Transition Trajectory for Equilibrium Droplet Formation

Andreas Nußbaumer, Elmar Bittner, and Wolfhard Janke

Computational Quantum Field Theory
Institut für Theoretische Physik
Universität Leipzig

Computation of Transition Trajectories and Rare Events in Non-Equilibrium Systems

Centre Blaise Pascal, ENS de Lyon, 13 June 2012

Outline

1. Motivation
2. Theory
3. Monte Carlo (MC) Simulations
   - Square lattice NN Ising model
   - Triangular lattice Ising model
   - Square lattice NNN Ising model

Outline

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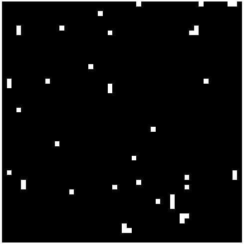
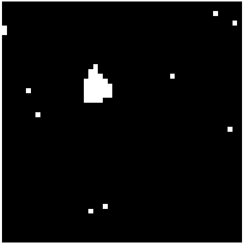
Evaporated



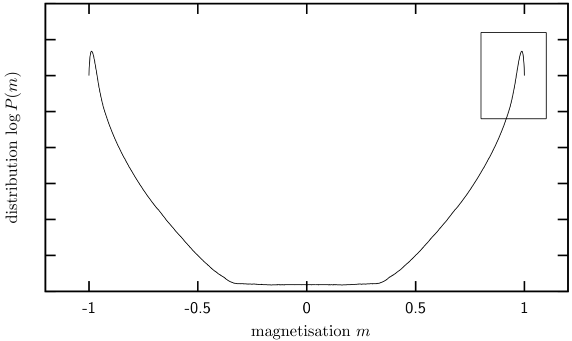
Condensed



Balancing fluctuations vs interface free energy, i.e.,
entropy vs energy

Droplet formation: nucleation of “wrong” phase

- fluid droplet in gas phase, or
- “$-$” Ising droplet in “$+$” phase



Fisher; Binder & Kalos; Furukawa & Binder; Pleimling & Selke; Neuhaus & Hager; . . .

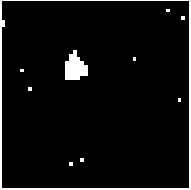
Biskup, L. Chayes & Kotecký, Europhys. Lett. **60** (2002) 21; Comm. Math. Phys. **242** (2003) 137

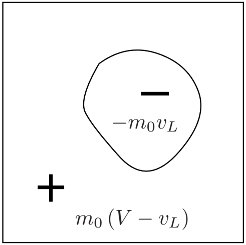
Theory: Equilibrium Droplet Formation

2D Ising model formulation

lattice gas:

- spin up = black = vacancy
- spin down = white = particle





$$M = -m_0 \underbrace{v_L}_{\text{droplet}} + m_0 (\underbrace{V - v_L}_{\text{background}})$$

$$\Rightarrow \quad \delta M \equiv M - M_0 = -2 v_L m_0$$

Gaussian fluctuations around peak:

$$\exp\left[-\frac{(\delta M)^2}{2V\chi}\right] = \exp\left[-\frac{(2m_0 v_L)^2}{2V\chi}\right]$$

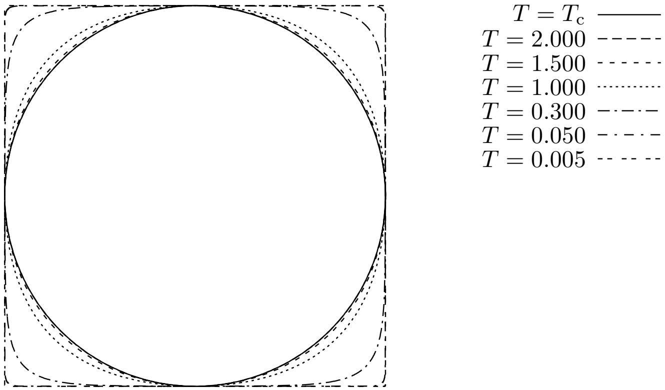
$\chi = \chi(\beta) = \beta V \left[\langle m^2\rangle - \langle m\rangle^2\right] =$ susceptibility

Interface free energy of droplet:

$$\exp\left[-\tau_\mathrm{W}\sqrt{v_L}\,\right]$$

$\tau_\mathrm{W} = \tau_\mathrm{W}(\beta) =$ interfacial free energy per unit volume of optimal Wulff shaped droplet

2D Ising model Wulff shapes at various temperatures:



$\Rightarrow$ for $1.0 \lesssim T \leq T_c \approx 2.27$ the Wulff shape is almost isotropic

