Artificial spin-ice & vertex models

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Why this topic ?

- Materials of possible technological importance
- that pose challenging

  problems in experimental physics,

  questions of fundamental interest,

and need(ed) the development of theoretical physics/mathematics tools.

Nice interplay between theory & experiment.

Interesting questions on out of equilibrium dynamics & equilibration.

Plan

- Materials
- Vertex models
- Statics: cavity method & Monte Carlo (MC) simulations
- Order by disorder: cavity method, low-T expansion & MC simulations
- Questions on dynamics: sample preparation & equilibration ?

Artificial spin-ice

Metamaterials: designed in the laboratory.

Artificial spin-ice

Metamaterials

Arrays of nano/micro-scale magnets

single domain magnetic islands

placed at the edges of a tiling or

the edges of a planar graph

Parameters specified by design

Artificial spin-ice

Metamaterials

Arrays of micro/nano-scale magnets

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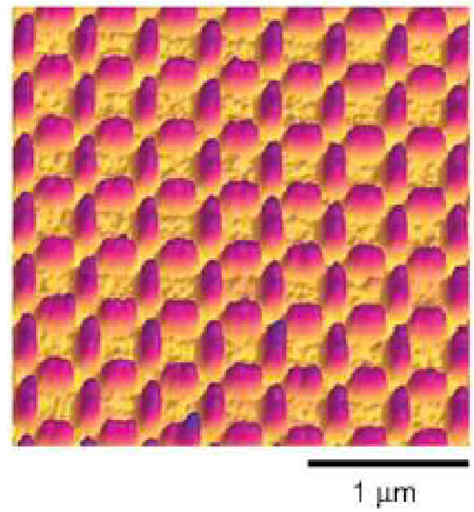
Parameters specified by design

Image: atomic foce microscopy



Square lattice

Wang et al 06

Artificial spin-ice

Metamaterials

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single domain magnetic islands

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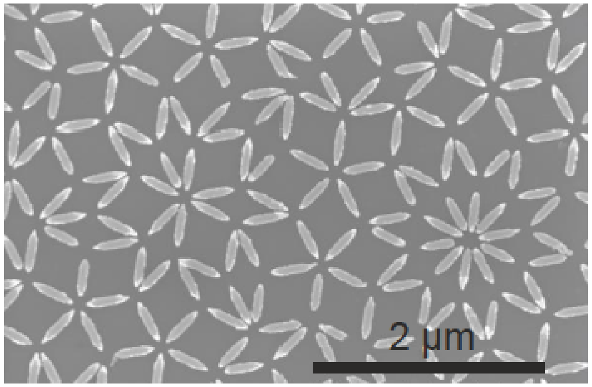


Penrose tiling

Marrows et al 14

Artificial spin-ice

Metamaterials

Arrays of micro/nano-scale magnets

single domain magnetic islands

placed at the edges of a tiling

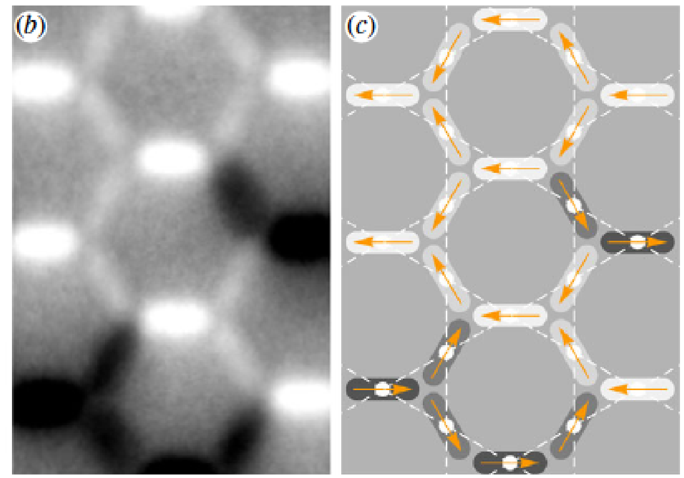
the edges of a planar graph

Material such that Ising spins

Construction $\Rightarrow$ along the edges

Photoelectron emission microscopy

(More about fabrication later)



Honeycomb lattice

Hügli et al 15

Artificial spin-ice

Metamaterials

Arrays of micro/nano-scale magnets

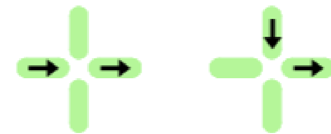
single domain magnetic islands

placed at the edges of a tiling or

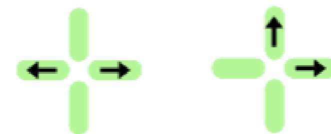
the edges of a planar graph

Ising spins along the links

e.g., square geometry



Favorable Pair Alignments



Unfavorable Pair Alignments

The islands meet at each vertex ; local dipolar interactions are frustrated ; that is to say, they cannot be satisfied simultaneously.

It is not possible to find a configuration of the spins that join at a vertex that minimises all pair contributions to the total energy.

Artificial spin-ice

Metamaterials

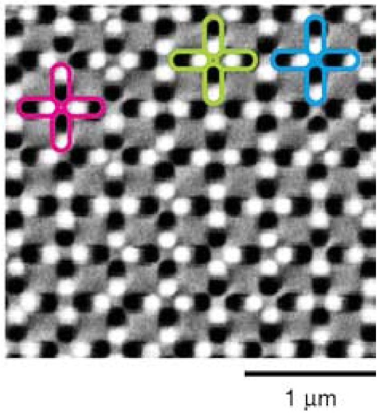
Arrays of nanoscale magnets

single domain magnetic islands

placed at the edges of a tiling or

the edges of a planar graph

Ising spins along the links



Magnetic force microscopy

Local dipolar interactions are $\boxed{\text{geometrically frustrated}}$

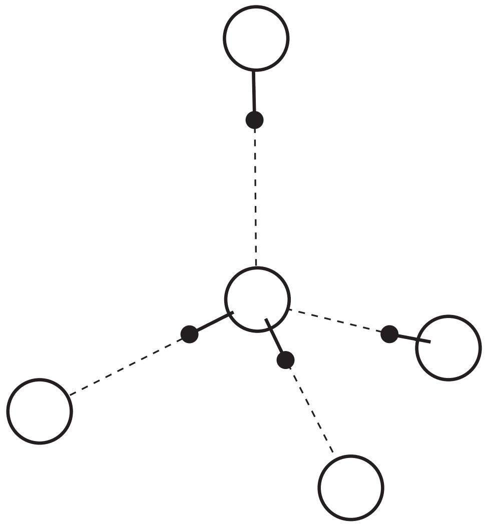
no quenched disorder

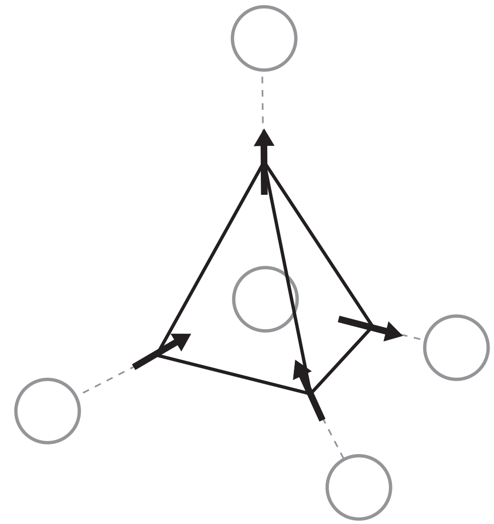
It is not possible to find a configuration of the spins that join at a vertex that minimises all pair contributions to the total energy.

$\boxed{\text{Macroscopic degeneracy of the ground state and metastable states}}$

Natural ices

Single cell unit - tetrahedron - in water-ice and spin-ice





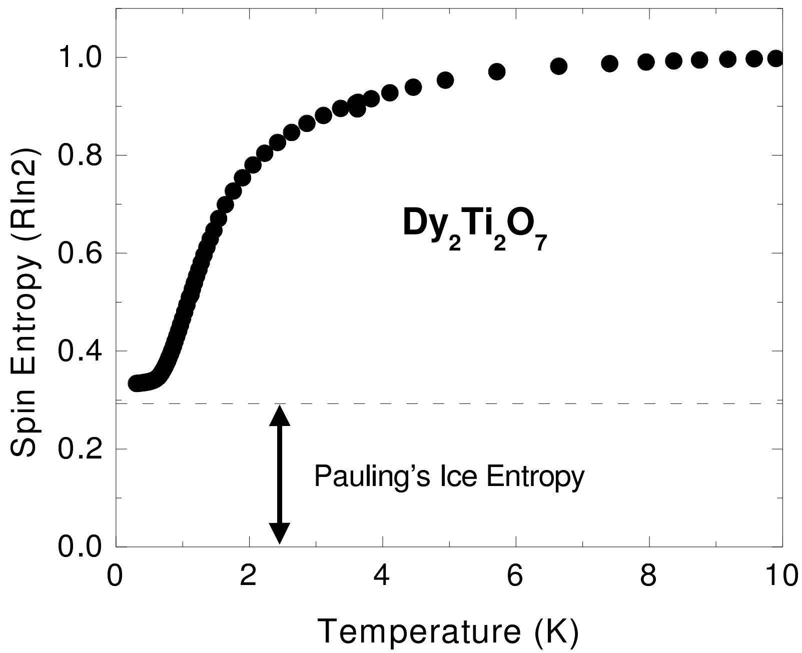
Water-ice: coordination four lattice. **Bernal & Fowler 33** rules, two H near and two far away from each O.

Spin-ice: four (Ising) spins on each tetrahedron forced to point along the axes that join the centres of two neighbouring units (Ising anisotropy). Local interactions imply the two-in two-out ice rule

e.g. $Dy_2\ Ti_2\ O_7$ **Harris, Bramwell, McMorrow, Zeiske & Godfrey 97**

Natural spin-ice entropy

$$\boxed{\Delta S = \int_{T_1}^{T_2} dT' \, \frac{C(T')}{T'}}$$



Counting argument

Pauling 35

2-near 2-far H

(2-in 2-out arrows)

equally probable

Pauling's ice entropy

Ramírez, Hayashi, Cava, Siddharthan & Shastry 99.

Very similar to **Giauque & Stout 33** for water ice.

