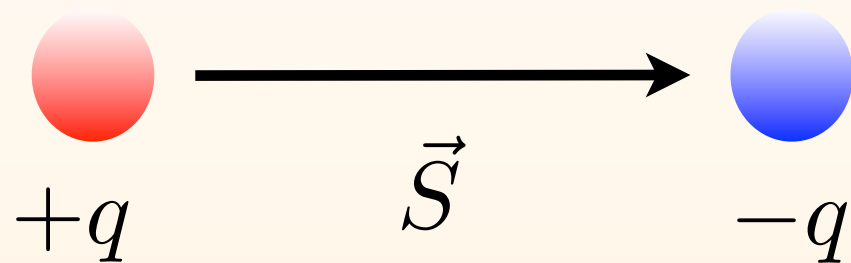
Ramirez, Hayashi, Cava, Siddharthan & Shastry 1999

Thermal excitations in spin-ice

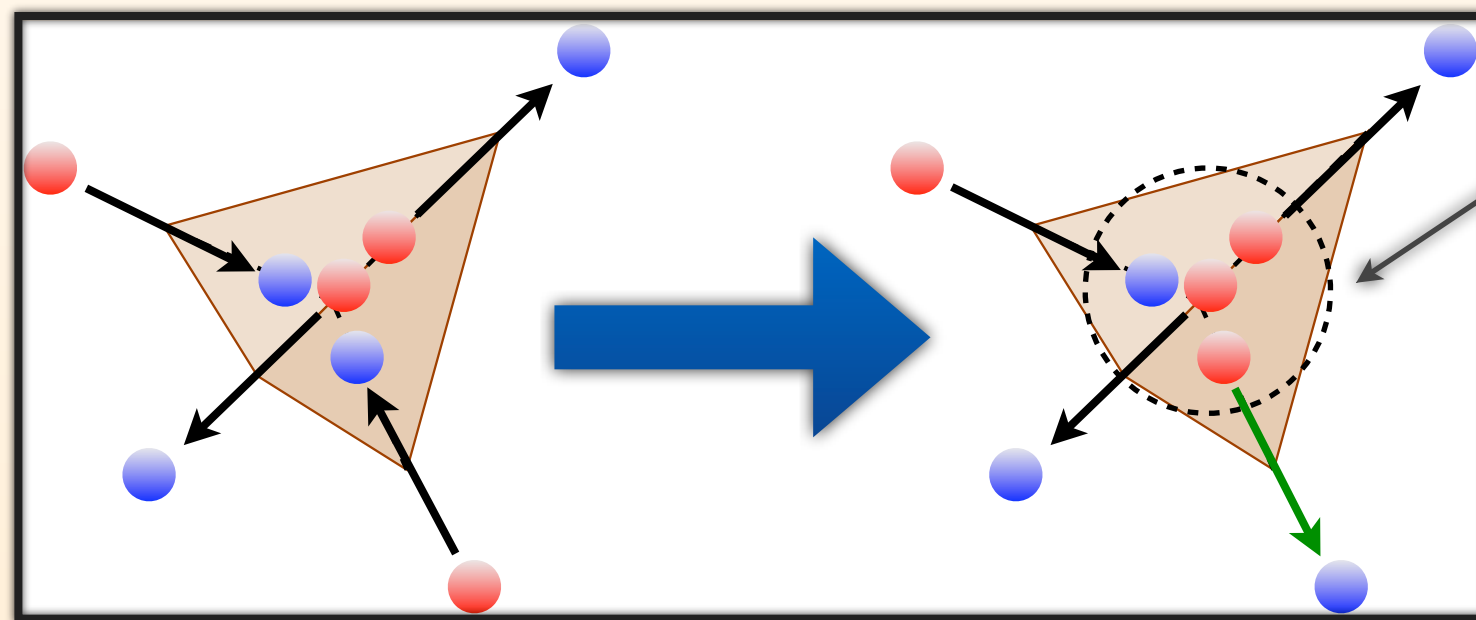
$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + Da^3 \sum_{i < j} \frac{\vec{S}_i \cdot \vec{S}_j}{r_{ij}^3} - 3 \frac{(\vec{S}_i \cdot \vec{r}_{ij})(\vec{S}_j \cdot \vec{r}_{ij})}{r_{ij}^5} \approx \sum_{(\alpha, \beta)} V_{\alpha\beta}$$

Pyrochlore lattice
= dipoles

Diamond lattice
= monopoles



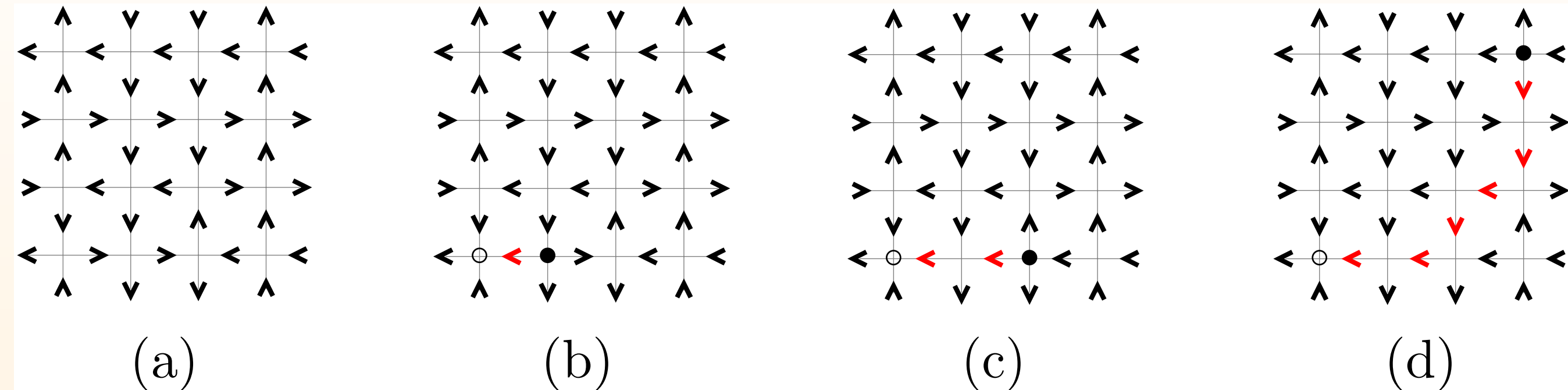
Thermal excitations
violating the ice rules =



magnetic monopoles

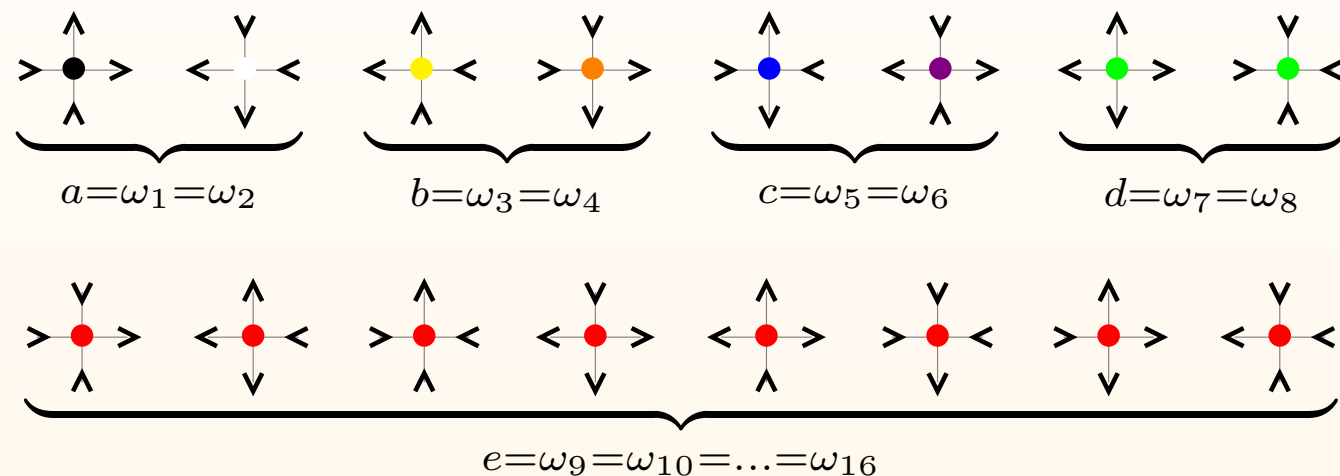
$\Rightarrow$ Ice configurations $\equiv \{q_\alpha = 0\}$

Magnetic monopoles in spin-ice

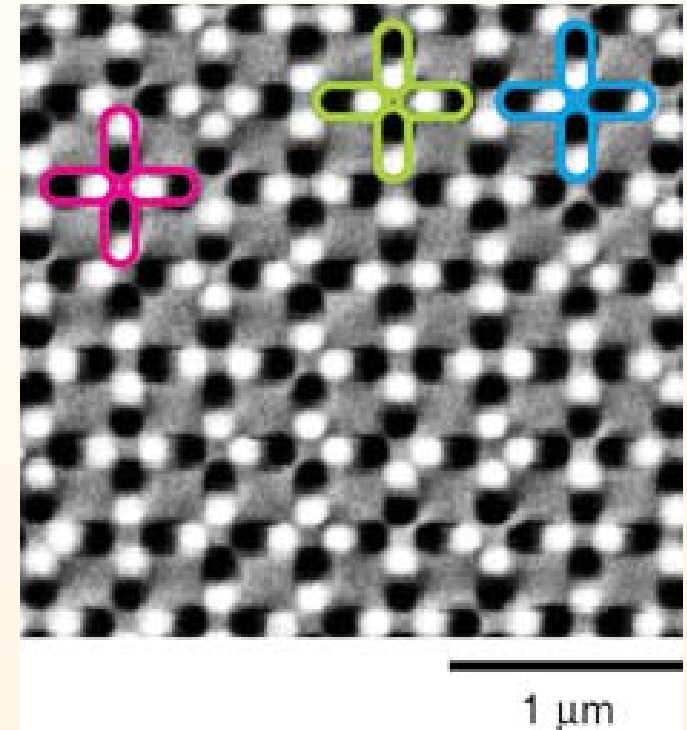


- If all the 2 in - 2out vertices are equivalent, the only energy cost comes from the $1/r$ **Coulomb interaction**.
- Finite energy to separate two monopoles to infinity = *de-confined*
→ *Fractionalisation in 3D*

2D experiments: Artificial Spin-Ice



from Wang et al., Nature 2008



Experimental motivation:

1. direct visualisation of **defects'** dynamics

Mengotti, Heyderman, Rodríguez, Nolting, Hügli, Braun 2011.

2. vertex weights can be tuned $\rightarrow a = b = c$

Moller & Moessner 2006

3. A-thermal system: energy barrier $\sim 10^5 K$;

$\rightarrow$ **effective thermodynamics** can be recovered

Nisoli, Li, Ke, Garand, Schiffer, Crespi 2010;

Morgan, Stein, Langridge, Morrows 2011.

Equilibrium.

Sixteen-vertex model (numerics)

Allow defects $\Rightarrow d = e \neq 0$

Conjecture: (numerics)

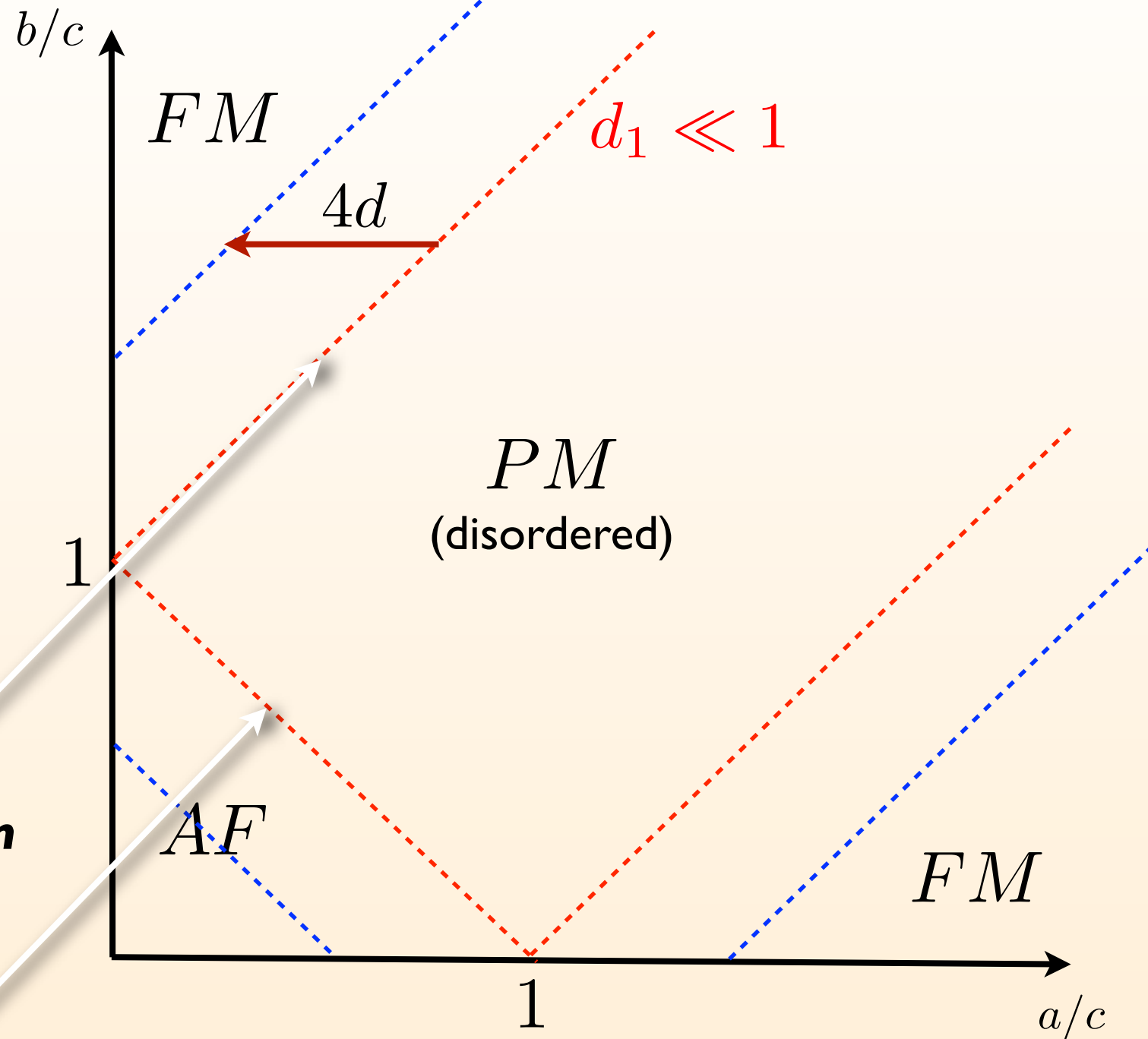
$$\Delta_{16} = \frac{a^2 + b^2 - c^2 - (3e + d)^2}{2(ab + c(3e + d))}$$

$$e = 0 \longrightarrow \Delta_8 = \frac{a^2 + b^2 - c^2 - d^2}{2(ab + cd)}$$

$\Delta_{16} > 1$ **ordered** FM phase
continuous phase transition

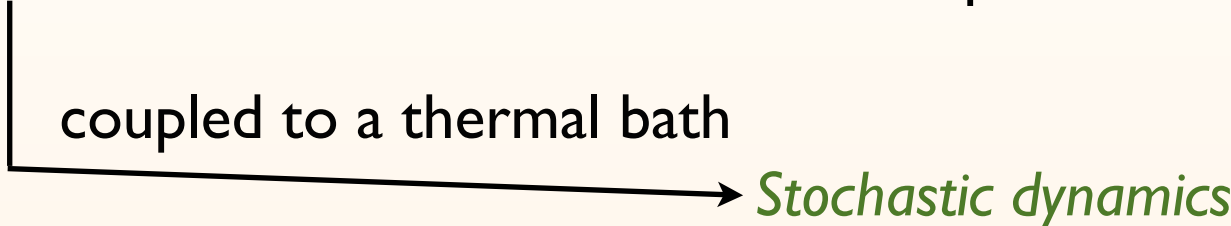
$1 > \Delta_{16} > -1$ **disordered** PM phase
continuous phase transition

$\Delta_{16} < -1$ **ordered** AF phase



Phase ordering dynamics after a quench.