Artificial spin-ice - model

Instead of dipolar interactions, a simpler modelling

Metamaterials

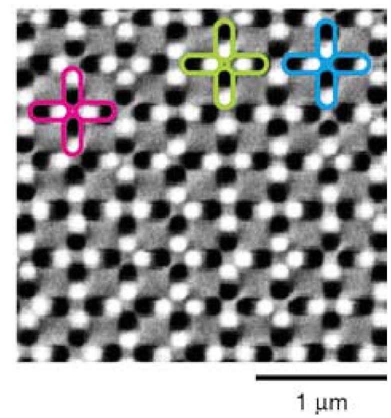
Arrays of nanoscale Ising magnets

single domain magnetic islands

placed at the edges of a tiling or

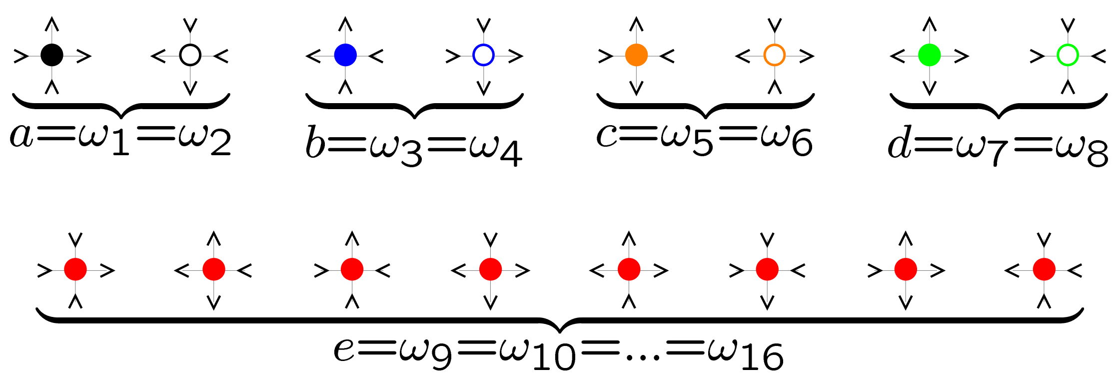
the edges of a square lattice

Parameters specified by design



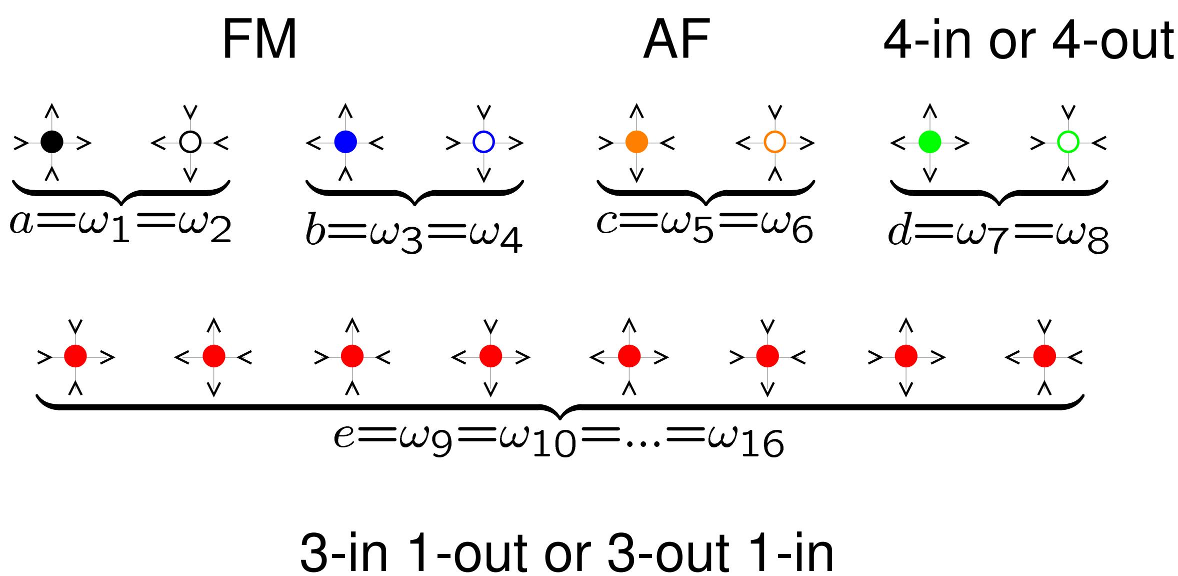
Magnetic force microscopy

Local approx: $2d$ vertex model with experimentally relevant parameters



The $2d$ 16 vertex model

with 3-in 1-out vertices: non-integrable system



(Un-normalized) statistical weight of a vertex $\omega_k = e^{-\beta\epsilon_k}$

In the model a, b, c, d, e are free parameters (usually, c is the scale)

In the experiments ϵ_k depend on the sample and,

typically, $\boxed{\epsilon_{\rm AF} < \epsilon_{\rm FM} < \epsilon_{\rm 3in-1out} < \epsilon_{\rm 4in}}$

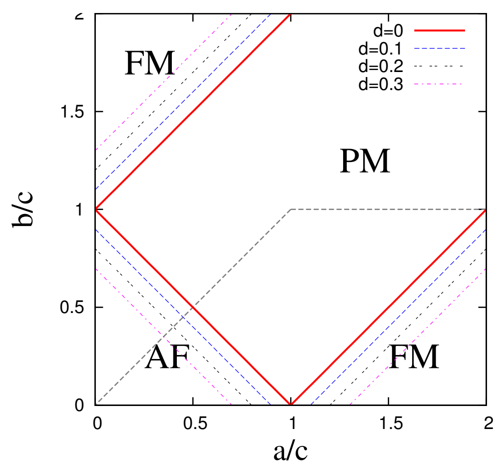
The energies ϵ_k could be tuned differently by adding fields, vertical off-sets, etc.

Static properties

What did we know ?

- **6 and 8 vertex models.**

  Integrable systems techniques (transfer matrix + Bethe Ansatz), mappings to many physical (e.g. quantum spin chains) and mathematical problems.



Phase diagram

critical exponents

ground state entropy

boundary conditions effects

etc.

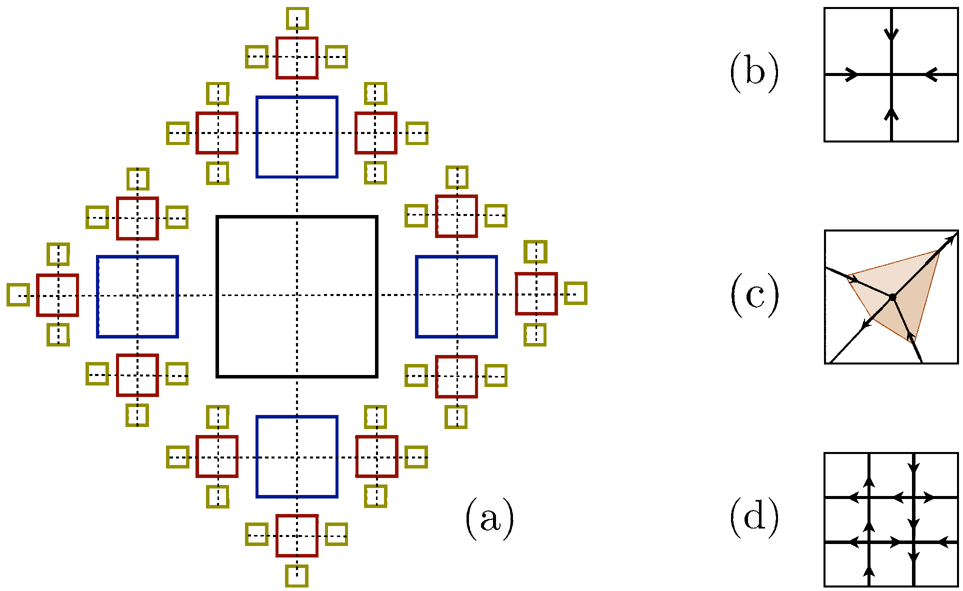
Lieb 67 ; Baxter *Exactly solved models in statistical mechanics* **82**

- **16 vertex model.**

  Integrability is lost. Not much interest so far.

Equilibrium analytic

Bethe-Peierls or cavity method



Correct phase diagram, Pauling's entropy at spin-ice point & improvements towards Lieb's result with unit plaquettes, etc.

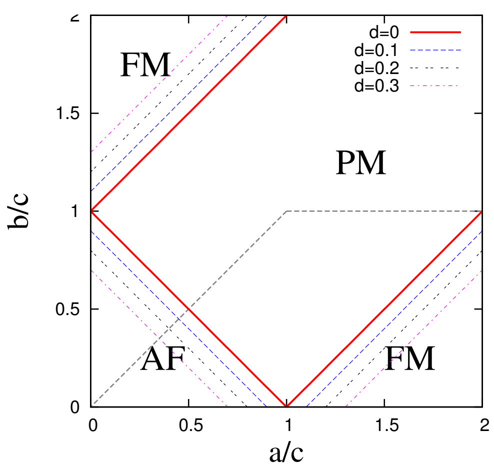
Foini, Levis, Tarzia & LFC 12

Static properties

With cavity method and Monte Carlo

- **6 and 8 vertex models.**

  Exact phase diagram (though different order of some transition lines)



Phase diagram

$\neq$ critical exponents

$\simeq$ ground state entropy

boundary conditions effects

etc.

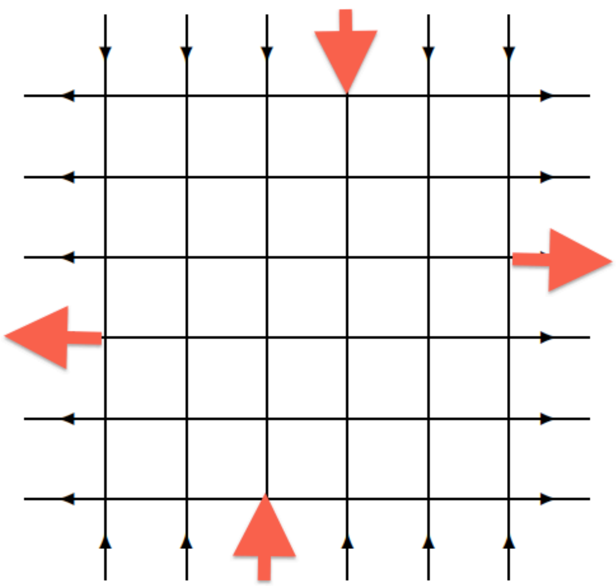
- **16 vertex model.**

  Integrability is lost. Phase diagram

Six-vertex model

with domain-wall boundary conditions

Strongly constrained model: non-trivial effect of boundary conditions.



Global parameters in D phase

$f^{D}_{\mathrm{dwBC}} > f^{D}_{\mathrm{pBC}}$

Korepin & Zinn-Justin 00

Macroscopic phase separation

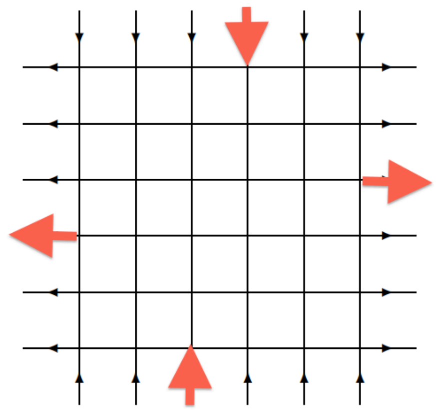
external frozen region

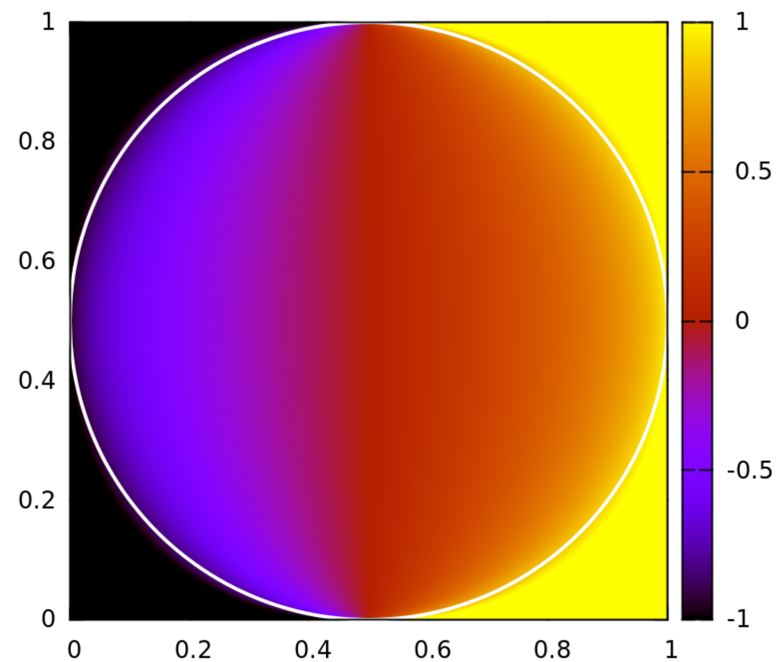
internal thermal region

arctic curve between the two

Six-vertex model

with domain-wall boundary conditions





$$\Delta \equiv (a^2 + b^2 - c^2)/(2ab)$$

$= 0$ Disordered phase

$a = b$ free-fermion case

Color code : Bethe-Peierls polarization of horizontal arrows

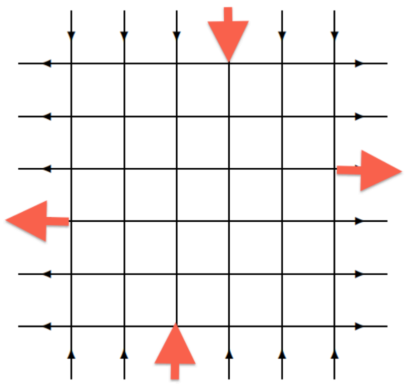
White curve : analytic arctic circle.

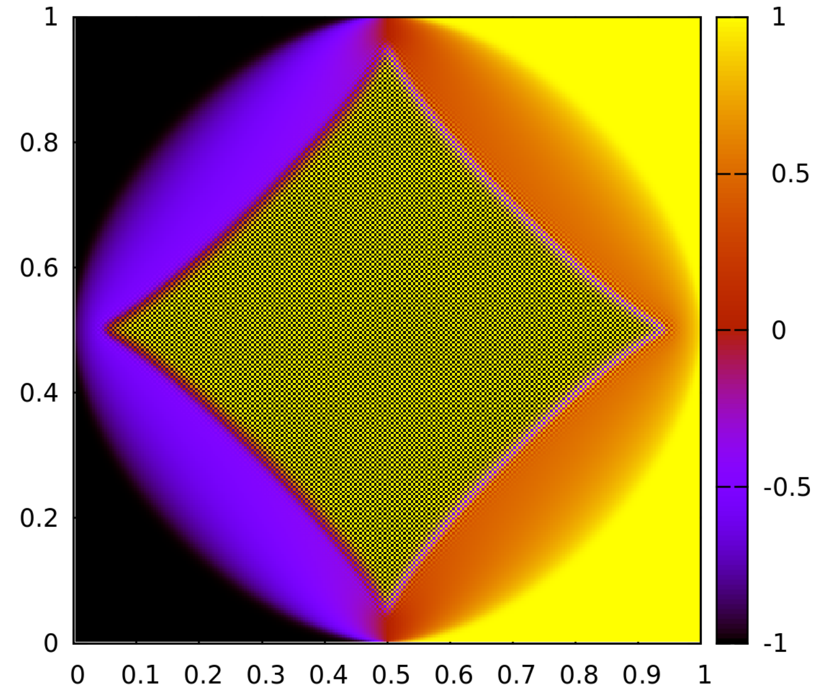
Elkies et al. 92-96 ; Jokusch et al. 98 ; Colomo & Pronko 08-14 ; Sportiello

LFC, Gonnella & Pelizzola 14

Six-vertex model

with domain-wall boundary conditions





$$\Delta \equiv (a^2 + b^2 - c^2)/(2ab)$$

< -1 Anti-ferromagnetic

$a = b = 1$

$c = 2.5$

Color code : BP polarization of horizontal arrows

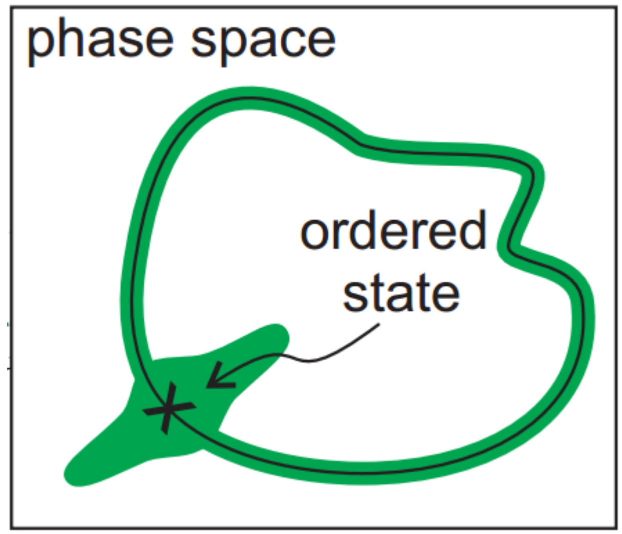
Double phase separation : frozen – thermal disordered - AF

Colomo, Pronko & Zinn-Justin 10 ; Sportiello

LFC, Gonnella & Pelizzola 14

Order by disorder

Classical result in statistical physics

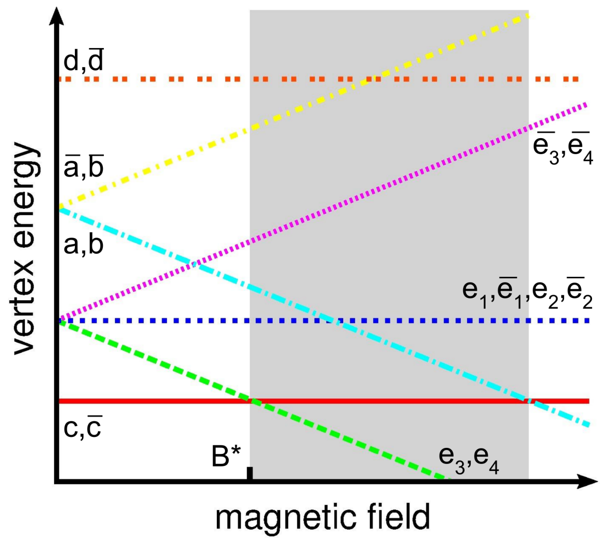


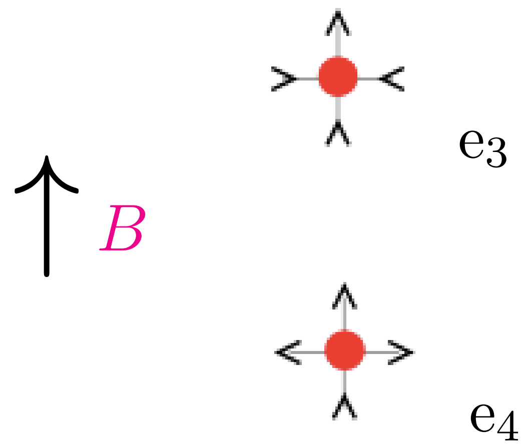
Degenerate manifold of ($T = 0$) ground states. The ordered one **x** is selected by the low temperature fluctuations since its excitations are much more numerous.

Villain, Bidaux, Carton & Conte 80

Order by disorder

In $2d$ spin-ice samples





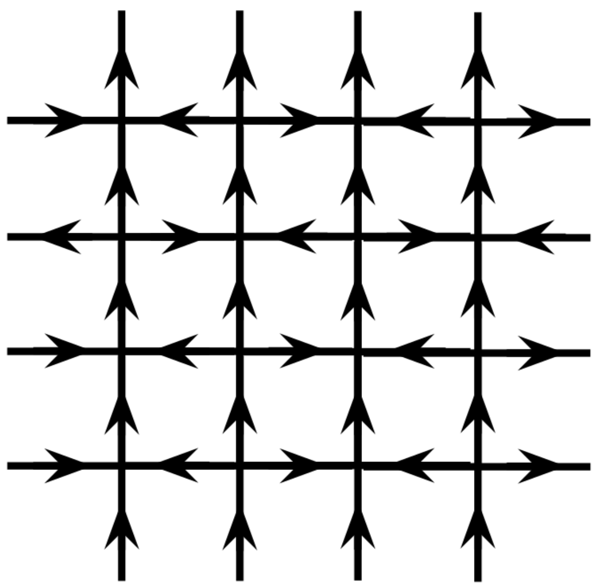
Imagine an unusual energy hierarchy at $B = 0$ with the 3in-1out and 3out-1in (called e) the first excited vertices

Apply a vertical magnetic field such that this pair of 3in-1out 3out-1in vertices become the lowest energy ones at B^*

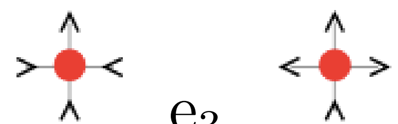
Work at $B \gtrsim B^*$

Order by disorder

Ground states made of e_3 and e_4



$\uparrow B$



Vertical arrows point up

On each line horizontal

arrows alternate right - left

staggered two-in / two-out

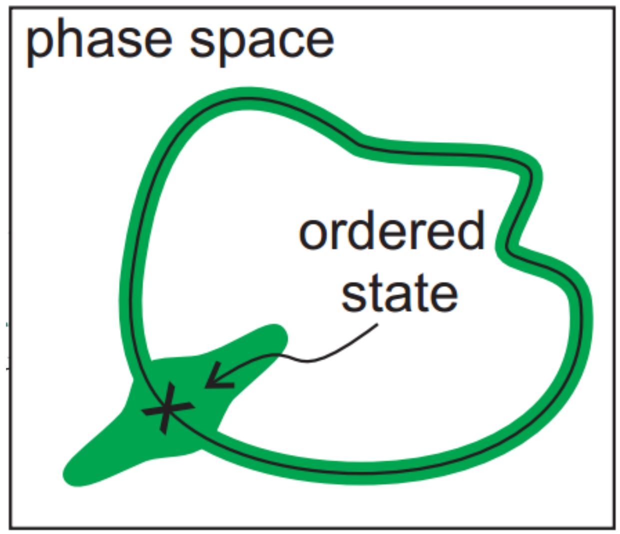
the starting one is free

Subextensive but large ground state entropy :

$S_0 = L \ln 2$, two independent choices for each line.