Evolution of the system across a phase transition.

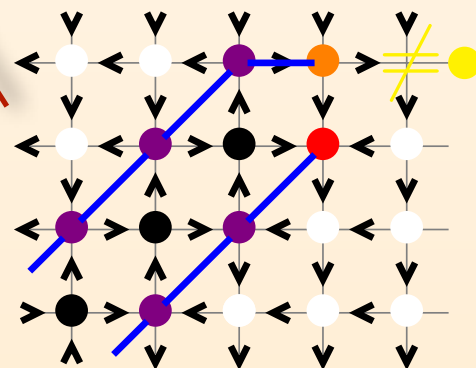
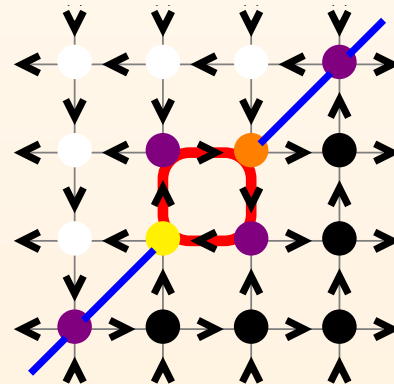
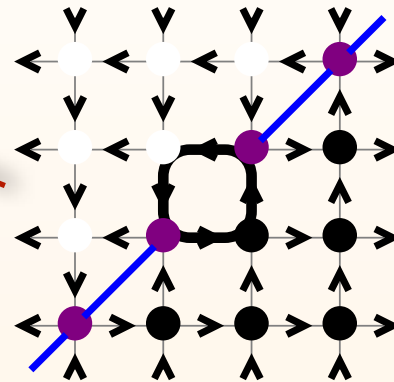
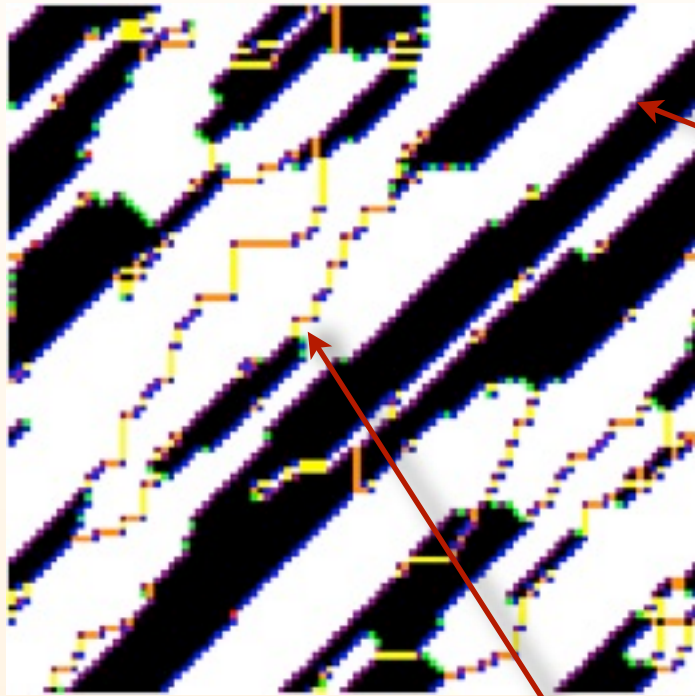
- Give updating rules: **Non-conserved** order parameter (single spin flips)

coupled to a thermal bath *Stochastic dynamics*
- Prepare the system in a **disordered** equilibrium state and **quench** it into a known equilibrium **ordered symmetry broken** phase
 *Competition between opposite orders* *Slow dynamics* $L(t) \sim t^z$
- **Dynamical scaling theory**: at late times, there is a single length scale $L(t)$ such that:

$$C(t, t_w) = \langle s_i(t) s_i(t_w) \rangle \simeq M_{eq}^2 F_C \left(\frac{L(t)}{L(t_w)} \right)$$

$$G(r, t) = \langle s_i(t) s_j(t) \rangle \simeq M_{eq}^2 F_G \left(\frac{r}{L(t)} \right)$$

Quench into the FM phase.

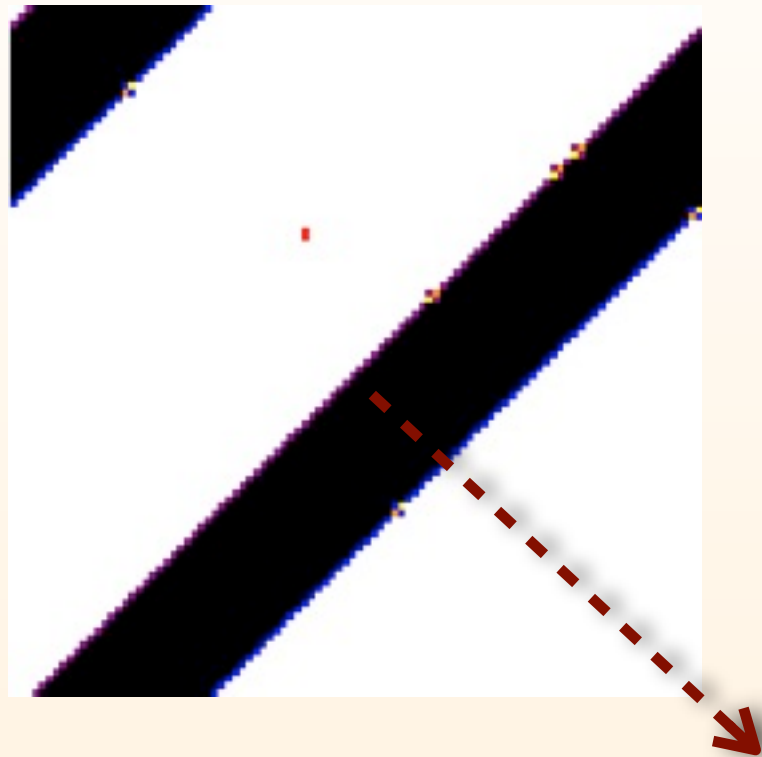
Dynamic mechanisms



- **anisotropy** $a \neq b$ tends to create **diagonal domain walls** made of AF vertices.
- **loop fluctuations** are the elementary moves that do not break the ice-rules.
- ‘corners’ of domains cannot have a neighboring a-vertex. Avoiding defects, this explains the presence of strings.
- **Strings connect two domains** and mediate their growth.

Quench into the FM phase.

Dynamic mechanisms

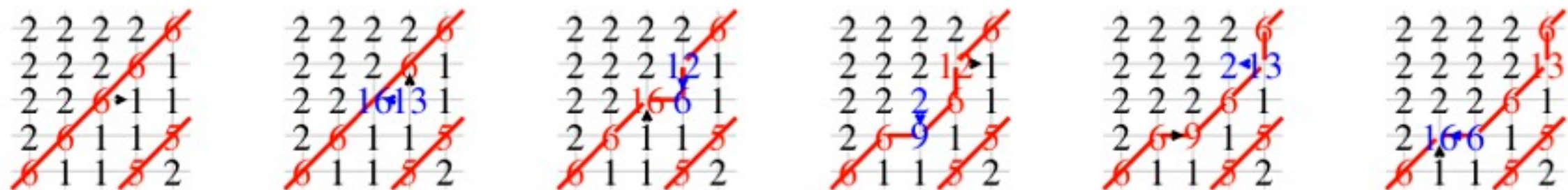


- once the bands are created we must **create a pair of defects** and made them move along the walls to restore the equilibrium configuration.

→ Extremely slow process $T \sim L$

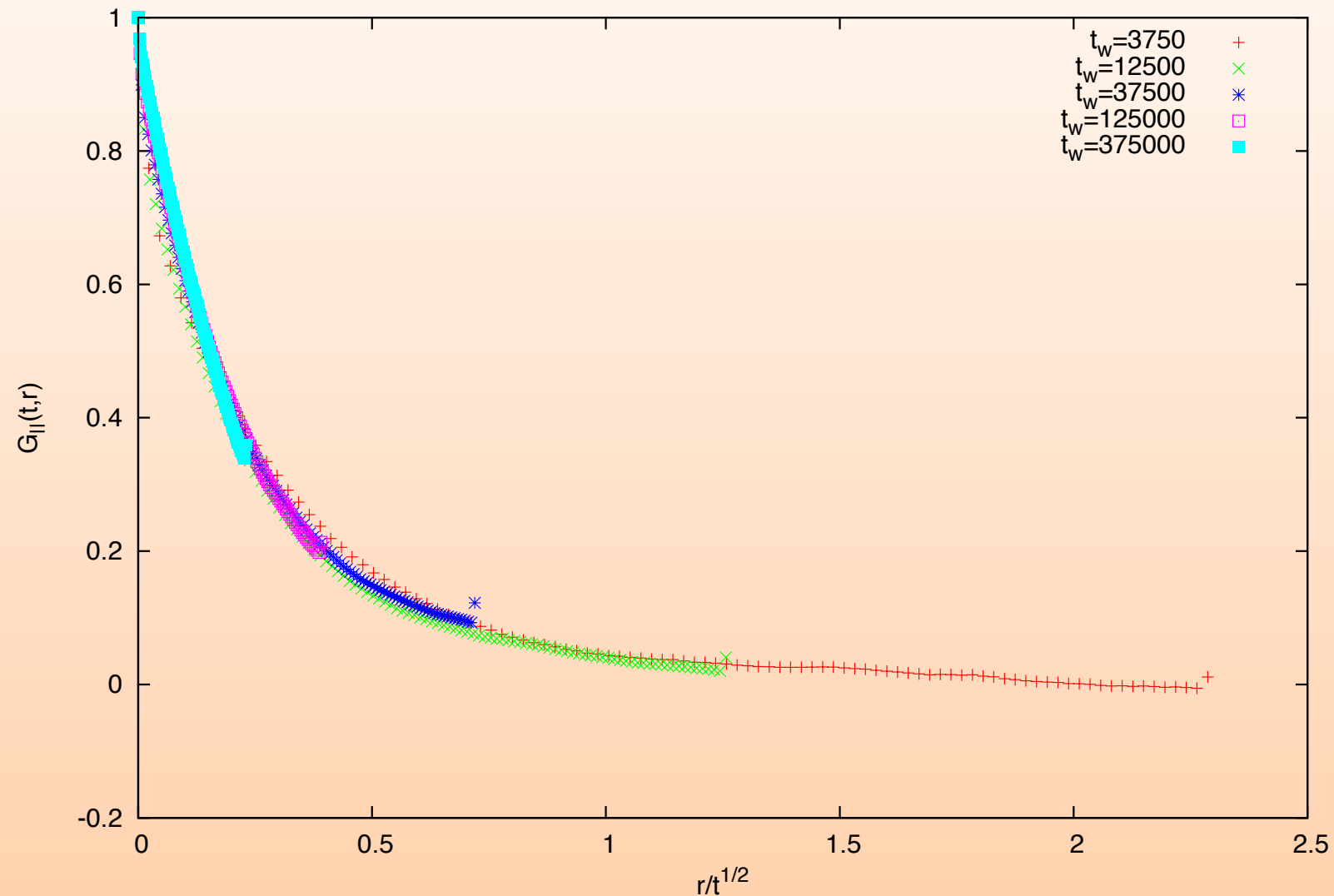
(diverging at the thermodynamic limit)

Equilibrium is reached when magnetic order percolates in the $\perp$ direction.



Out-of-equilibrium.

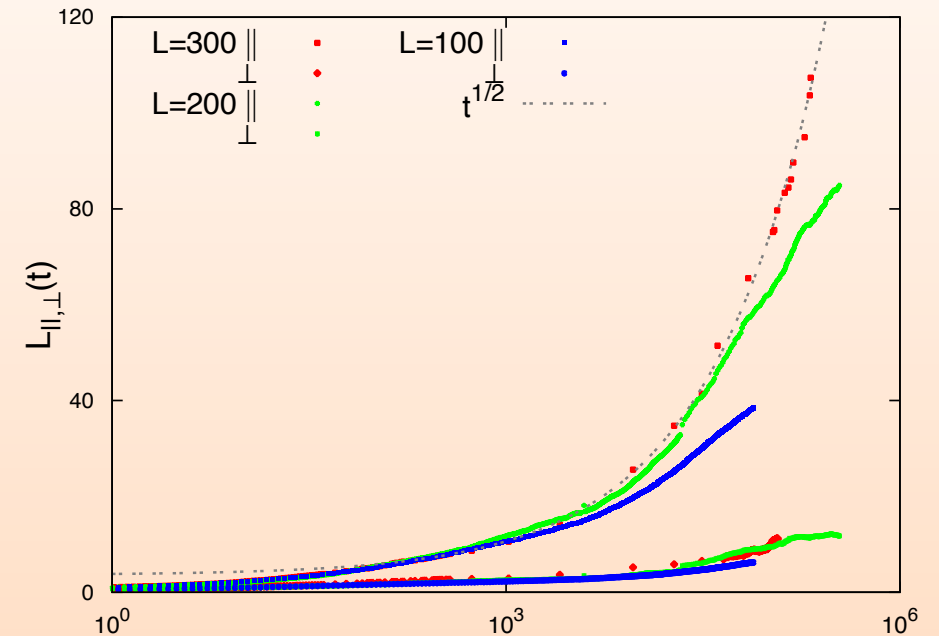
Quench into the FM phase.



L=200

Two-point self correlation function in the $||$ direction:

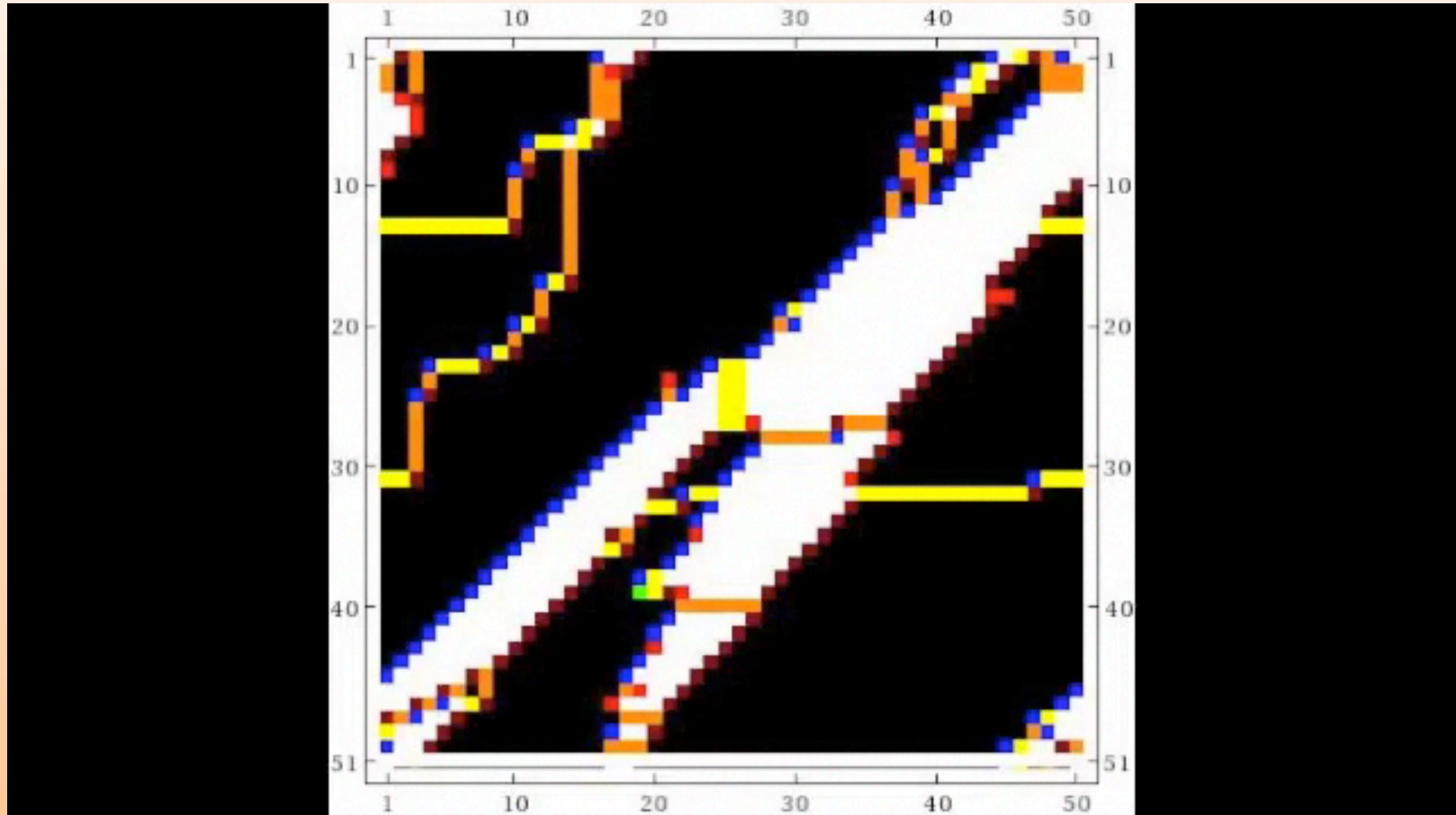
$$G_{||}(t, r) = \sum_{i,j} \langle S_{i,j}(t) S_{i+\frac{r}{\sqrt{2}}, j+\frac{r}{\sqrt{2}}}(t) \rangle$$



Out-of-equilibrium.

Quench into the FM phase.

Evolution from a D i.c. to $a = 5, b = 1, e = 10^{-7}, d = e^2$

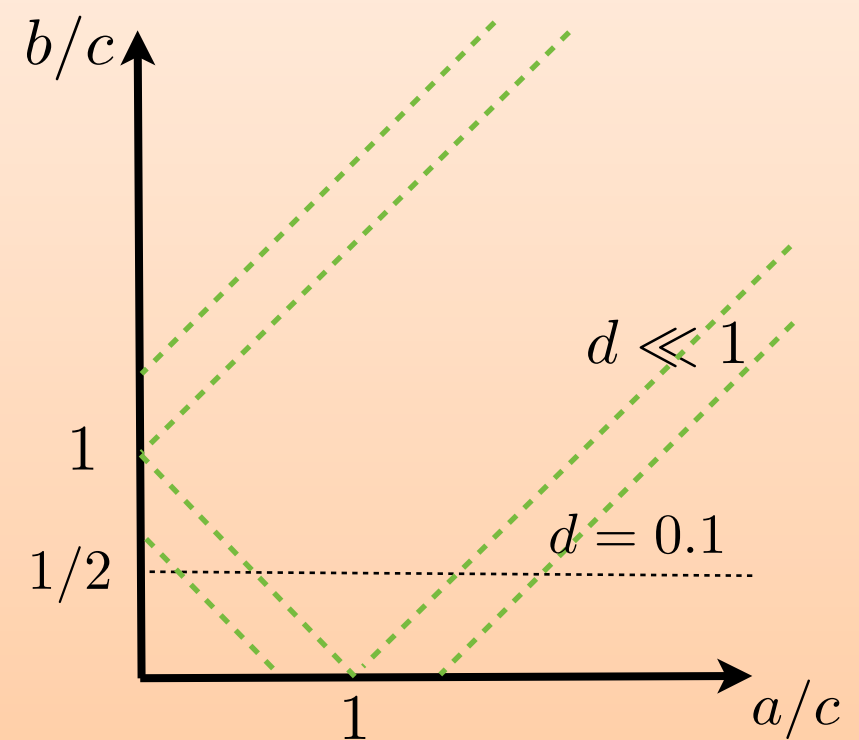
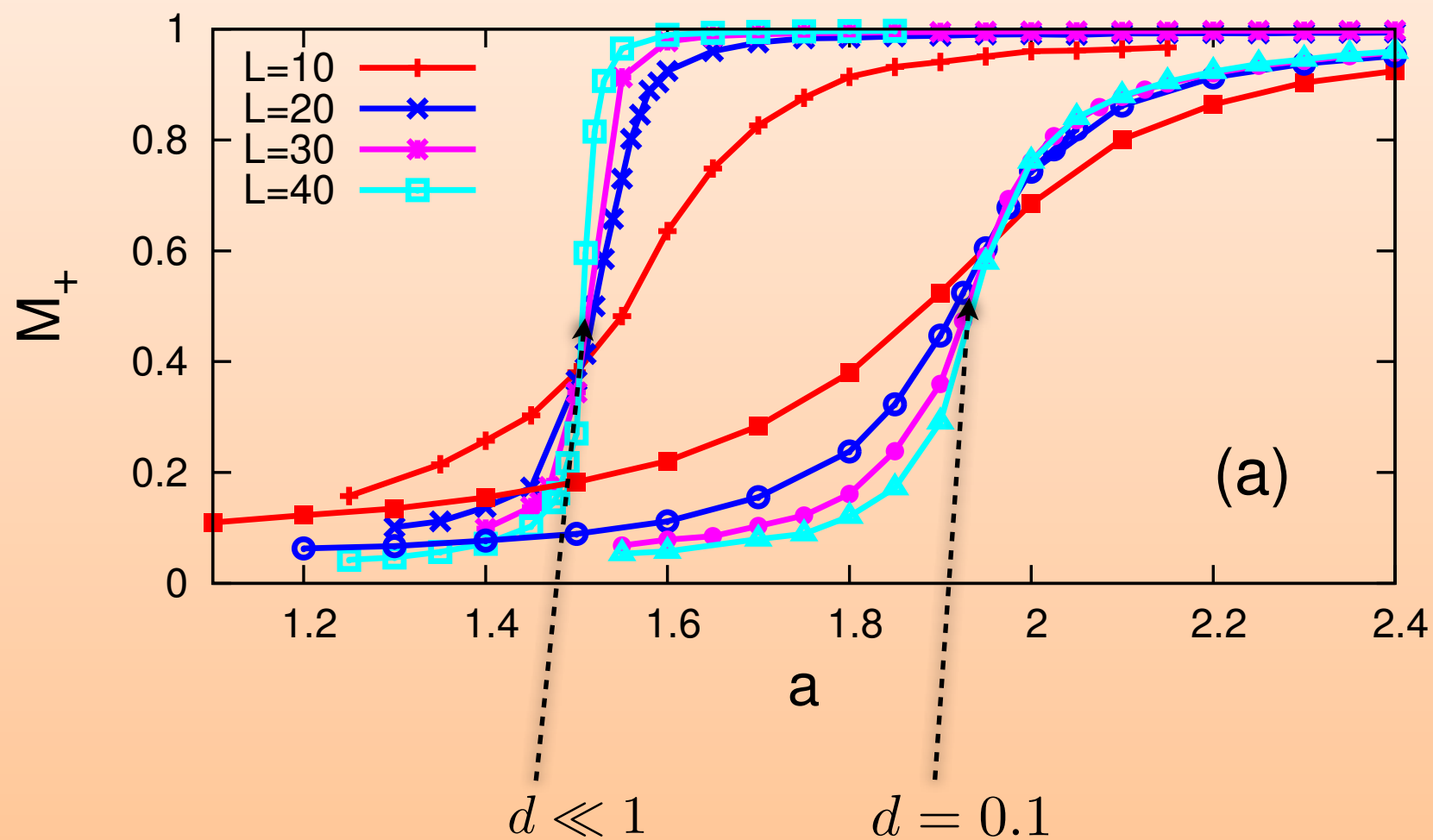


Equilibrium.

Sixteen-vertex model

Allow defects $\Rightarrow d = e \neq 0$

Example: $b = 1/2, c = 1$



→ The FM transition gets “smoother” by increasing the weight of the defects

Equilibrium.

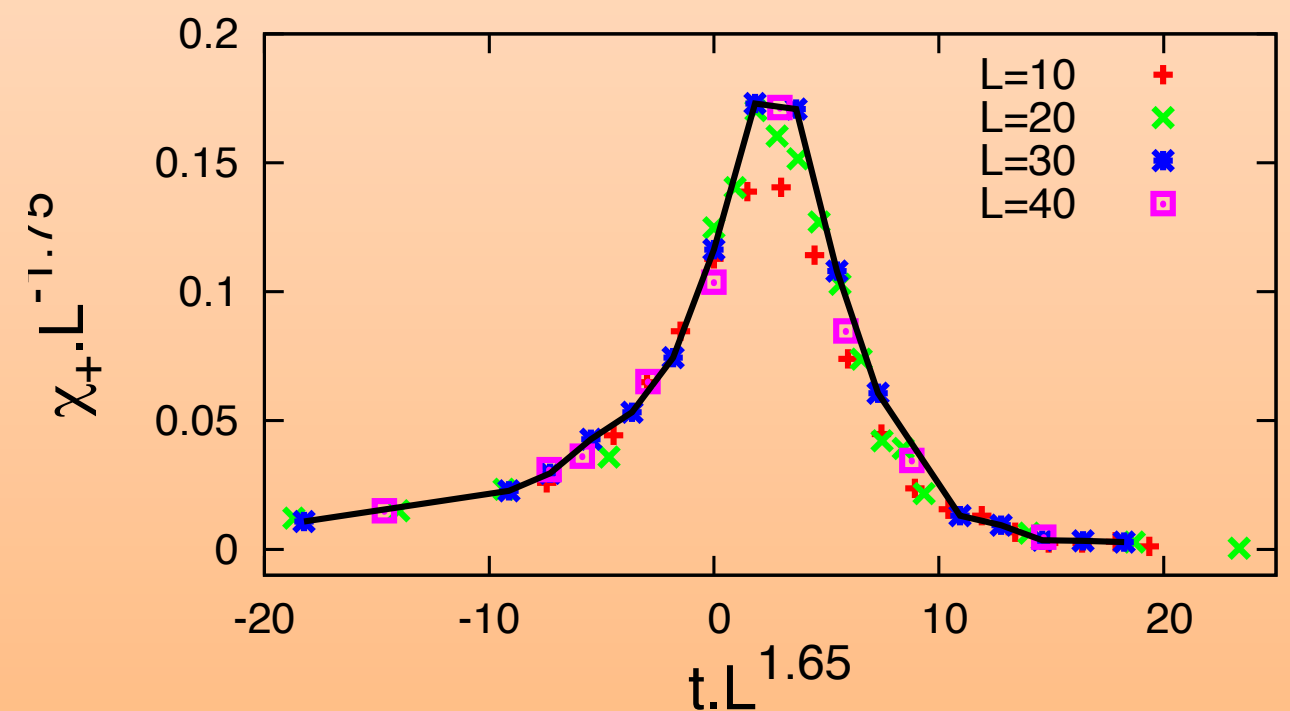
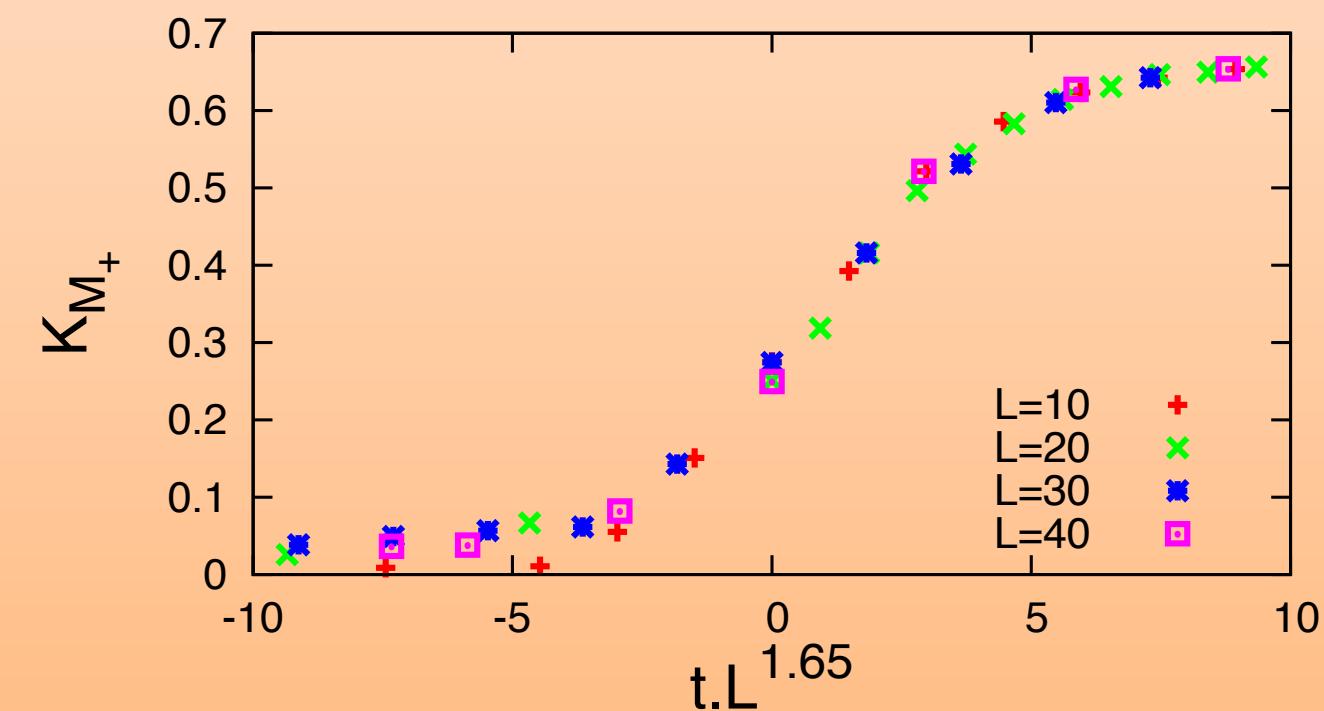
Sixteen-vertex model