Order by disorder

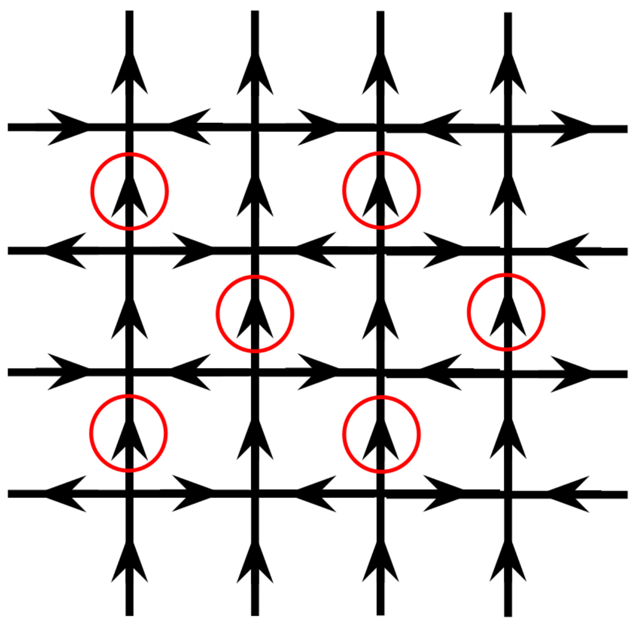
Classical result in statistical physics



Degenerate manifold of ($T = 0$) ground states.

Order by disorder

Two special ground states



$\uparrow B$

Vertical arrows point up

On each line horizontal

arrows alternate right - left

staggered two-in / two-out

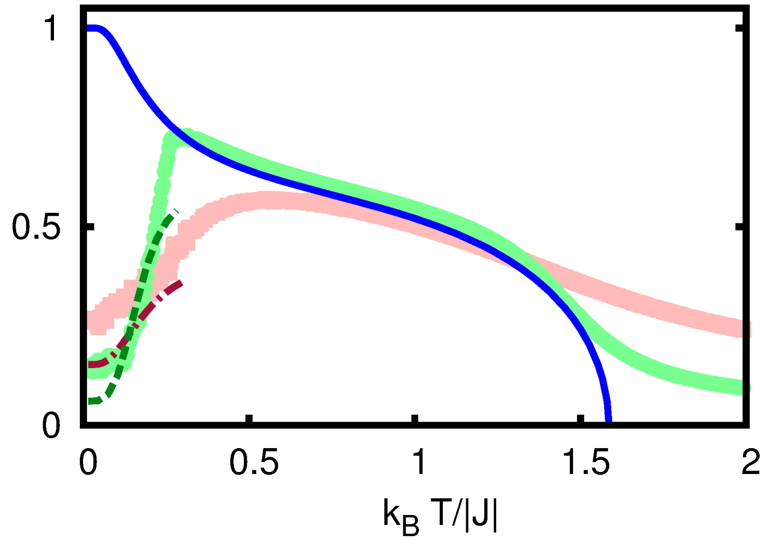
staggered AF order of lines

The encircled arrows can be turned at low energetic cost for $B \gtrsim B^*$ at low T

(a pair of e_3 - e_4 vertices into a pair of AF vertices)

Order by disorder

Analytical & numerical



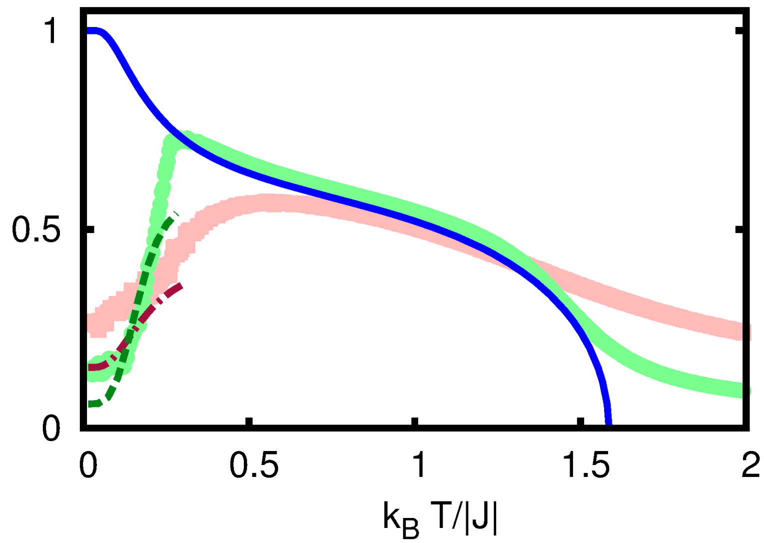
Blue line: cavity method results. Green and pink : solid lines simulations for two L, dashed lines low-T expansion of an effective $1d$ AF Ising model

$$H = J_{\text{eff}} L \sum_{i=1}^{L} s_i s_{i+1} \qquad\qquad J_{\text{eff}} = (4\beta)^{-1} e^{-2\beta\epsilon}$$

coupling the first spins on each row (the rest of the row is fixed by it).

Order by disorder

Exploiting finite size effects



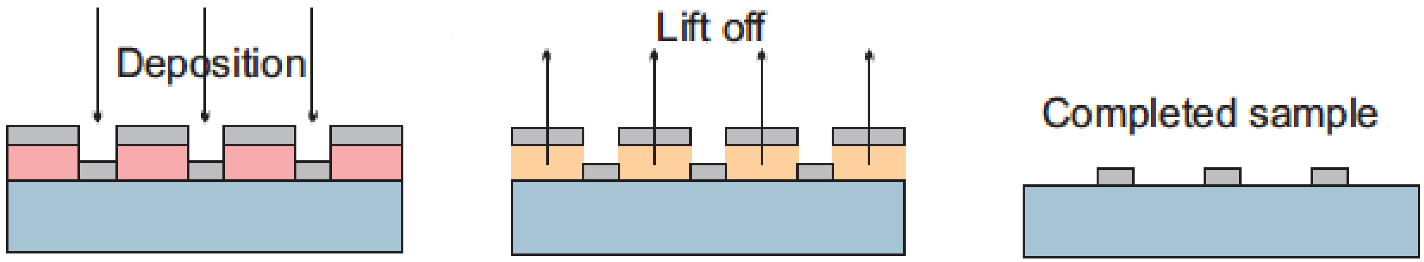
Blue line: cavity method results. Green and pink : solid lines simulations for two L, dashed lines low-T expansion of an effective $1d$ AF Ising model

Guruciaga, Tarzia, Ferreyra, LFC, Grigera & Borzi 16

Artificial spin-ice

Back to experiments: as-grown samples

- Lattice is written with electron beam lithography.
- Magnetic material is gradually poured as in the sketch.



- β is ambient inverse temperature
- By choosing ℓ, material, vertical off-set and other tricks:

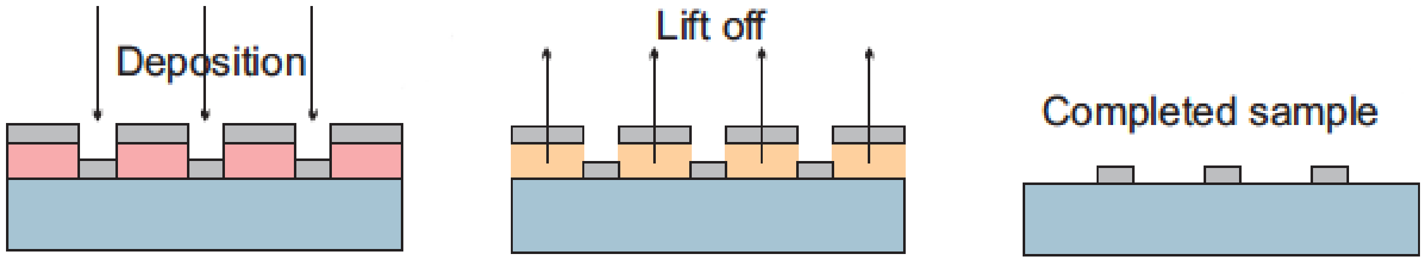
$\mathrm{e}_{\mathrm{vertices}}$ hierarchy

Our proposal: try to see ObD

Artificial spin-ice

Back to experiments: as-grown samples

- Lattice is written with electron beam lithography.
- Magnetic material is gradually poured as in the sketch.



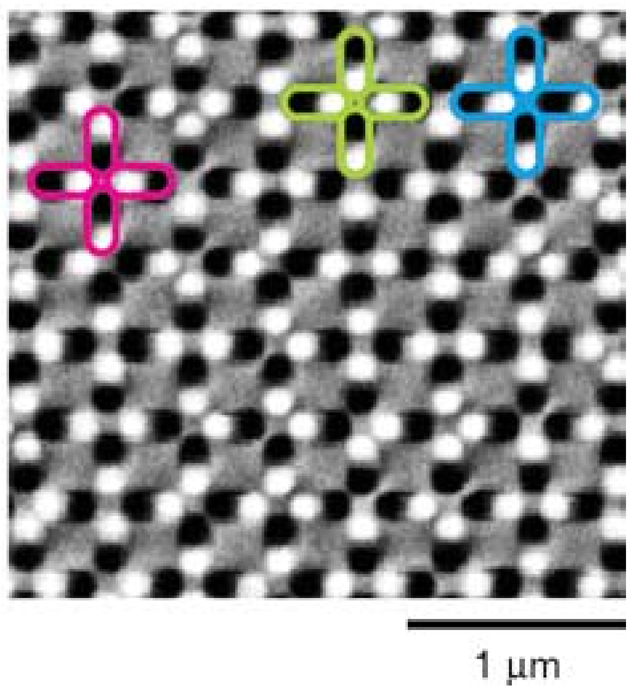
- Thermal fluctuations let the magnets flip until some size is reached.
- Configurations are henceforth blocked.

(Magnetic field annealing is also used.)

Note the similarity with granular matter & effective measure ideas.

Vertex density

Equilibrium number distribution ? How many of each kind ?



Signalled in this image

Pink : an AF vertex

Green : a 3-in 1-out vertex

Blue : a FM vertex

No 4-in nor 4-out vertices

Magnetic force microscopy

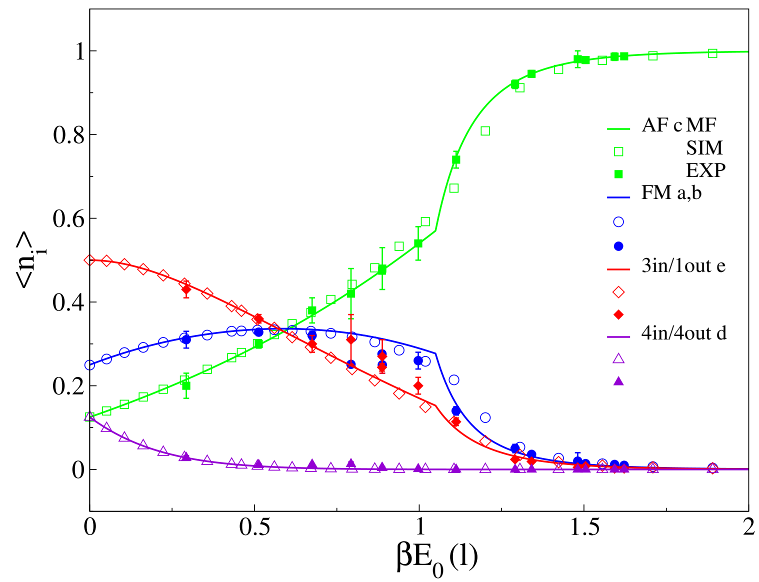
Wang et al 06

Does one sample the Gibbs-Boltzmann distribution function at β ?