Finite size scaling:

$$K_{M_+} = 1 - \frac{\langle M_+^4 \rangle}{3\langle M_+^2 \rangle^2} \sim \Phi_K(tL^{1/\nu})$$

$$\chi_+ \sim \Phi_{chi_+}(tL^{\gamma/\nu})$$

Distance from the transition: $t = \frac{a - a_c}{a}$



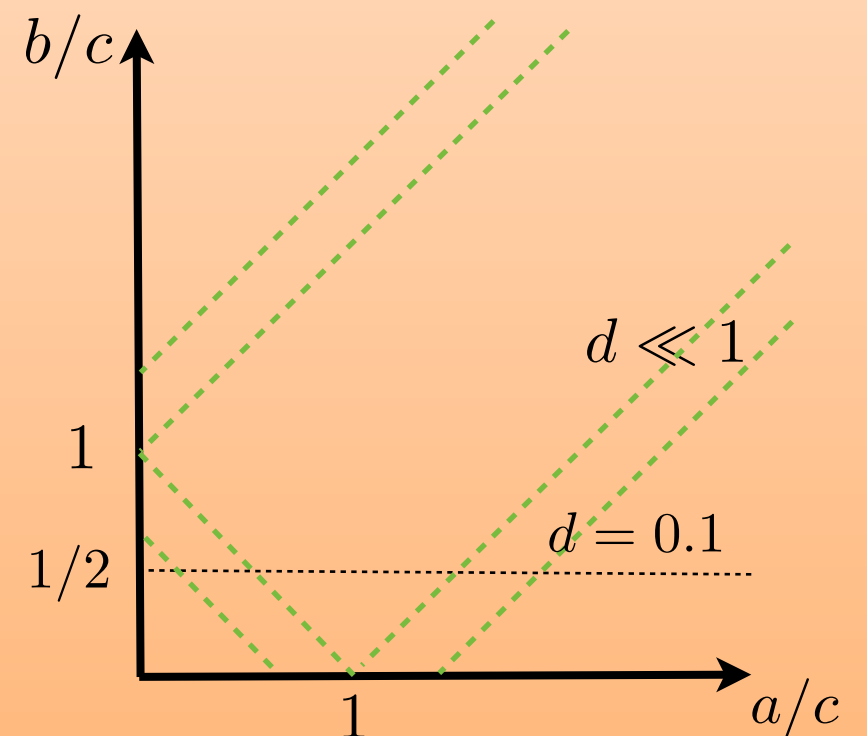
Sixteen-vertex model

Ex: critical exponents for the FM transition

	six-vertex	$2d$ Ising	SI ($d = e = 10^{-5}$)	SI ($d = e = 0.1$)
$\hat{\gamma} = \gamma/\nu$	$7/4$	$7/4$	$= 1.75 \pm 0.02$	$= 1.75 \pm 0.02$
$\hat{\beta} = \beta/\nu$	$1/8$	$1/8$	$\approx 0.125 \pm 0.05$	≈ 0.125
$\hat{\alpha} = (2 - \alpha)/\nu$	2	2	$= 2.00 \pm 0.15$	≈ 2
γ	$7/8$	$7/4$	$= 1.06 \pm 0.03$	$= 1.75 \pm 0.18$
β	$1/16$	$1/8$	$= 0.050 \pm 0.014$	≈ 0.125
α	1	0	$= 0.84 \pm 0.23$	≈ 0
ν	$1/2$	1	$= 0.60 \pm 0.02$	$= 1.0 \pm 0.1$

Define new exponents : $M_+ \sim \xi^{-\hat{\beta}}$

Consistent with scaling relations



Sixteen-vertex model

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Exponents depend on the vertex weights

Sixteen-vertex model

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Exponents depend on the vertex weights

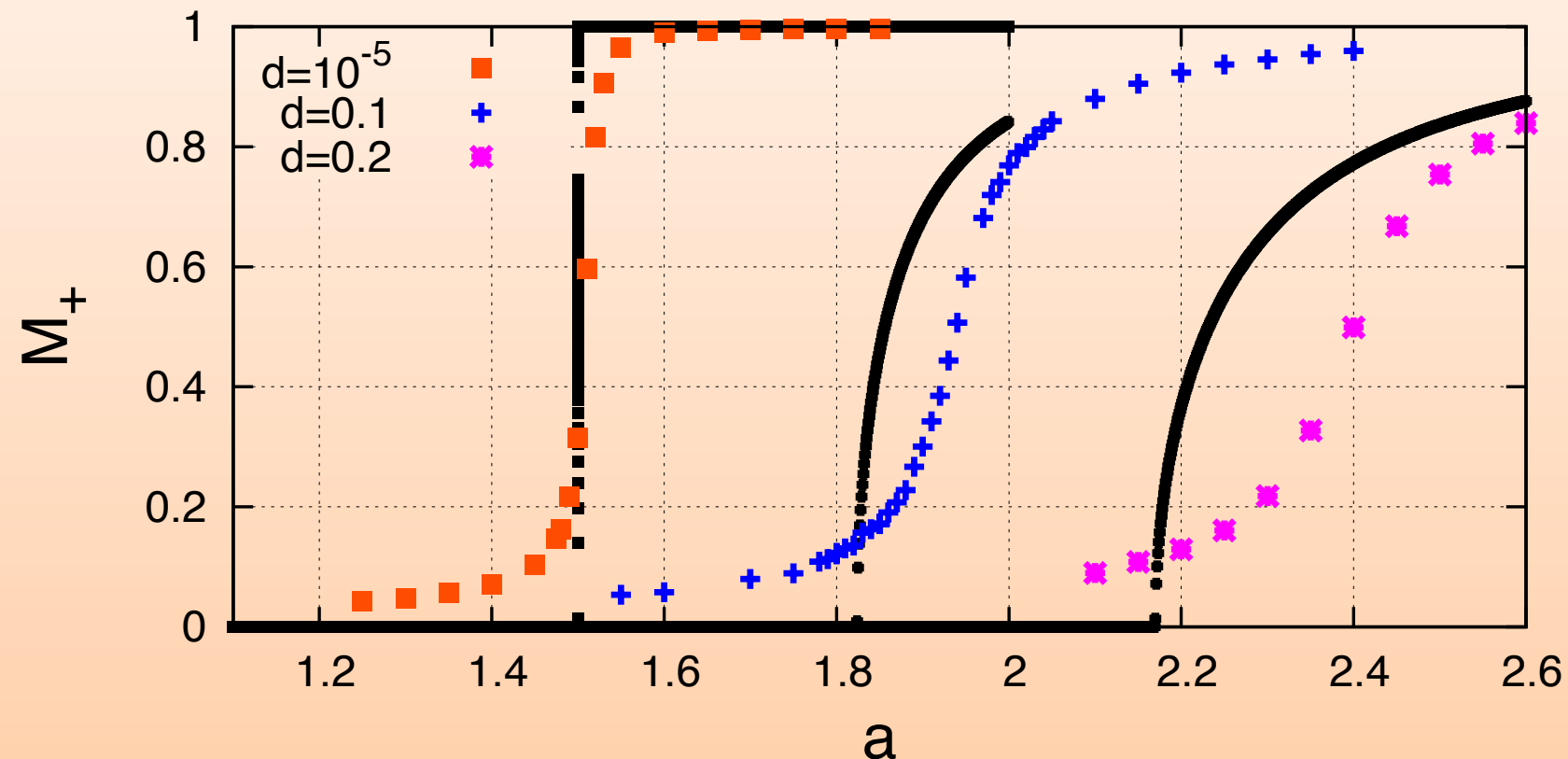
$\hat{\gamma}, \hat{\alpha}, \hat{\beta}$ does not!



Weak universality (Suzuki 1974)

Spin-ice on a tree graph (cavity method)

Cavity vs. numerical results (sixteen-vertex model)



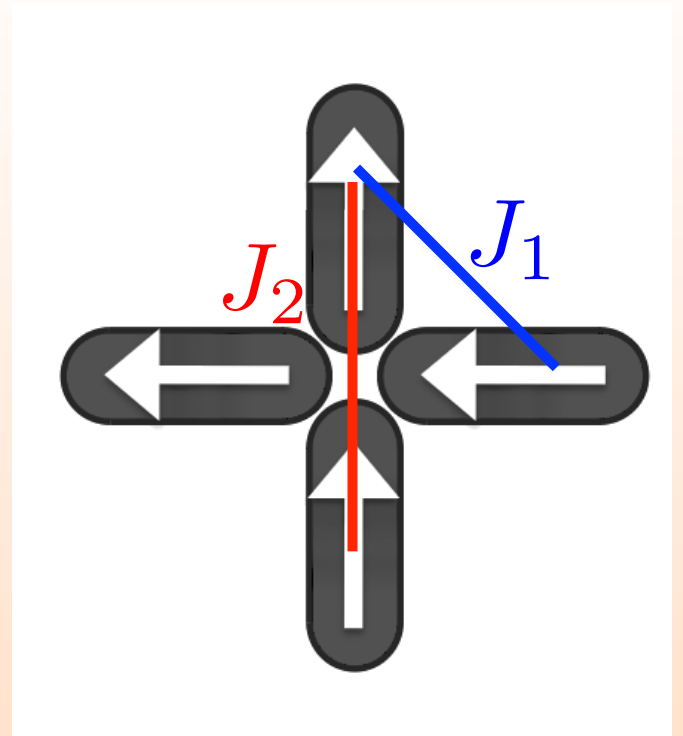
1. The approx. becomes worse when increasing the weight of the **defects** and the transition gets “softer”.

2. The location of critical surfaces obtained by the cavity calculation are almost parallel to the six-vertex ones (as predicted by MC)

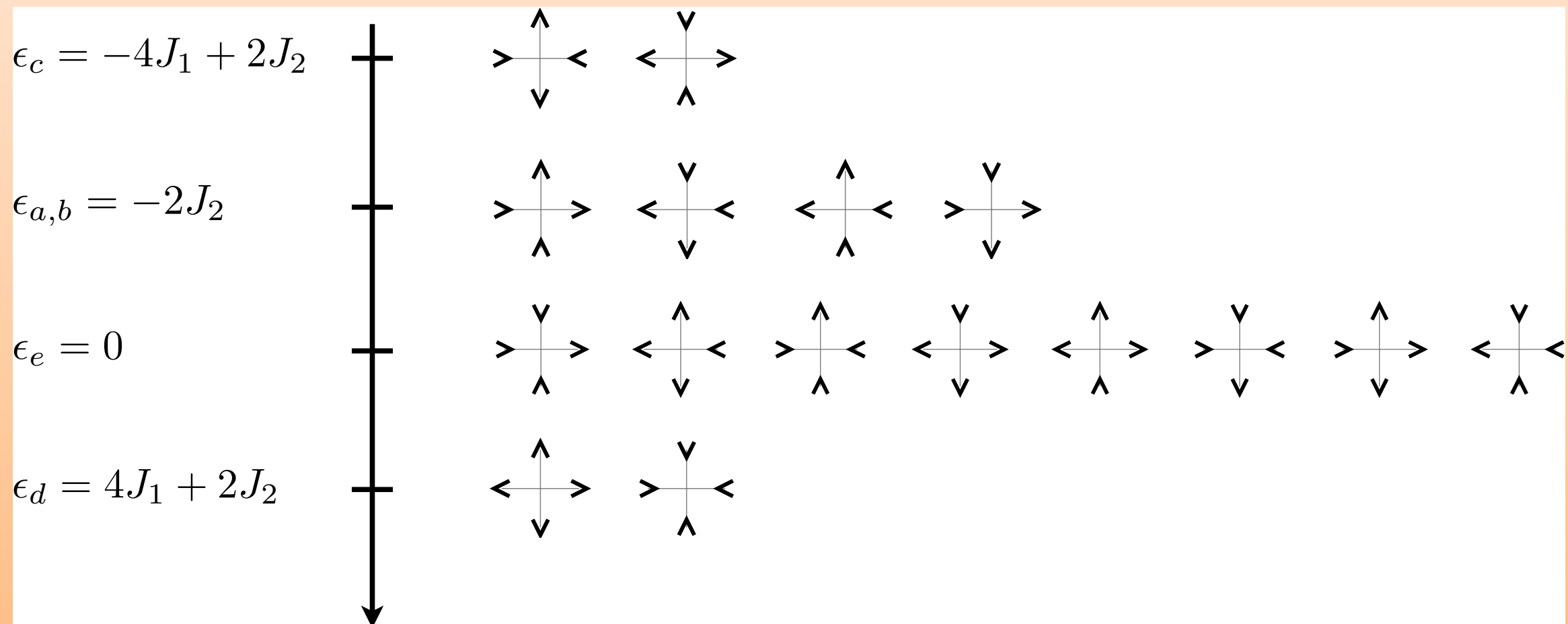
Artificial spin ice

Wang et al., Nature 439 (2006)

$$H = Dr_0^3 \sum_{i < j \in \mathcal{P}} \left(\frac{\mathbf{S}_i \cdot \mathbf{S}_j}{\|\vec{r}_{ij}\|^3} - 3 \frac{(\mathbf{S}_i \cdot \vec{r}_{ij})(\mathbf{S}_j \cdot \vec{r}_{ij})}{\|\vec{r}_{ij}\|^5} \right)$$



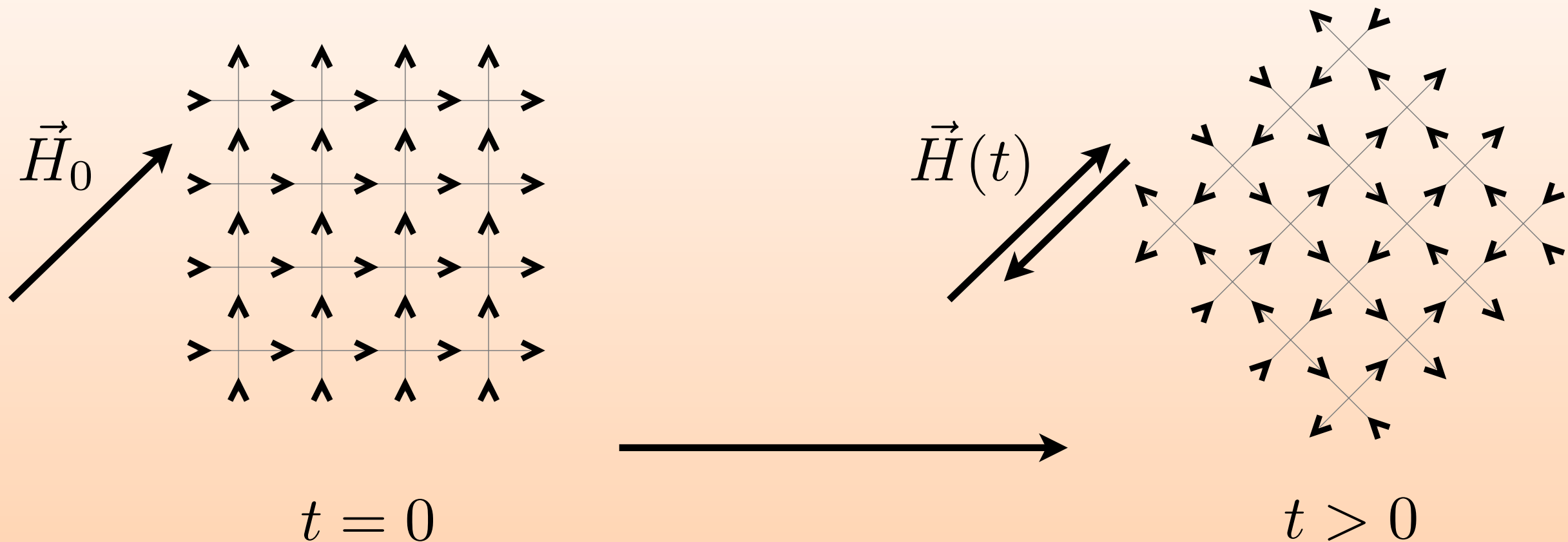
Energy levels



$\Rightarrow$ 2 in - 2 out vertices are not equivalent in the square lattice

'A-thermal' Artificial spin ice

(Nisoli et al. 2007-2008)



Demagnetisation protocol: $H(t = n\Delta t) = (-1)^n (H_0 - nH_s)$

- polarised initial configuration
- rotate the sample
- decrease magnetic field
- change polarity of the field after a cycle

Shearing and shaking in
granular matter ??

'A-thermal' Artificial spin ice

(Nisoli et al. 2007-2010)

Assume: (i) $E \approx ct$

(ii) vertices can be chosen **independently** (mean-field)

→ Construct an **Edwards' measure**

1. Count configurations $S(E, N) = \ln \Omega(E, N)$

2. Maximise the entropy under the constraint $E \approx ct$

Gives population of vertices created during the demagnetisation :

$$n_{\alpha} = \frac{\exp(-\beta_E \epsilon_{\alpha})}{Z(\beta_E)}$$

With $\frac{1}{T_E} = \frac{\partial S}{\partial E}$ **configurational 'temperature'**

'A-thermal' Artificial spin ice

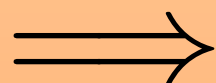
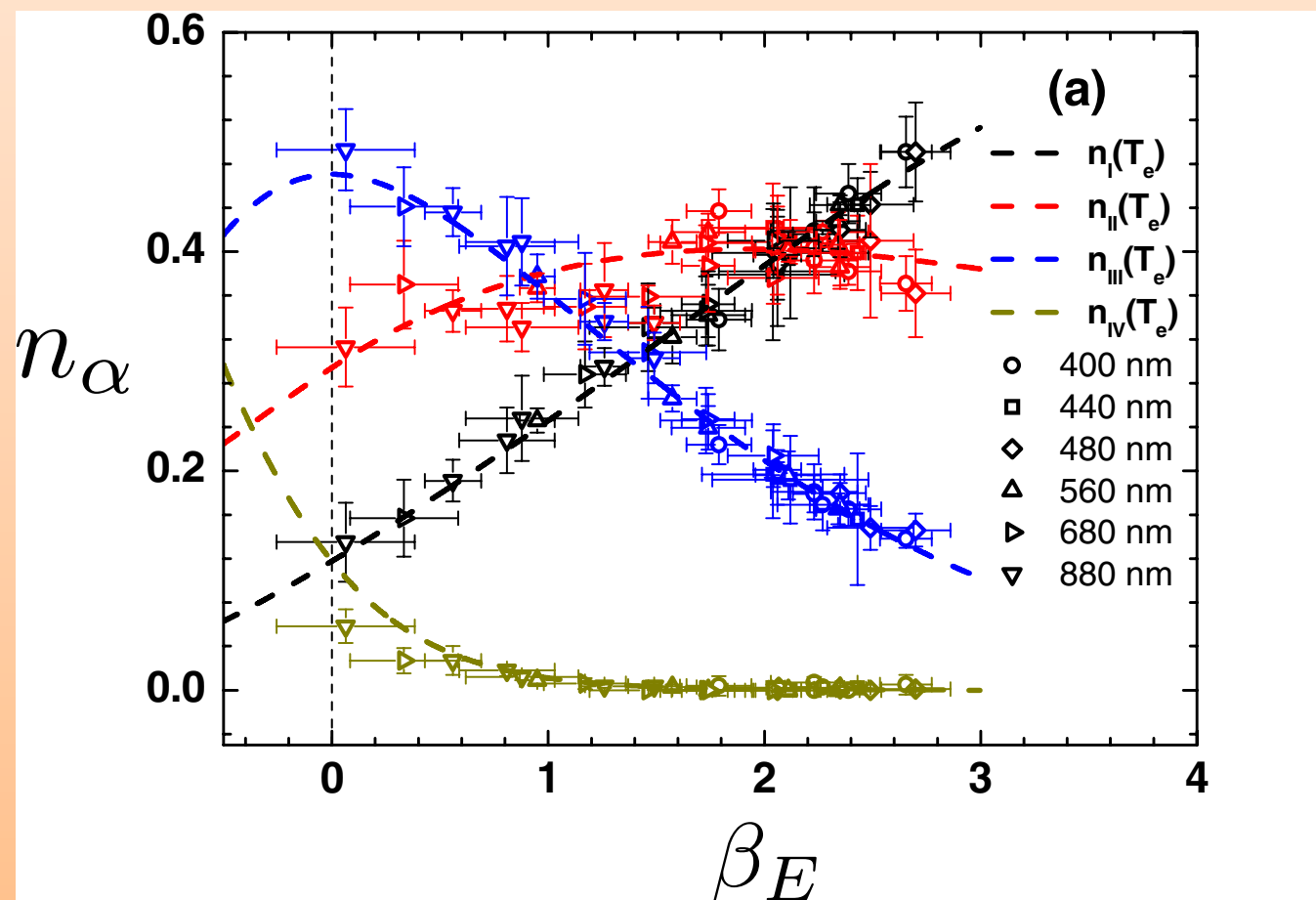
(Nisoli et al. 2007-2010)

Count vertices in the samples

$$n_\alpha = \frac{\exp(-\beta_E \epsilon_\alpha)}{Z(\beta_E)}$$

$$\beta_E = \ln \left(\frac{4n_c}{n_e} \right) (\epsilon_e - \epsilon_c)^{-1}$$

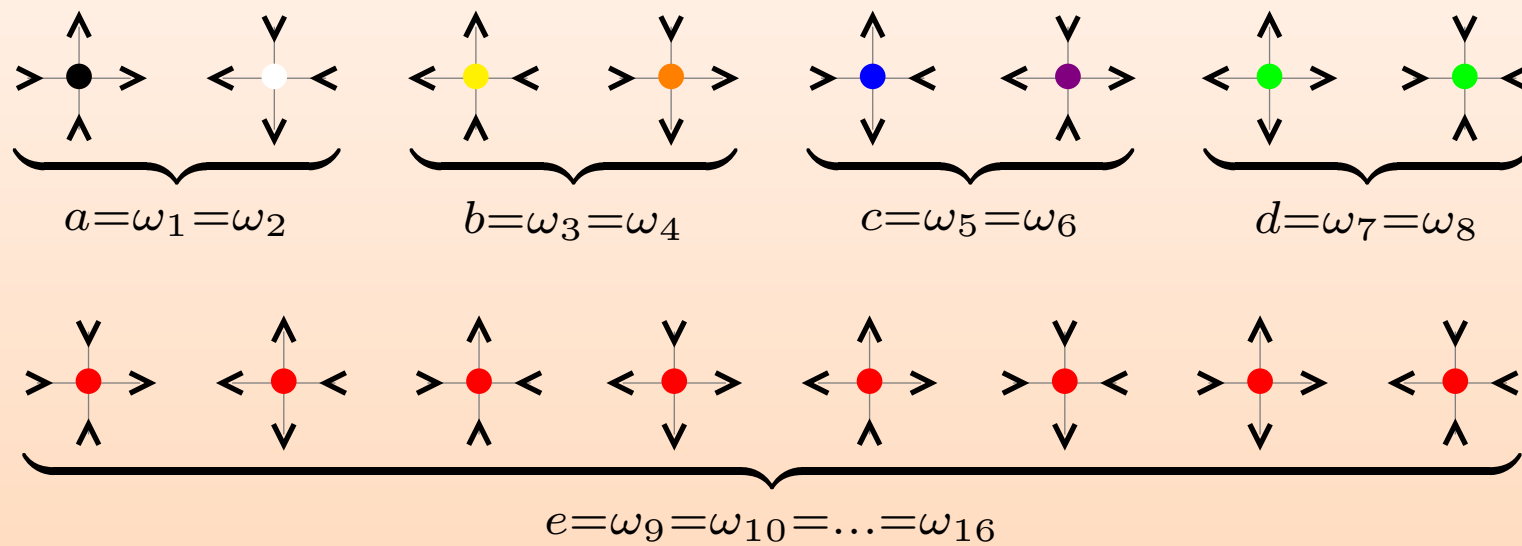
From: Nisoli et al., PRL 105 (2010)



Ground state cannot be reached with this procedure

'Thermal' Artificial spin ice

Special parametrisation of the 16-vertex model:



$$a = b = \exp(-\beta \epsilon_a)$$

$$c = \exp(-\beta \epsilon_c)$$

$$e = \exp(-\beta \epsilon_e)$$

$$d = \exp(-\beta \epsilon_d)$$

Energy of each vertex = approximation of the dipolar interactions
 $\Rightarrow$ High energy to the defects

Analytical calculation on the **tree of plaquettes**

+

Continuous Time **Monte Carlo** simulations

Our canonical temperature: $\beta = -\frac{\ln a}{\epsilon_a}$

Sixteen-vertex model

Allow defects $\Rightarrow d = e \neq 0$

Ice rules $\rightarrow$ collective paramagnet with $\xi_{eq} = \infty$

~~Ice rules~~ $\rightarrow$ disordered paramagnet? $\infty > \xi_{eq} > L$

How can we observe a difference?

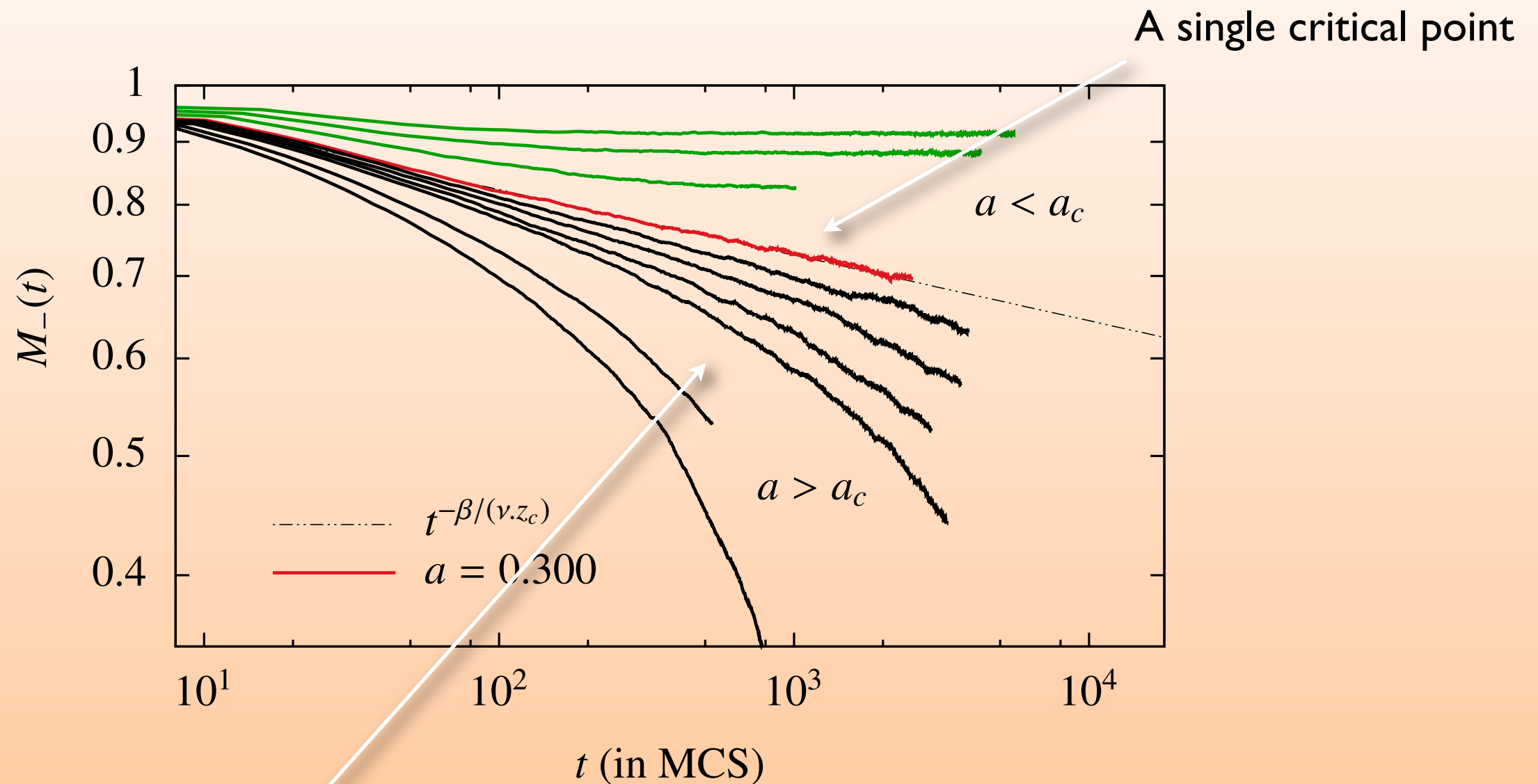
Non-equilibrium relaxation from an completely ordered state towards equilibrium in different phases

$$M_+(t) \left\{ \begin{array}{ll} \sim \exp(-t/\tau) & \text{disordered} \\ \sim t^{-\lambda} & \text{critical } \xi_{eq} = \infty \\ \sim M_+^{eq} \exp(-t/T) & \text{ordered} \end{array} \right.$$

power-law behaviour inside the SL phase

TEST criticality

'Thermal' Artificial spin ice

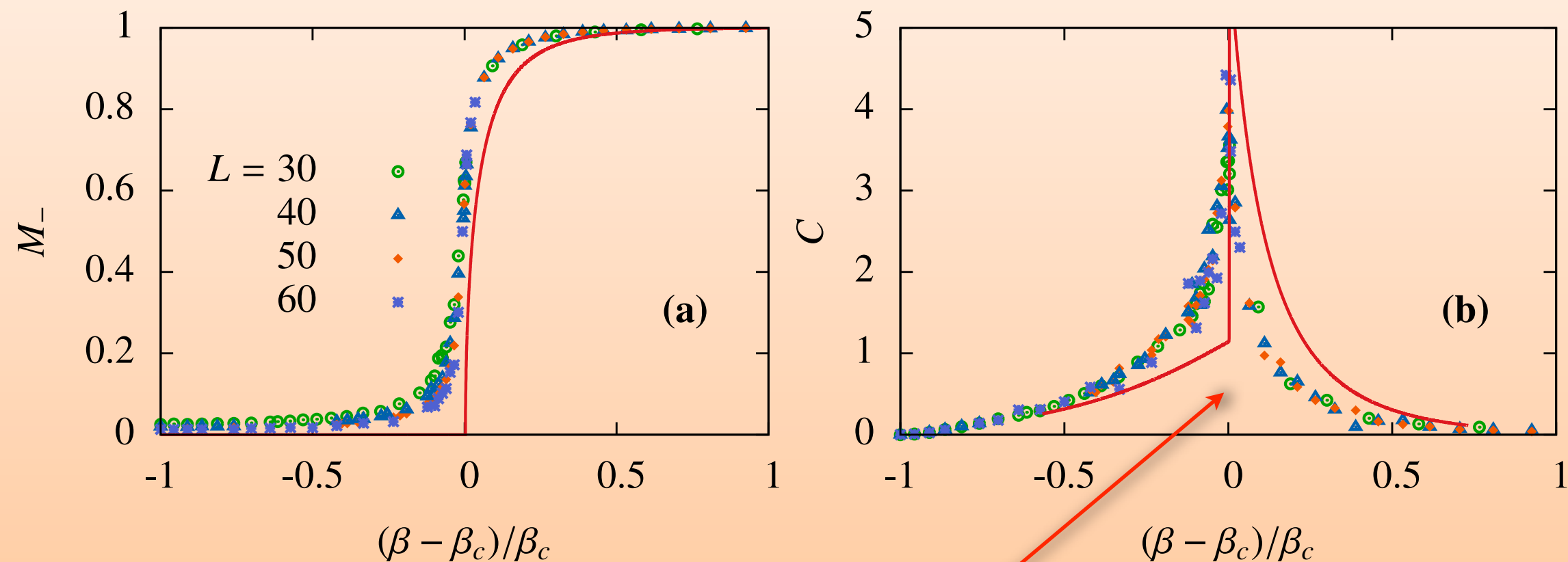


Non-critical correlation in the PM phase

⇒ The spin-liquid phase is lost as soon as a finite density of defects is present