Another measure ?

Vertex density

Across the PM-AF transition – numerical, analytic and exp. data



Disordered AF

PM - AF transition

AF vertices

FM vertices

3-in 1-out & 3-out 1-in e-vert.

4-in & 4-out d-vertices

Each set of vertical points, $\beta E_0(\ell)$ value, corresponds to a different sample (varying lattice spacing ℓ or the compound). $\epsilon_{\text{vertices}} = \overline{f}(\ell) = f(\epsilon_{\text{AF}})$

Agreement seems perfect but not enough to prove equilibrium...

Levis, LFC, Foini & Tarzia 13 ; experimental data courtesy of **Morgan** *et al.* **12**

Quench dynamics

A simpler setting

- Take an initial condition in equilibrium at, e.g. $\boxed{T_0 \to \infty}$ that corresponds to equal probability of all kinds of vertices
- Evolve it with a set of parameters a, b, c, d, e in the phases PM, FM or AF: an infinitely rapid quench at $t = 0$.
- Concretely, we use **stochastic dynamics**:

  with single spin flip updates with the usual heat-bath rule,

  and a continuous time MC algorithm (to reach long time scales).

  Relevant dynamics experimentally (contrary to loop updates used to study equilibrium in the 8 vertex model)

Levis & LFC 11, 13

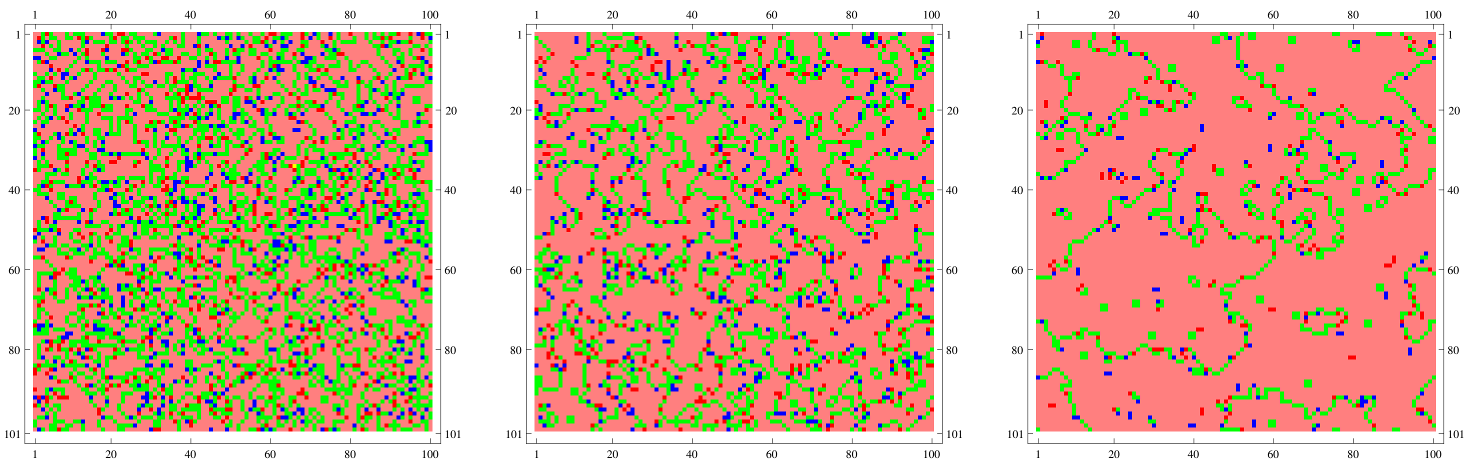
Dynamics in AF phase

Snapshots – coarsening

Color code. Orange background : AF order of two kinds ;

green FM vertices, red-blue defects.

Initial state coarsening states



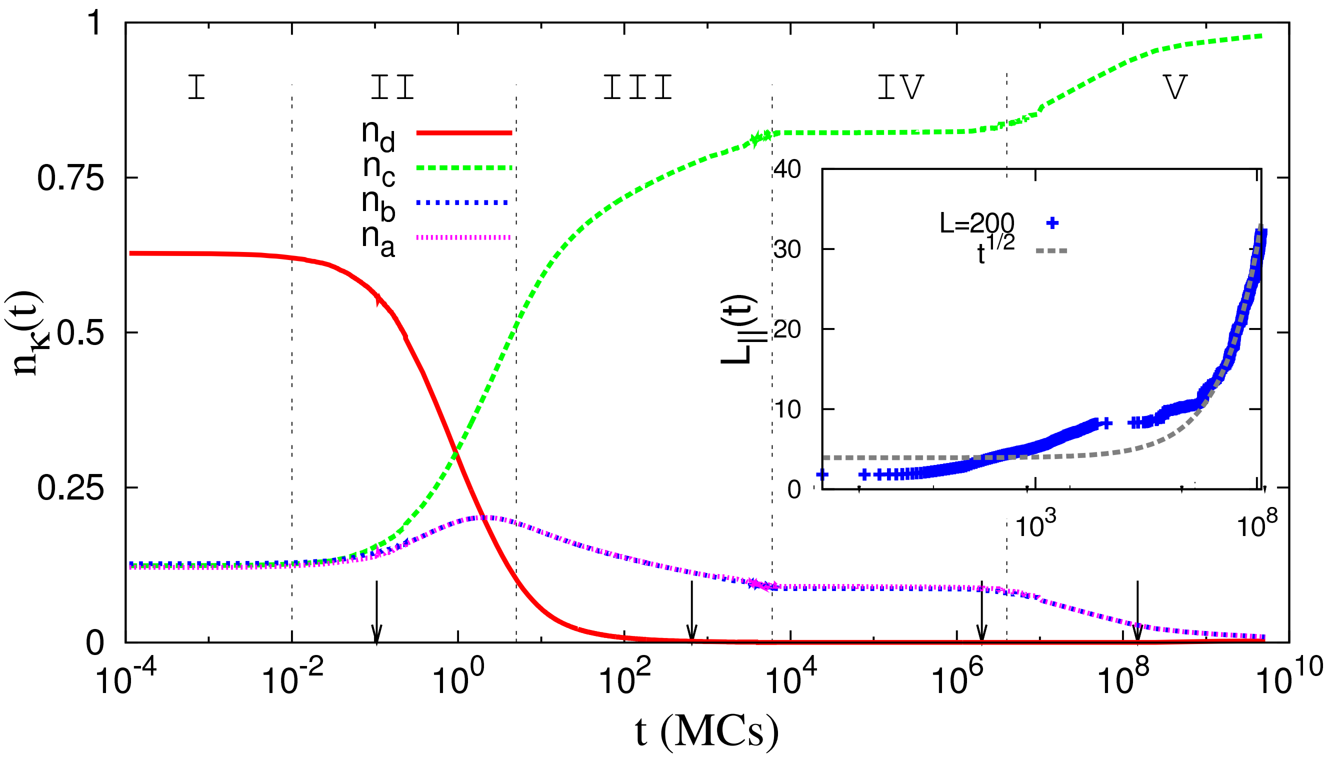
Isotropic growth of AF order for this choice of parameters

$\boxed{c \gg a = b}$ AF vertices are energetically preferred ;

there is no anisotropy imposed.

Dynamics in AF phase

Density of defects & growing length ($a = b$ and $d = e$ here)



Isotropic growth of AF order (for $a = b$) with $\boxed{L(t) \simeq t^{1/2}}$

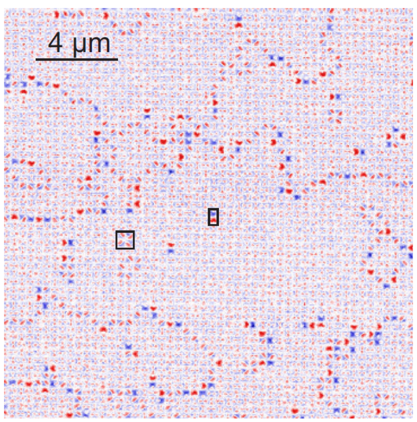
Dynamics in AF phase

Snapshots – experiment vs. numerics

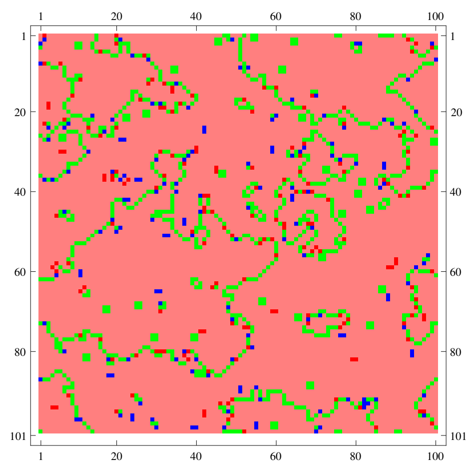
Color code. Orange background: AF order of two kinds;

green FM vertices, red-blue defects.

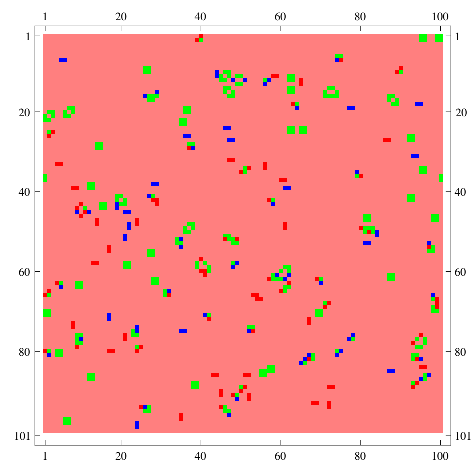
Magnetic force microscopy



coarsening state



equilibrium state



Interfaces between the two staggered AF orders

A statistical and geometric analysis of domain walls & defects should be done to conclude on equilibration or not.

Summary

Classical geometrically frustrated magnetism

spin-ice in two dimensions

$2d$ vertex models

Problems with analytic, numeric and experimental interest

Summary of results

- Materials
- Vertex models
- Statics
  - Phase diagrams (beyond integrable cases)
  - Macroscopic separation under domain wall boundary conditions
  - Order by disorder
- Dynamics
  - Coarsening
  - Equilibration

Square lattice artificial spin-ice

Local energy approximation $\Rightarrow$ $2d$ 16 vertex model

Just the interactions between dipoles attached to a vertex are added.