'Thermal' Artificial spin ice

Numerics vs. Cavity calculation

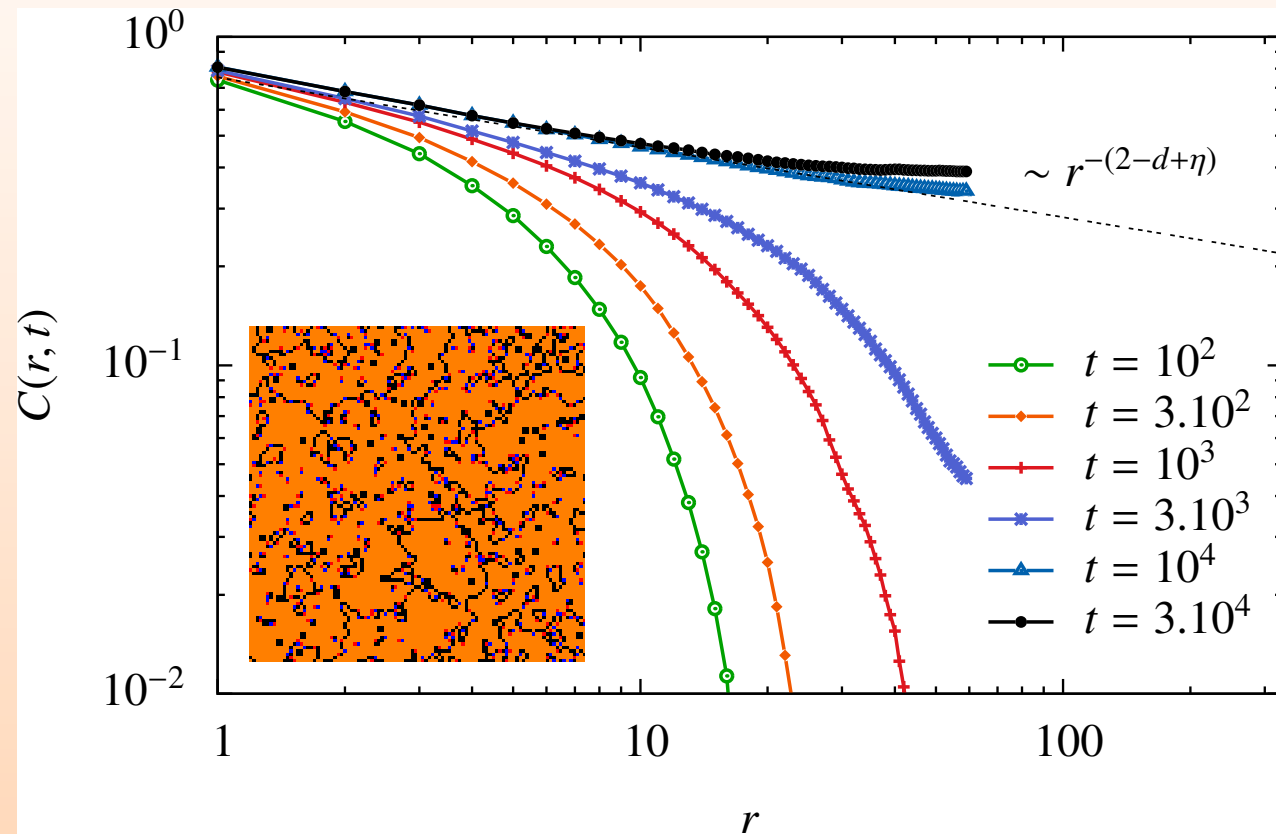


Second order phase transition at $\beta_c \approx 2.65$

→ Compare with experiments

Levis, Cugliandolo, Foini, Tarzia In preparation (2012)

'Thermal' Artificial spin ice

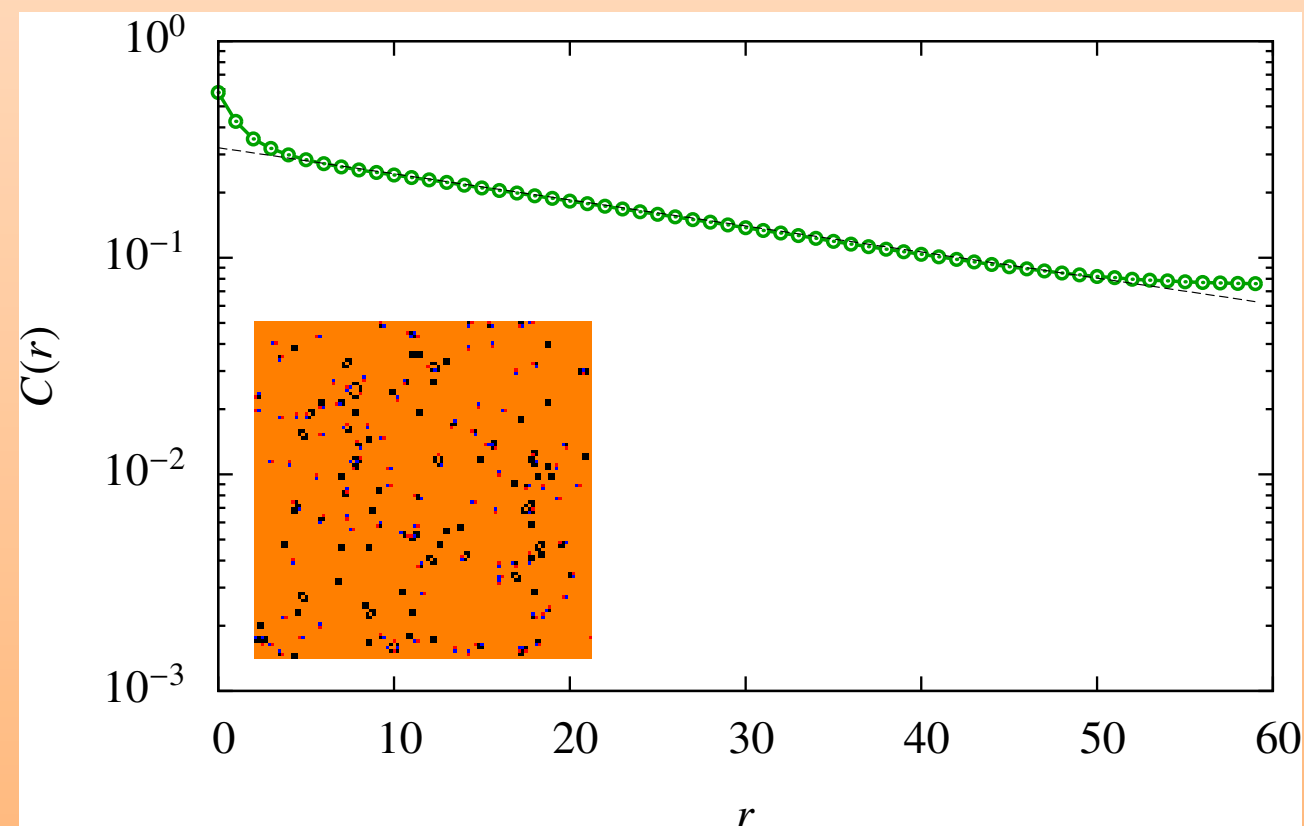


Two-point space-time correlations:

$$C(r, t) \propto \langle \sum_{i,j} S_{i,j}(t) S_{i+r,j+r}(t) \rangle$$

← $\beta \approx \beta_c$

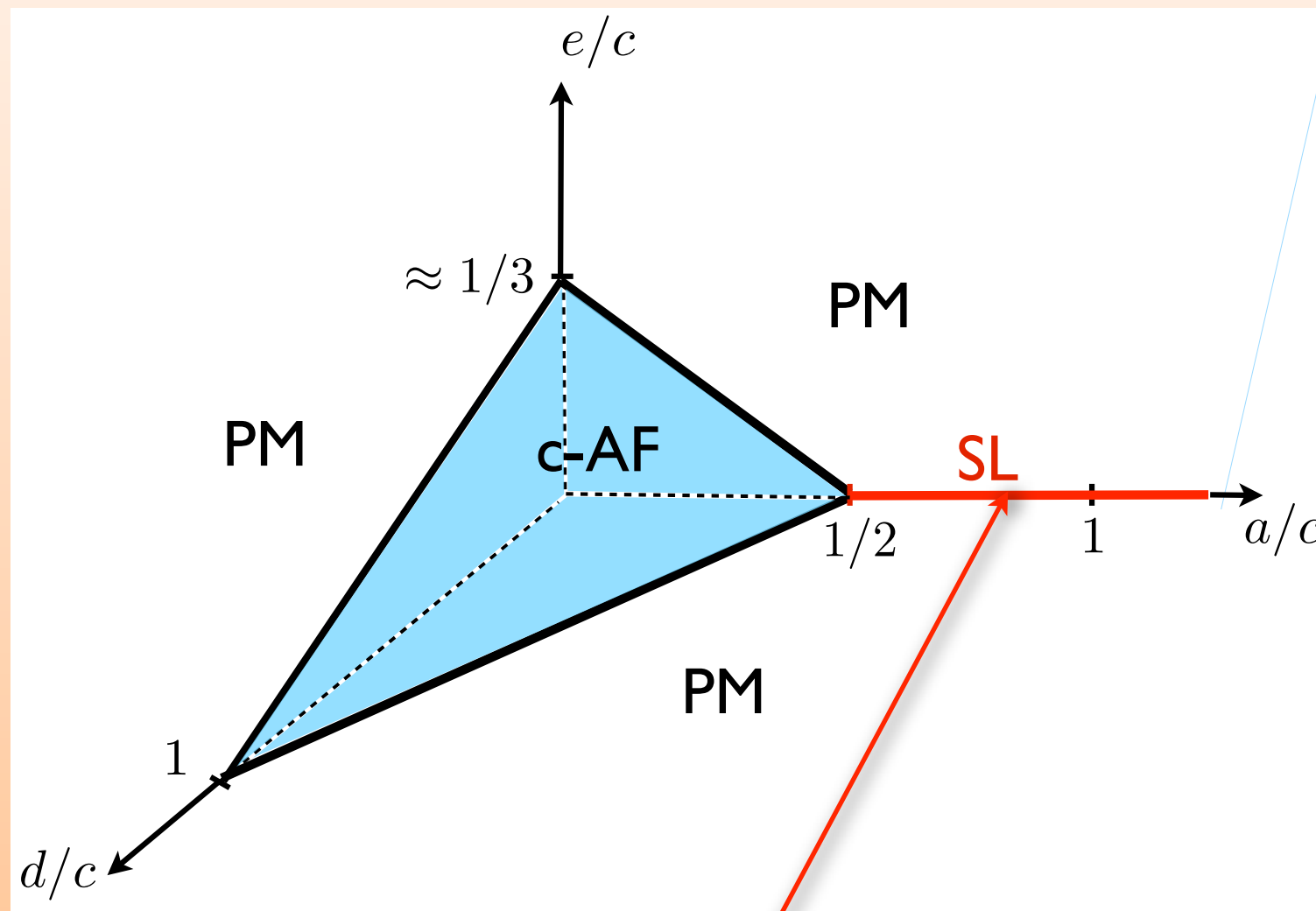
Slowing down close to the critical point



← $\beta > \beta_c$

'Thermal' Artificial spin ice

Phase diagram of ASI (extensive numerics + cavity)



The criticality of the SL phase is lost as soon as $d, e > 0$

Conclusion & outlook.

1. Investigate the variation of critical exponents in the 16V model by a real-space **Renormalisation Group** approach.
2. Extend the mappings between **integrable vertex models** (6V and 8V) into **quantum spin chains** (XXZ and XYZ resp.) to the unconstrained 16V model. Then, use our understanding on the classical model to predict the behaviour of the quantum system?
3. Link between **configurational temperatures** in ASI and the **canonical temperature**? In experiments:
 - properties of the domain walls?
 - thermal equilibration?
 - growth rate (link with a cooling rate)

Conclusion & outlook.

4. **Defects' motion** in 2D (square or hexagonal).

Prepare the system into an 'ice-rule' configuration, then follow the motion of a pair of defects. Interaction?

Model for collective transport properties?