Dipole-dipole interactions. Dipoles are modeled as two opposite charges. Each vertex is made of 8 charges, 4 close to the center, 2 away from it. The energy of a vertex is the electrostatic energy of the eight charge configuration. With a convenient normalization, dependence on the lattice spacing ℓ :

$$\epsilon_{AF} = \epsilon_5 = \epsilon_6 = (-2\sqrt{2}+1)/\ell \qquad \epsilon_{FM} = \epsilon_1 = \cdots = \epsilon_4 = -1/\ell$$

$$\epsilon_e = \epsilon_9 = \ldots \epsilon_{16} = 0 \qquad \epsilon_d = \epsilon_7 = \epsilon_8 = (4\sqrt{2}+2)/\ell$$

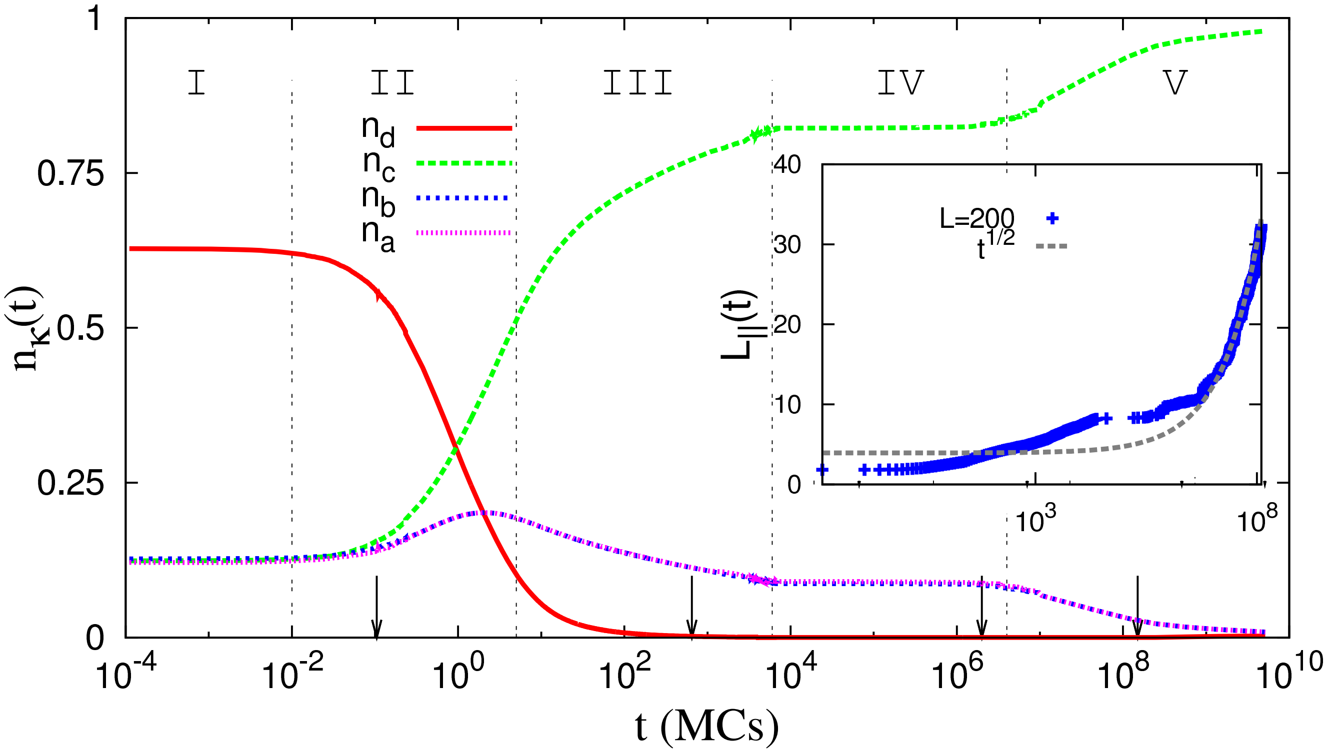
$$\boxed{\epsilon_{AF} < \epsilon_{FM} < \epsilon_e < \epsilon_d}$$

Nisoli *et al* 10

Energy could be tuned differently by adding fields, vertical off-sets, etc.

Dynamics in AF phase

Density of defects & growing length ($a = b$ and $d = e$ here)



Isotropic growth of AF order (for $a = b$) with $\boxed{L(t) \simeq t^{1/2}}$

Summary

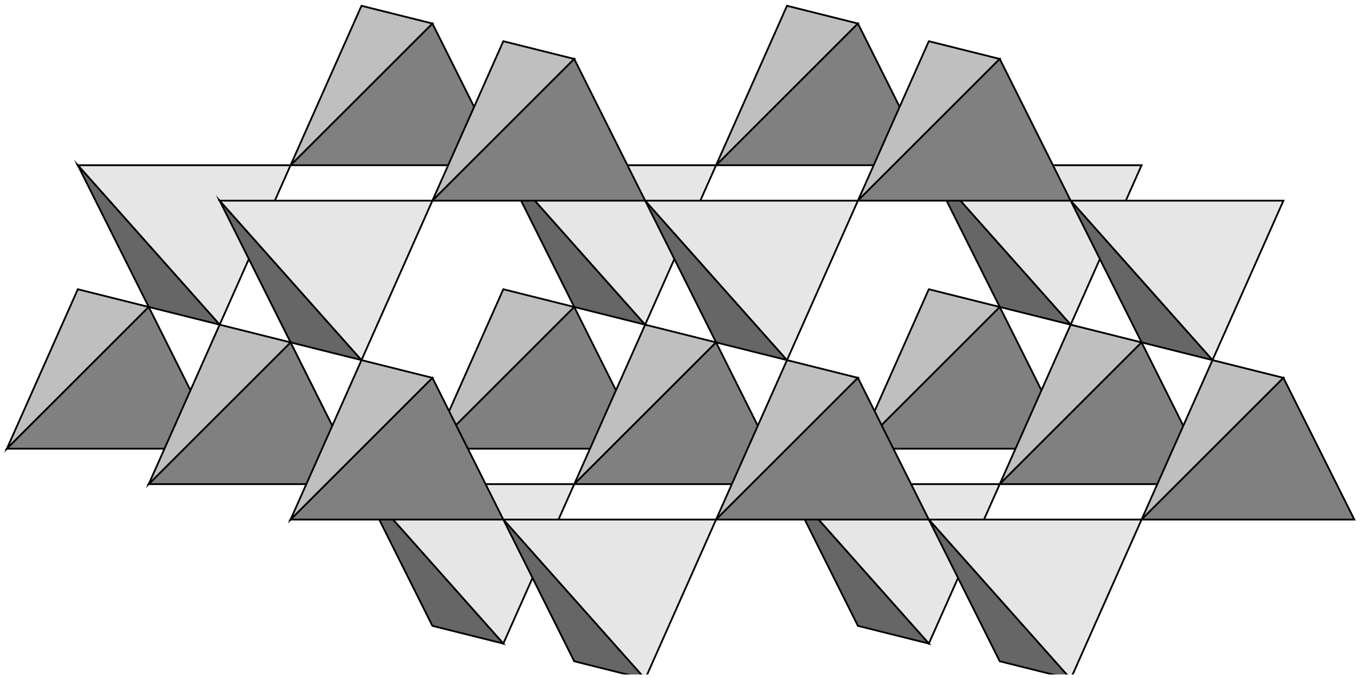
Classical frustrated magnetism ; spin-ice in two dimensions.

— $2d$ **vertex models** : problems with analytic, numeric and experimental interest. **Cfr. artificial spin-ice**

- Beyond integrable systems' methods to describe the **static** properties.
  — Some results of the Bethe-Peierls approximation are exact, others are at least very accurate. **Analytic challenge**
- Slow coarsening (or near critical in the disordered phase) **dynamics**.
  $L_{\parallel}^{\mathrm{FM}}(t) \simeq L_{\perp}^{\mathrm{FM}}(t) \simeq L^{\mathrm{AF}}(t) \simeq t^{1/2}$ **Analytically ?**
- Experiments : dynamics block, **non-equilibrium measures** ?
- Useful manipulation of **defects** (ice-breaking rule vertices).

Natural spin-ice

$3d$: the pyrochlore lattice



Coordination four lattice of corner linked tetahedra. The rare earth ions occupy the vertices of the tetrahedra ; **e.g. Dy$_2$ Ti$_2$ O$_7$**

Harris, Bramwell, McMorrow, Zeiske & Godfrey 97

Artificial spin-ice

Bidimensional square lattice of elongated magnets

Bidimensional square lattice

Dipoles on the edges

16 possible vertices

Experimental conditions in this fig. :

vertices w/ two-in & two-out arrows

with staggered AF order

are much more numerous

AF 3in-1out FM

Wang *et al* **06, Nisoli** *et al* **10, Morgan** *et al* **12**

Static properties

What did we do ?

- Equilibrium simulations with finite-size scaling analysis.

  — Continuous time Monte Carlo.

  e.g. focus on the **AF-PM transition** ; cfr. experimental data.

  AF order parameter : $\boxed{M_- = \frac{1}{2}\left(\langle|m_-^x|\rangle + \langle|m_-^y|\rangle\right)}$

  with $m_-^{x,y}$ the staggered magnetization along the x and y axes.

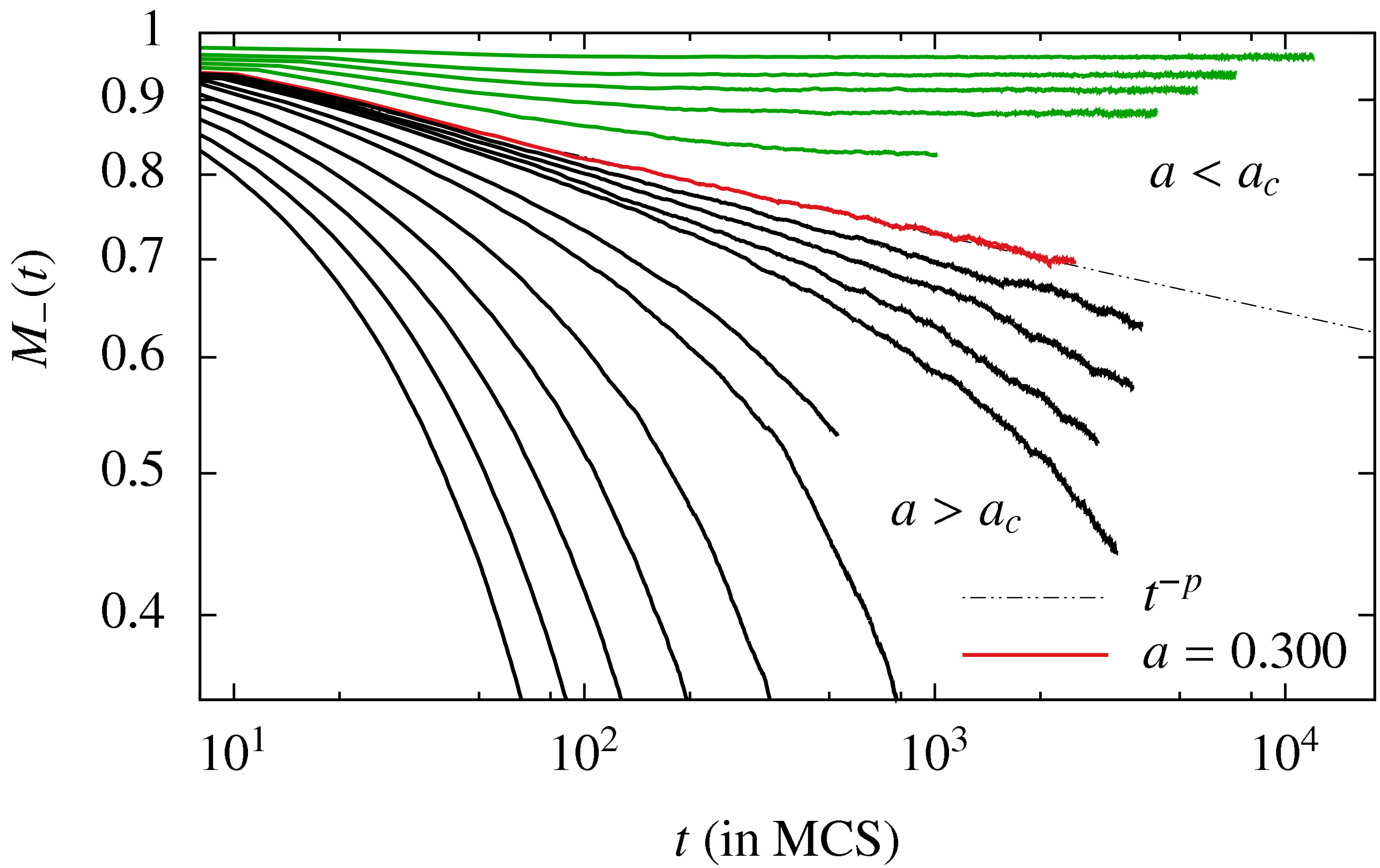
  — Finite-time relaxation $\boxed{M_-(t) \simeq t^{-\beta/(\nu z_c)}}$

- Cavity Bethe-Peierls mean-field approximation.