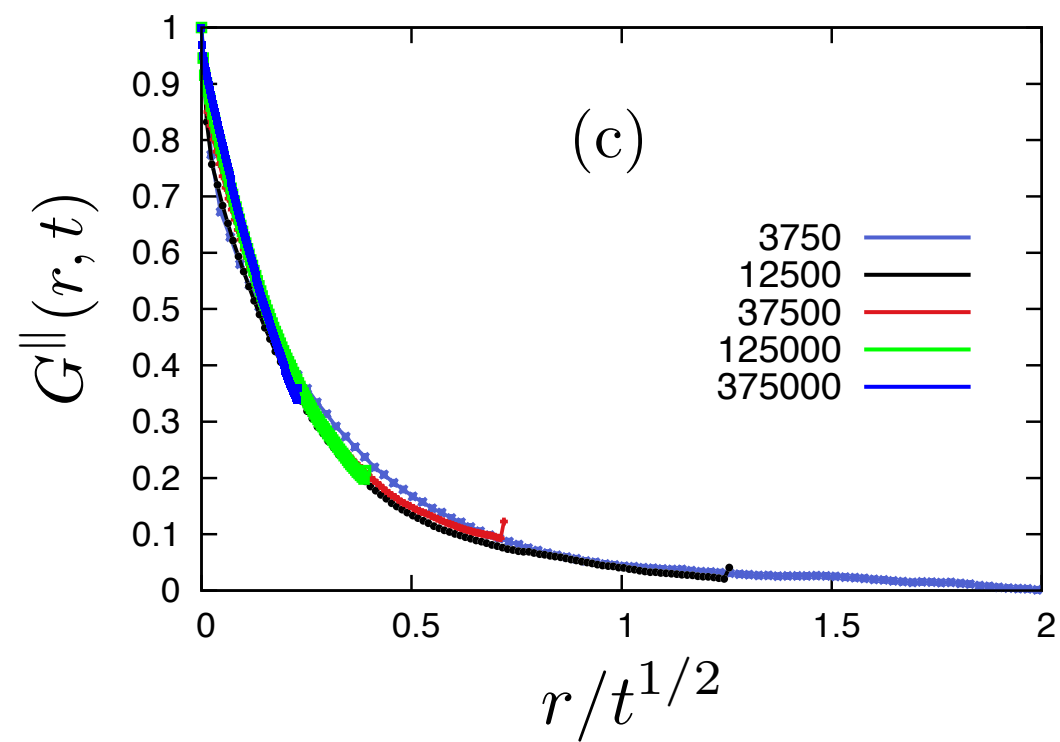
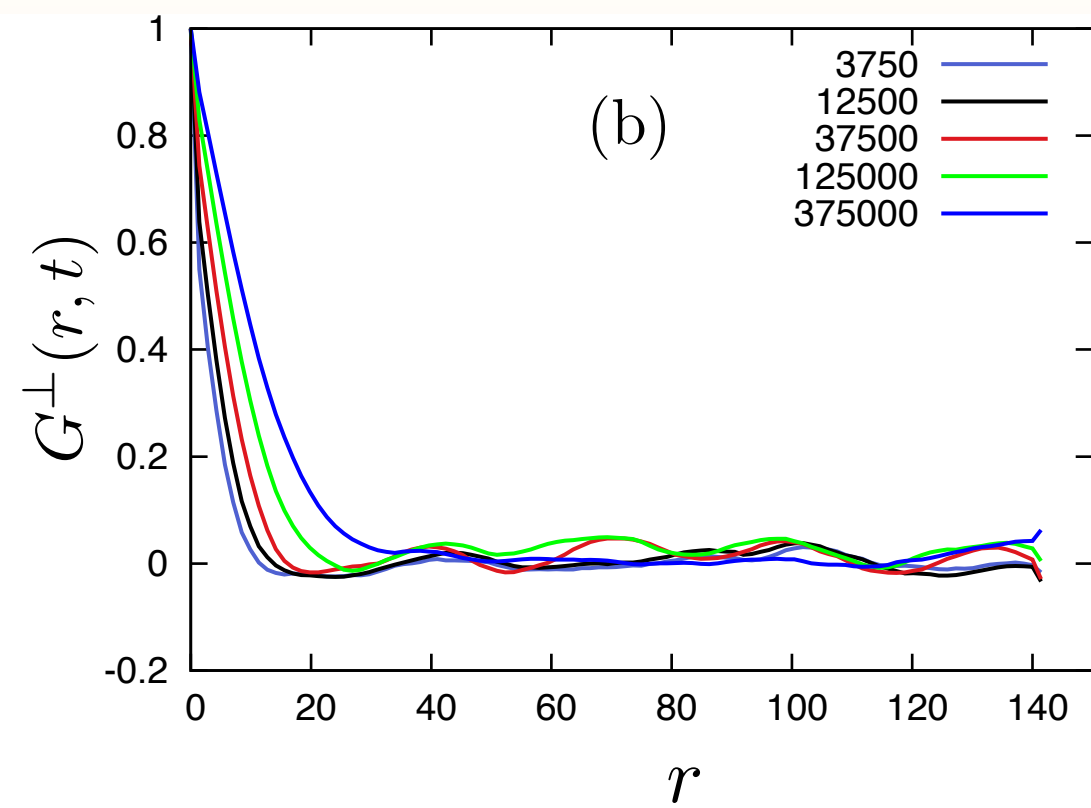
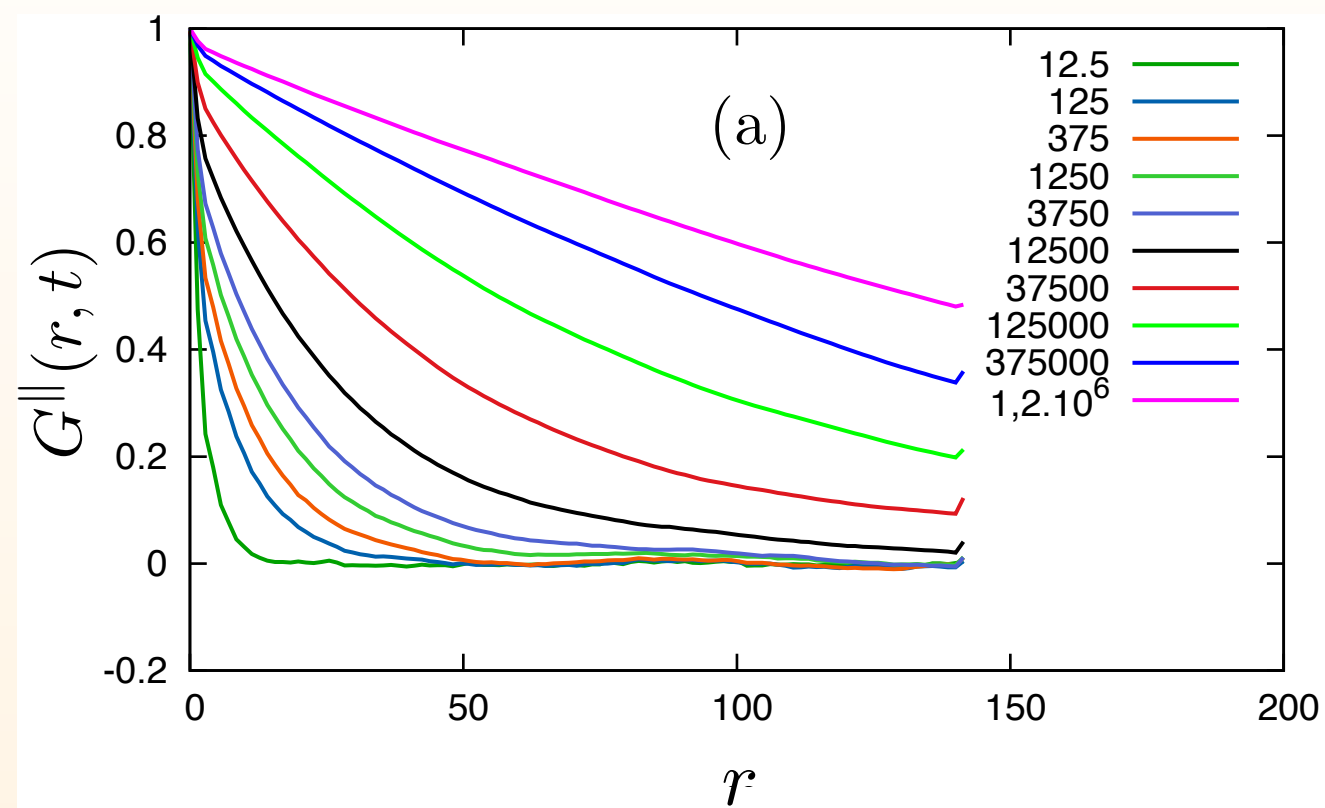
5. Effect of **boundary conditions** on the dynamics of hardly constrained models.

6. In particular, study the relaxation dynamics of the **six-vertex model with fixed boundary conditions** using local updates. **Topological glass?**

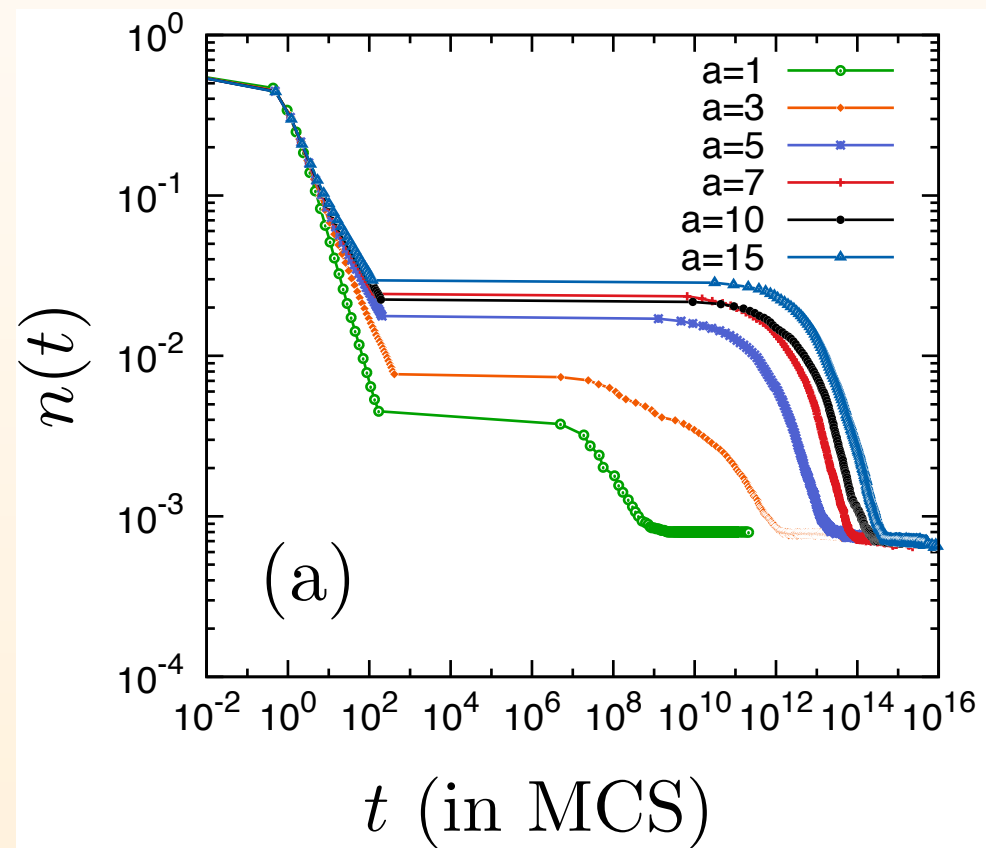
7. I. Use the same BP and CTMC approach to study the 16V model in an **external field**.

Extend the BP approach to deal with other **geometrically frustrated** stat. models (AF Ising, Kagome ice, colouring models, etc.).

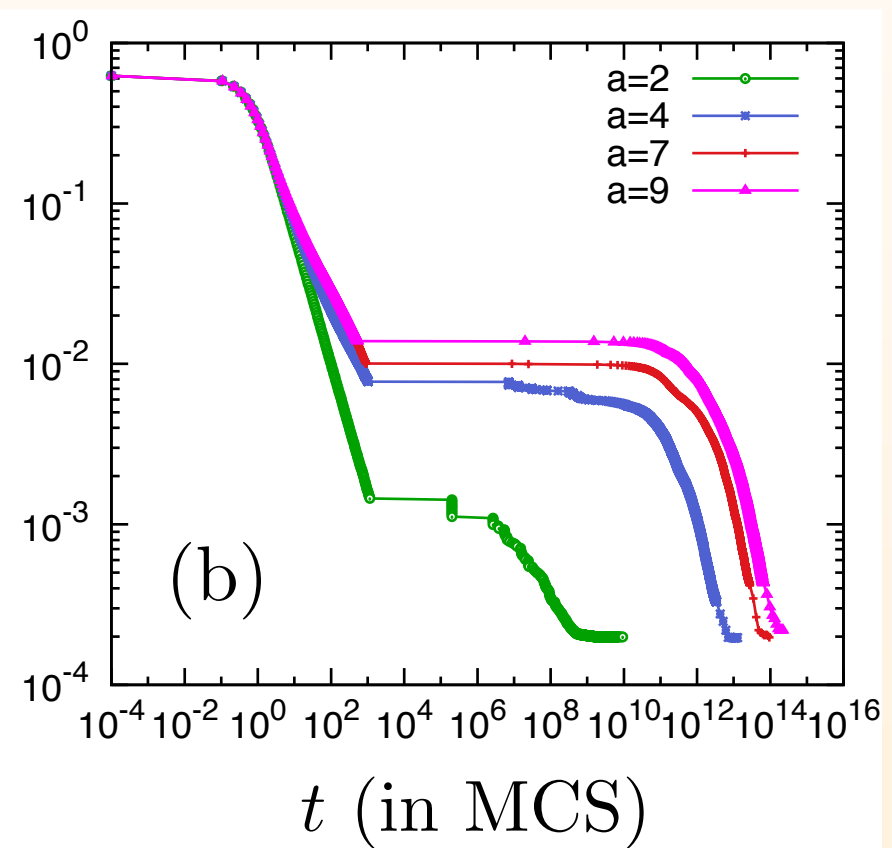
$$L = 200, a = 5, b = 1, d = e = 10^{-5}$$