  — The model is defined on a tree of single vertices or 4-site plaquettes

Finite time relaxation

Magnetization across the PM-AF transition



$a_c = e^{-\beta_c e_1} \simeq 0.3$ with $e_1 = 0.45 \;\Rightarrow\; \beta_c = 2.67 \pm 0.02$

Equilibrium analytic

Bethe-Peierls or cavity method

Write a (matrix) recurrence relation to compute the probability that the cavity site be occupied by each one of the six vertices.

Find the solutions as a function of the weigths ω_α.

Obtain the free-energy density.

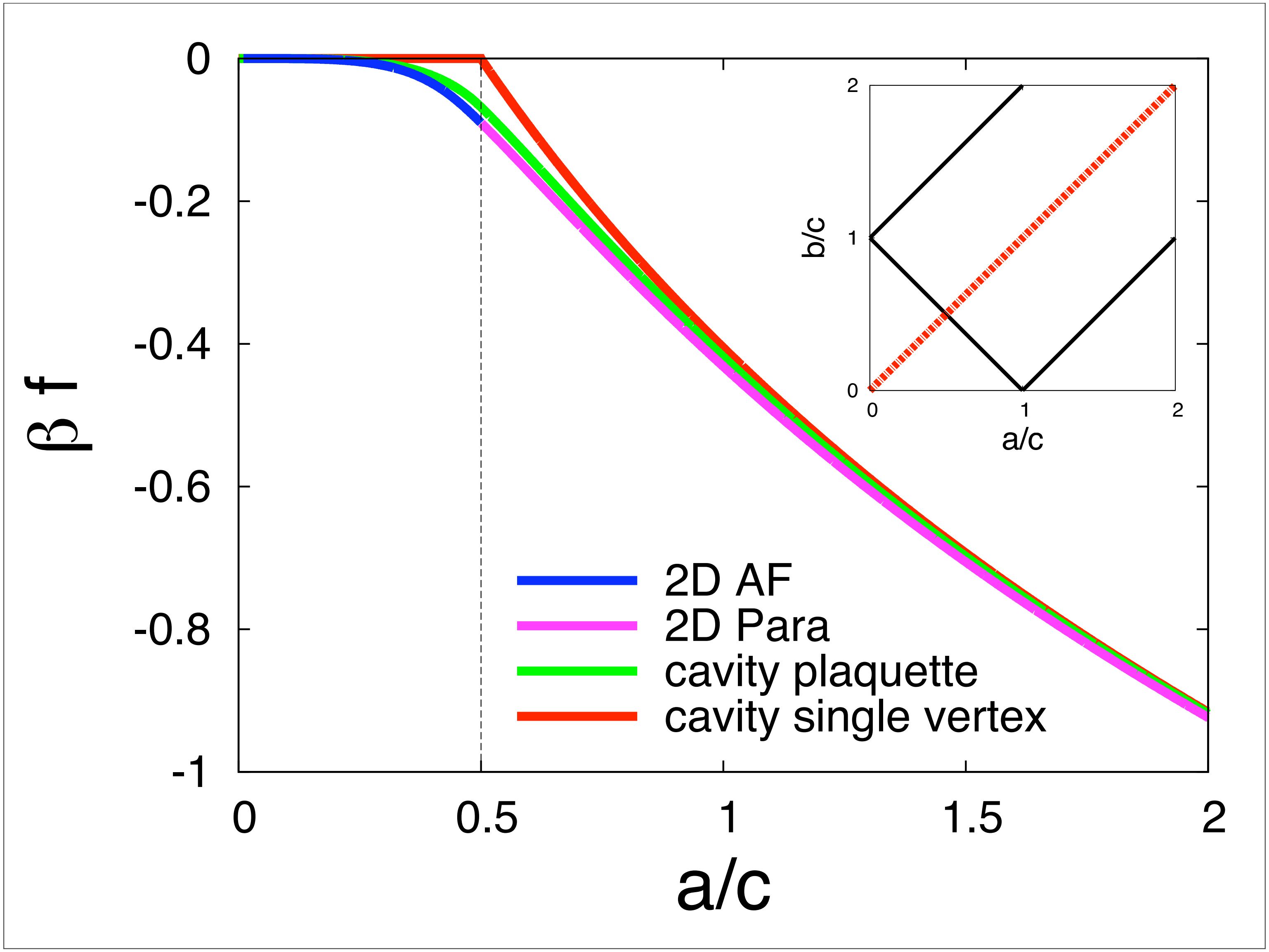
Look for transition lines.

This method can be applied to the 16 vertex model.

Foini, Levis, Tarzia & LFC 13

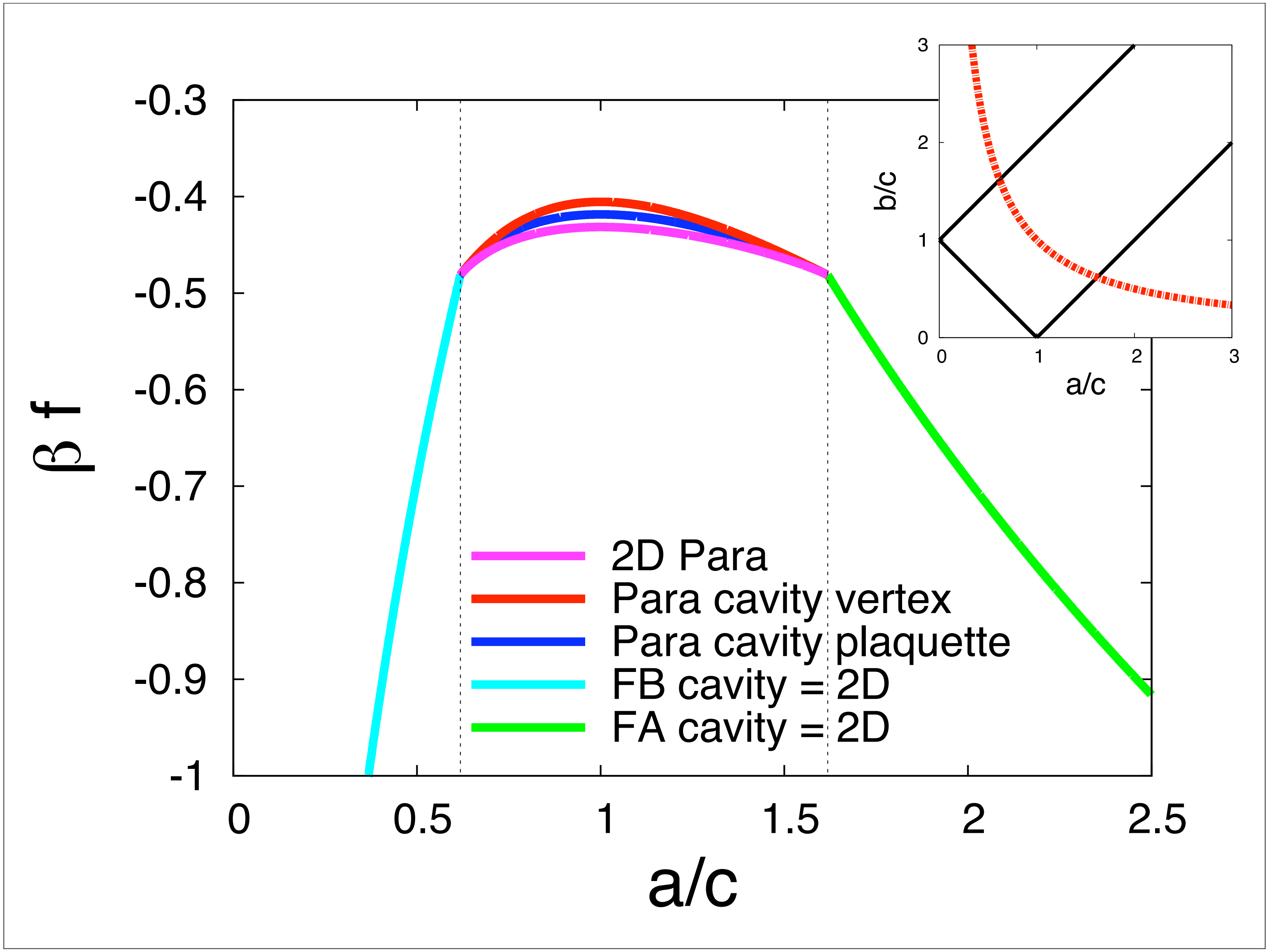
Equilibrium analytic

6 vertex : AF - D transition, cavity vs Baxter's exact solution



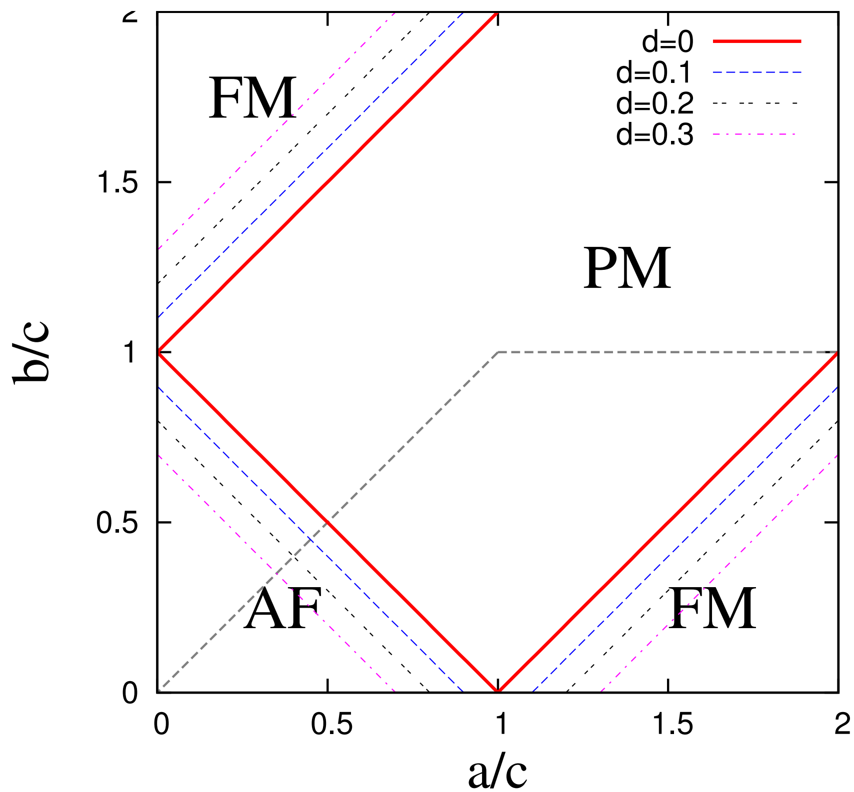
Equilibrium analytic

6 vertex : FM - D transition, cavity vs. Baxter's exact solution



The $2d$ 8 vertex model

Integrable system (transfer matrix + Bethe Ansatz)



No type e vertices.

2nd order phase transitions

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

$\Delta_8 = \pm 1$ transition lines

With three-in one-out vertices

Integrability

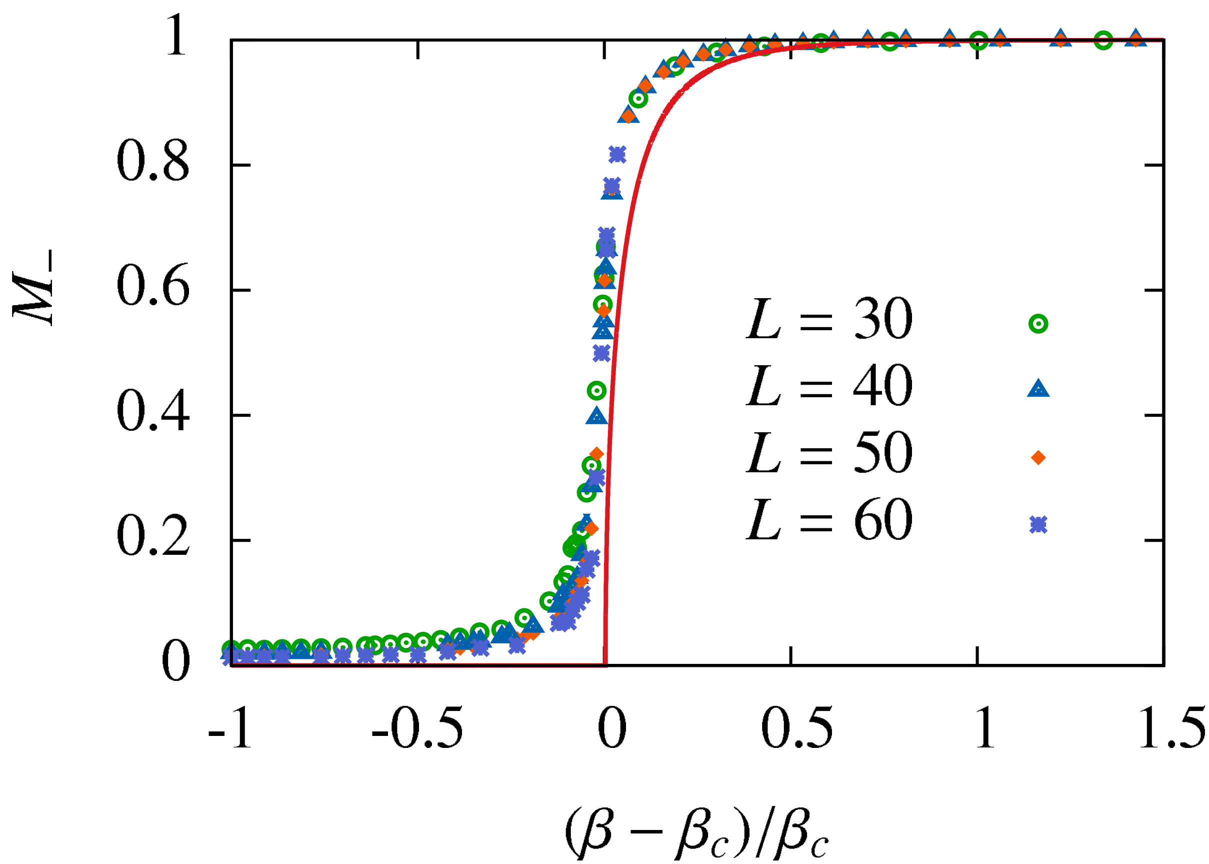
is lost.

Lieb 67 ; Baxter *Exactly solved models in statistical mechanics* **82**

Equilibrium CTMC

Magnetization across the PM-AF transition

Vertex energies set to the values explained above.

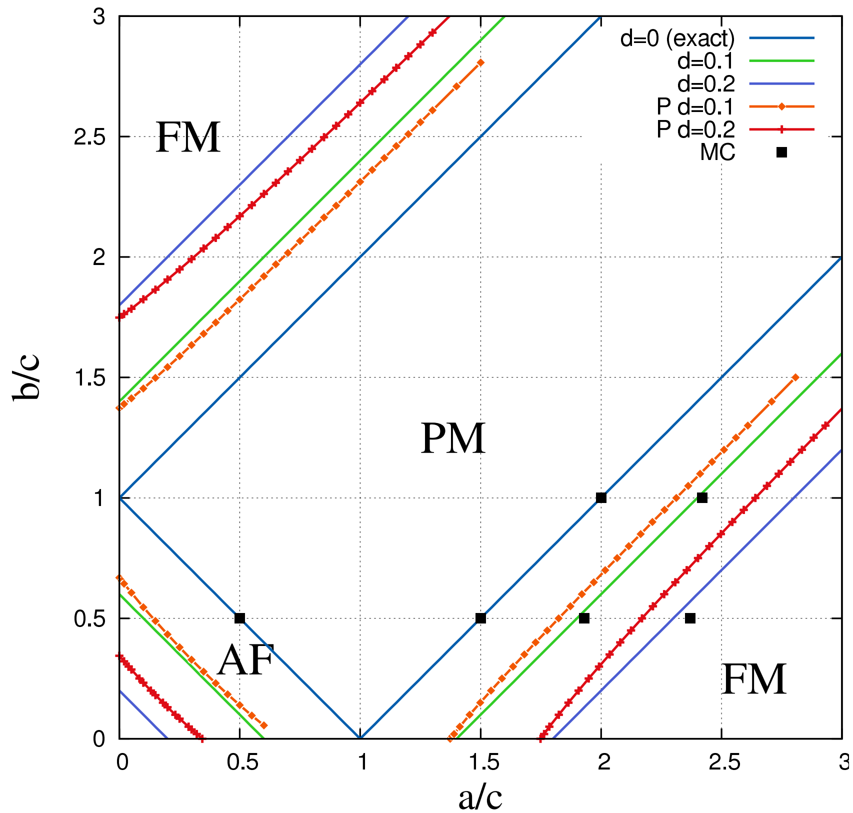


Solid red line from the Bethe-Peierls calculation.

Static properties

Equilibrium phase diagram 16 vertex model

- MC simulations & cavity Bethe-Peierls method



Phase diagram

critical exponents

ground state entropy

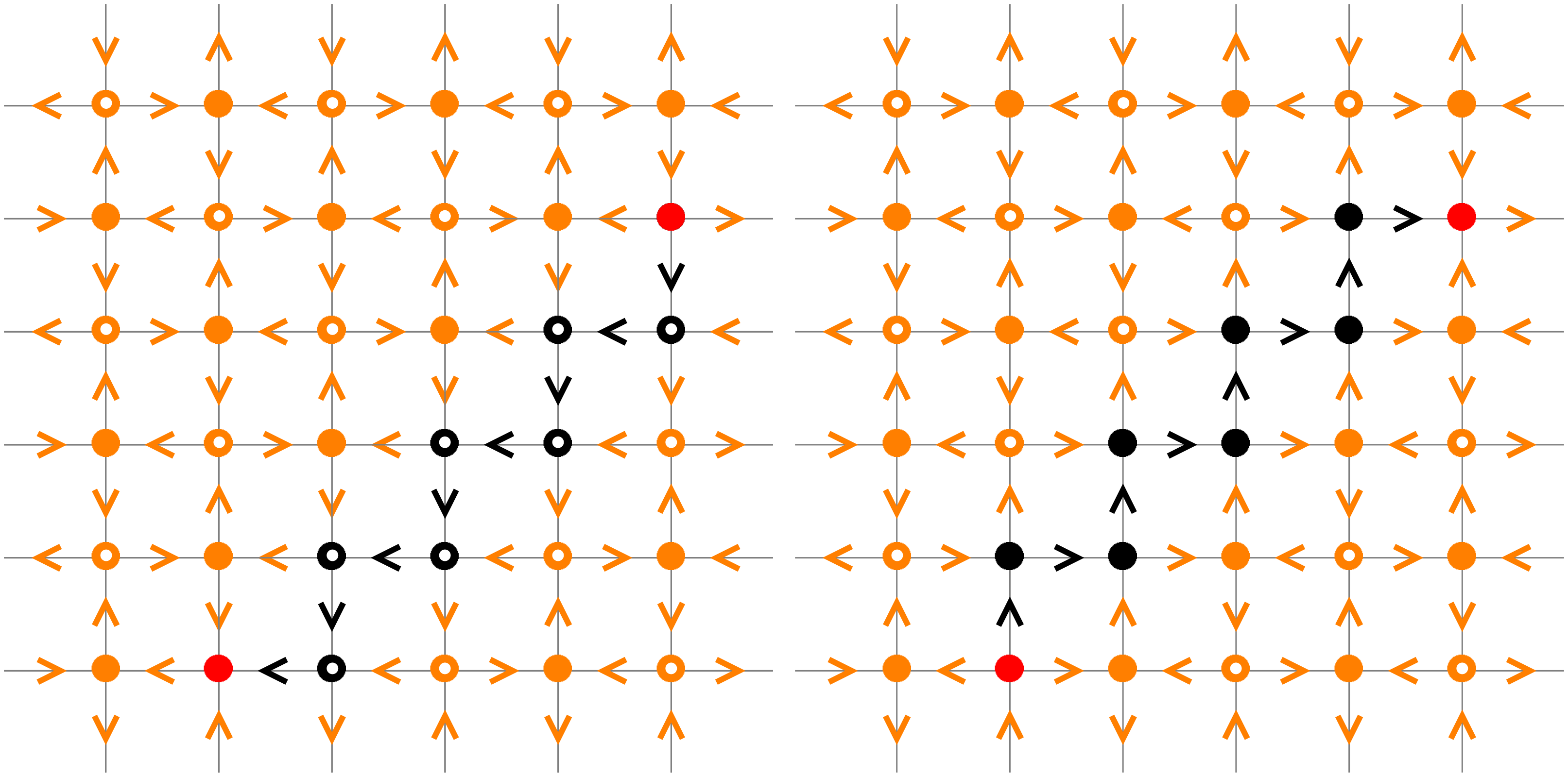
equilibrium fluctuations

etc.

Foini, Levis, Tarzia & LFC 12

Fluctuations

Sketch



The probability of such fluctuations can be estimated with the Bethe-Peierls calculation on a tree of four-site plaquettes !