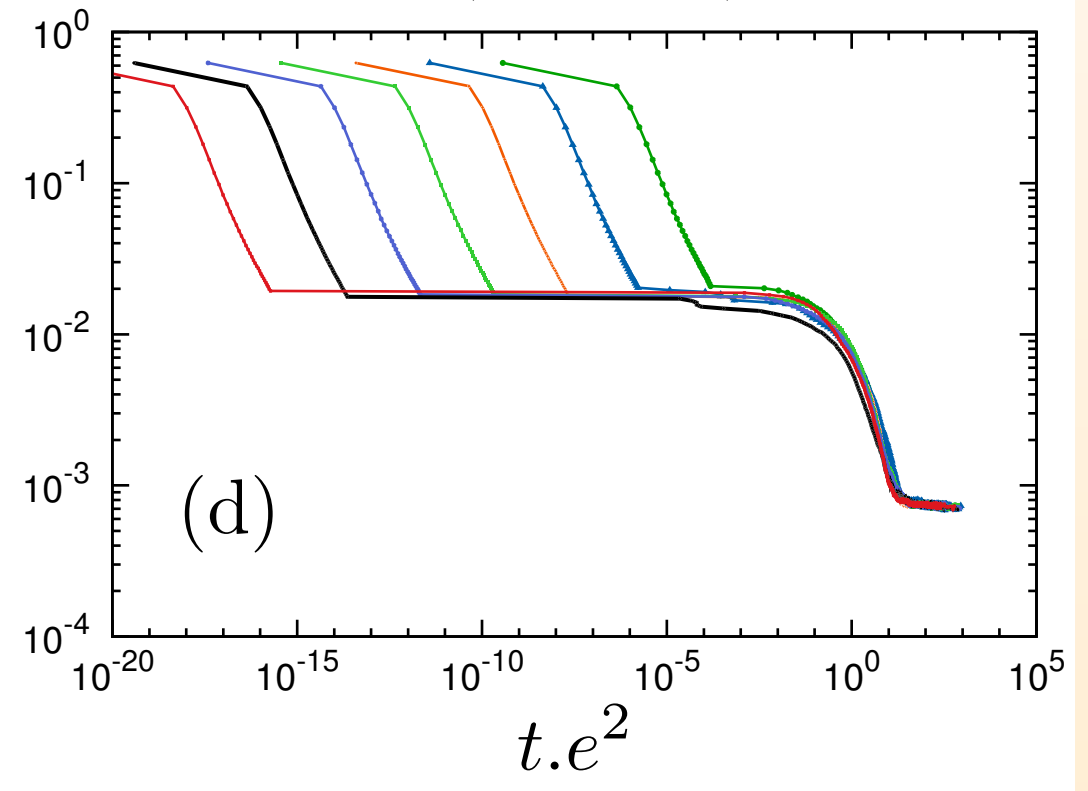
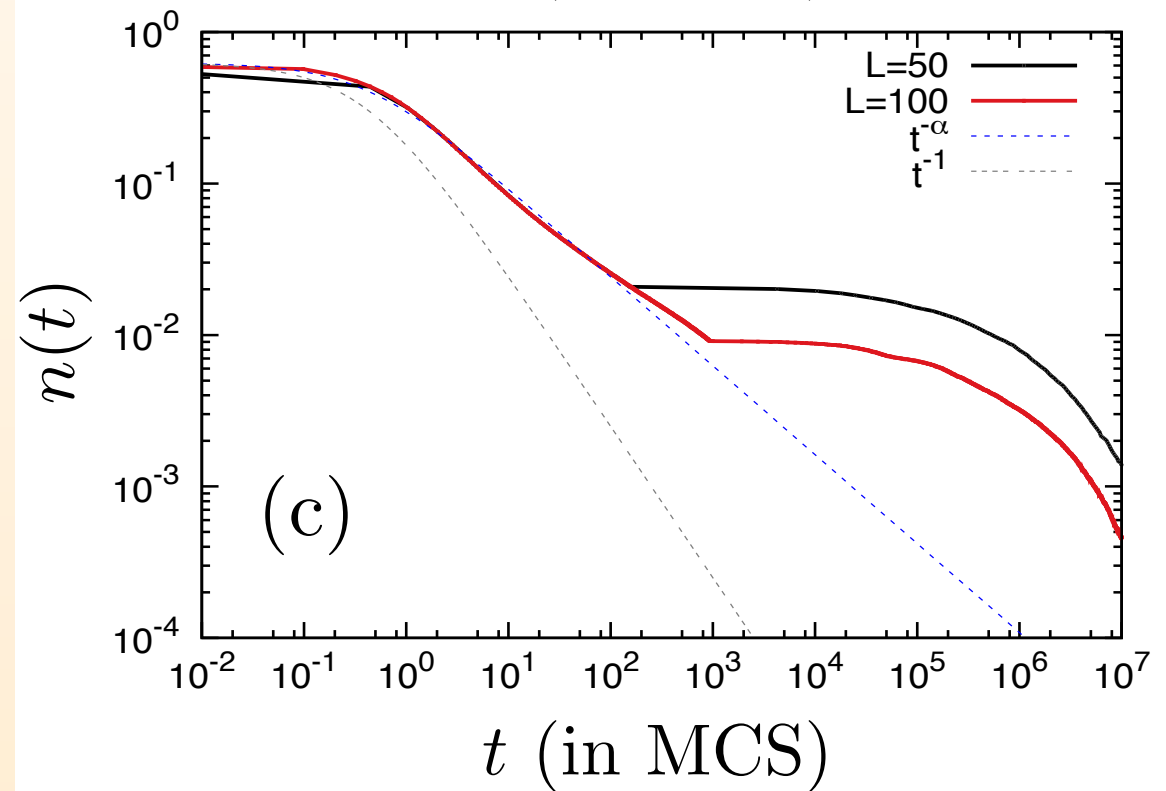
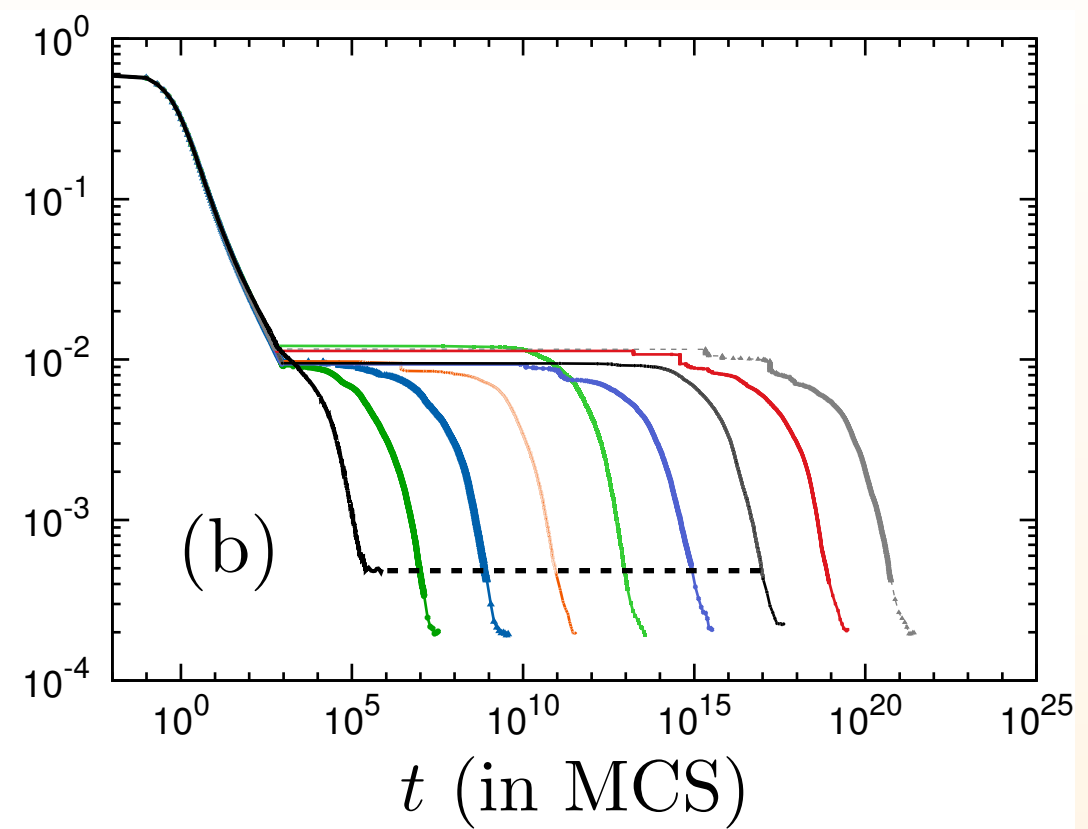
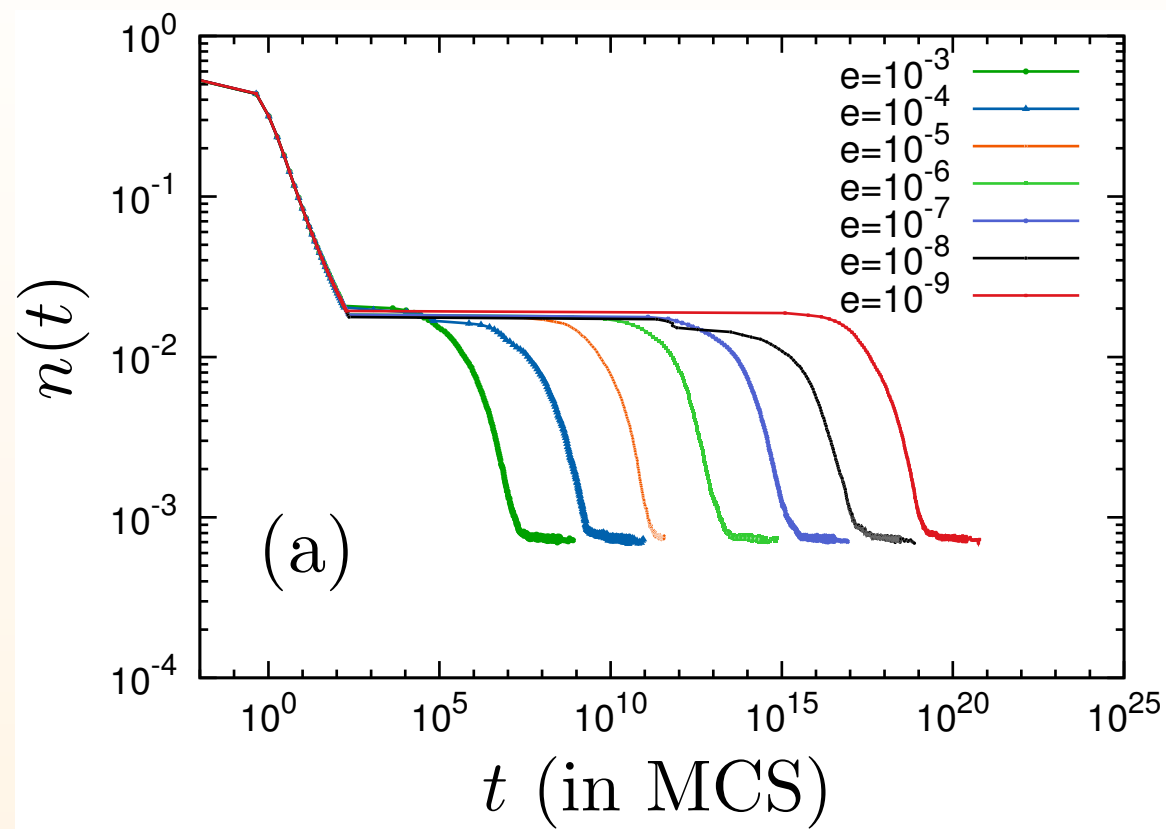
$$L = 50$$



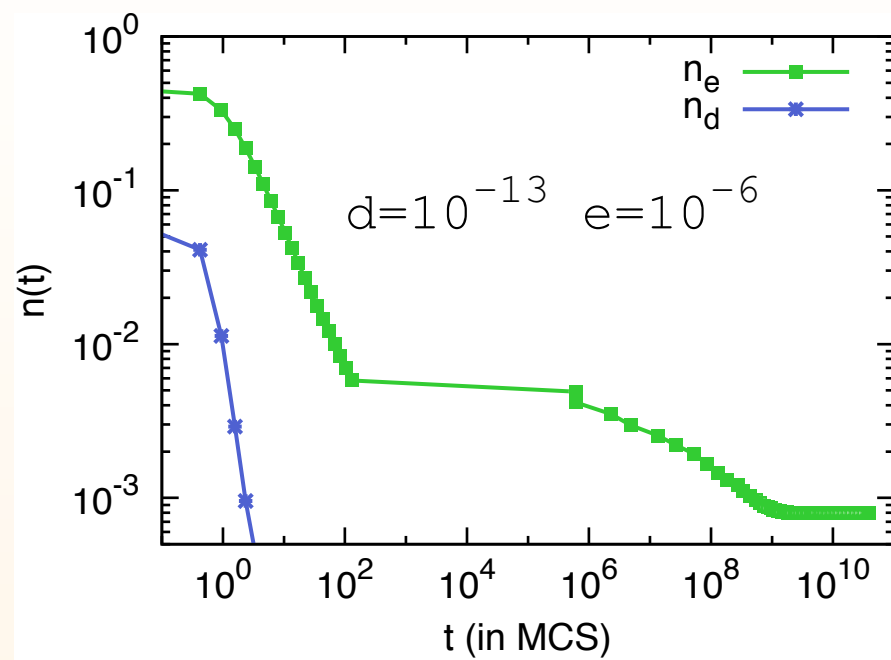
$$L = 100$$



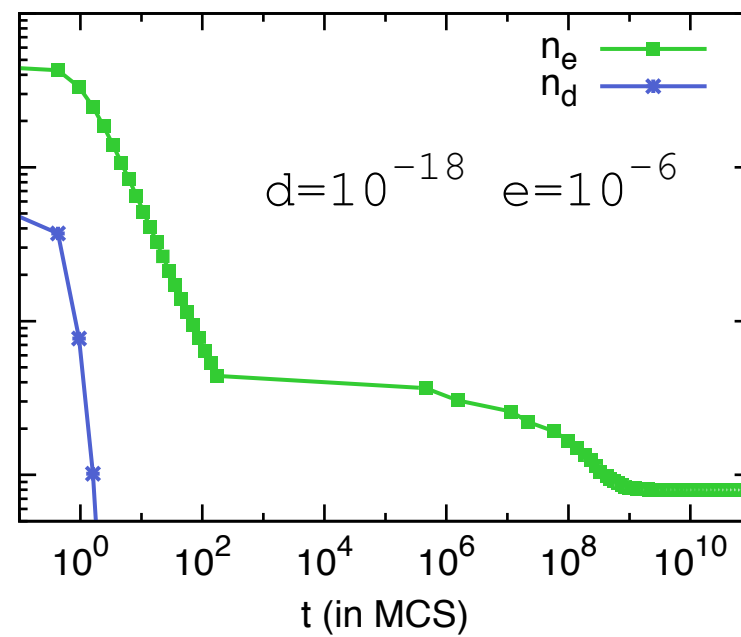
$$d = 10^{-18}, e = 10^{-6}$$

$L = 50$
 $L = 100$


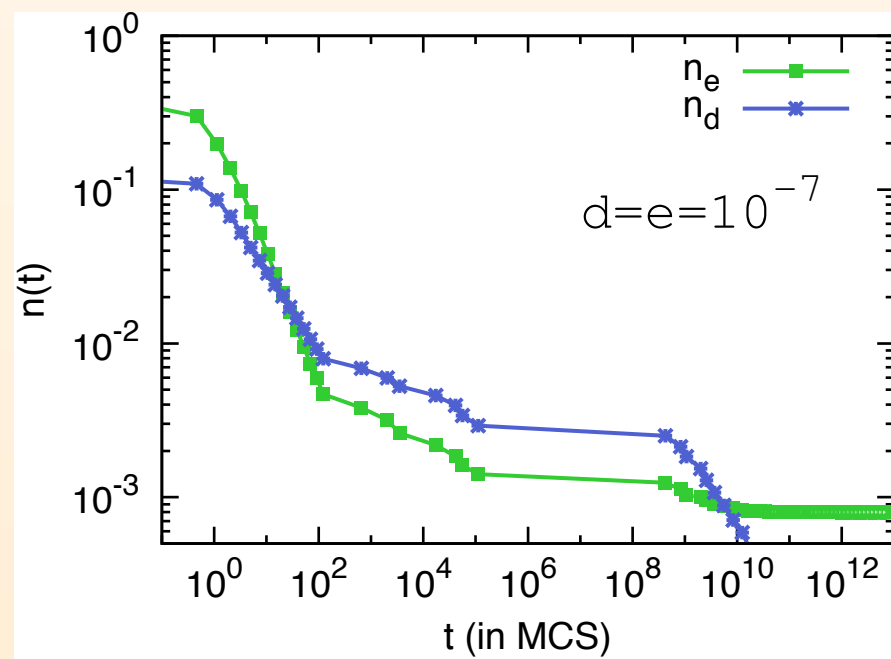
$$a = 5, b = 1, d = e^2$$



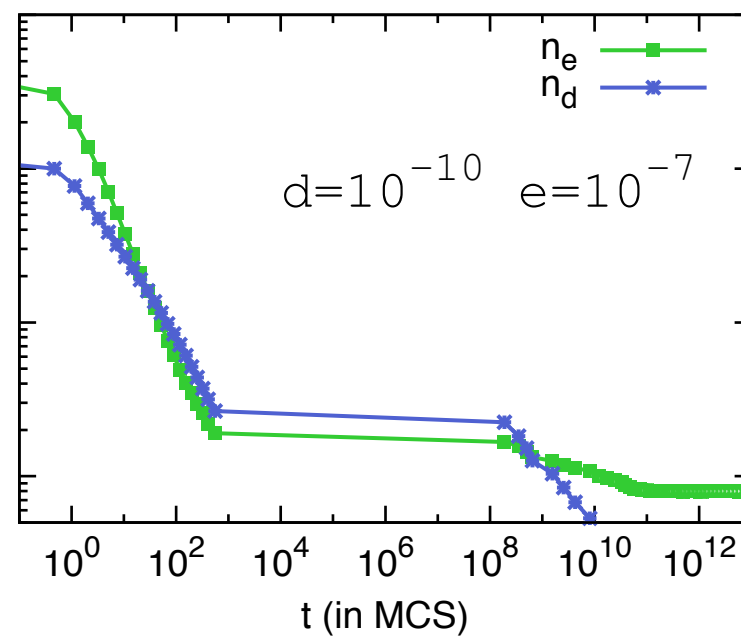
(a)



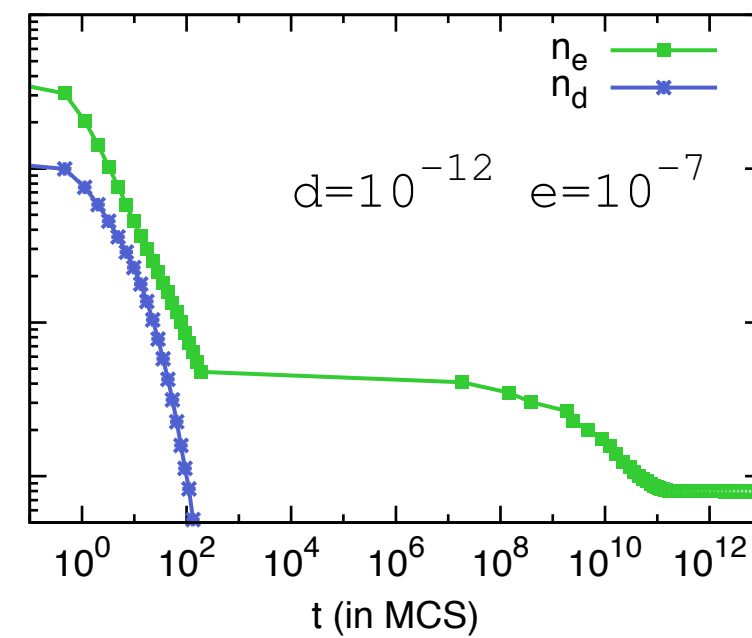
(b)



(a)



(b)



(c)