Balancing the exponents of the two limiting cases:

$$\Delta = \frac{(2m_0 v_L)^2/(2V\chi)}{\tau_W \sqrt{v_L}} = 2\frac{m_0^2}{\chi\tau_W}\frac{v_L^{3/2}}{V}$$

Terms are equally important for $\Delta \stackrel{!}{=} 1$:

$$\Rightarrow v_L \Rightarrow -\delta M = \theta V^{2/3} \qquad \text{with} \qquad \theta = \left(\frac{2\chi\tau_W}{\sqrt{2m_0}}\right)^{2/3}$$

- $-\delta M \gg \theta V^{2/3}$: droplet dominates
- $-\delta M \ll \theta V^{2/3}$: fluctuations dominate

"Isoperimetric reasoning" (Biskup *et al.*) shows that either of these two cases dominate – but no droplets of intermediate size can exist.

In general, a single large droplet of size v_d coexists with small fluctuations taking $v_L - v_d$ of the total excess.

- large droplet costs $e^{-\tau_W \sqrt{v_d}}$, absorbs fraction $\delta M_\mathrm{d} = -2 v_\mathrm{d} m_0$ of δM
- fluctuations cost $e^{-(\delta M - \delta M_d)^2/(2V\chi)}$

For large systems, probability for magnetization excess:

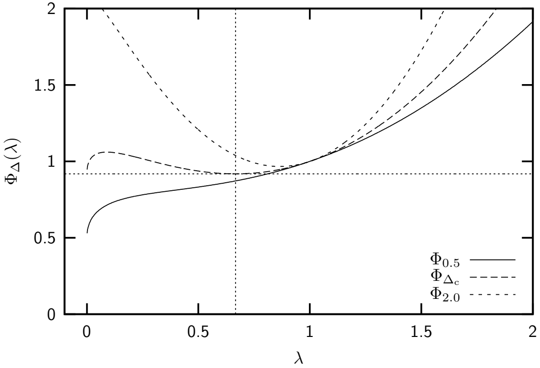
$$e^{-\tau_W \sqrt{v_\mathrm{d}} - \frac{(\delta M - \delta M_\mathrm{d})^2}{2V\chi}} = e^{-\tau_W \sqrt{\frac{-\delta M}{2m_0}} \Phi_\Delta(\lambda)}, \quad \Phi_\Delta(\lambda) = \left[\sqrt{\lambda} + \Delta(1-\lambda)^2\right]$$

where $\lambda = \delta M_\mathrm{d}/\delta M$ is the fraction taken up by the droplet.

$\Rightarrow$ Optimize $\Phi_\Delta(\lambda)$ in λ for given Δ

Recall: $\lambda = \delta M_{\rm d}/\delta M$, $\Delta = 2\frac{m_0^2}{\chi\tau_{\rm W}}\frac{v_L^{3/2}}{V}$

- $\Delta < \Delta_c$: $\lambda_{\rm min} = 0$
- $\Delta = \Delta_c = (1/2)(3/2)^{3/2} \approx 0.92$: $\lambda_{\rm min} = \lambda_c = 2/3$
- $\Delta > \Delta_c$: $\lambda_{\rm min} > 2/3$

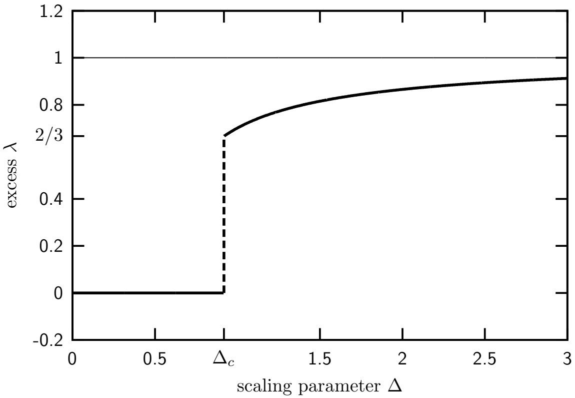


General d: $\Delta_c = \frac{1}{d}\left(\frac{d+1}{2}\right)^{\frac{d+1}{d}}$, $\lambda_c = \frac{2}{d+1}$

Solution:

$\lambda = \delta M_{\mathrm{d}}/\delta M \simeq$ droplet size

$\Delta = 2\frac{m_0^2}{\chi\tau_{\mathrm{W}}}\frac{v_L^{3/2}}{V} \simeq$ scaled magnetization ($\Delta = 0$: peak location)



Biskup *et al.*, Europhys. Lett. **60** (2002) 21; Comm. Math. Phys. **242** (2003) 137

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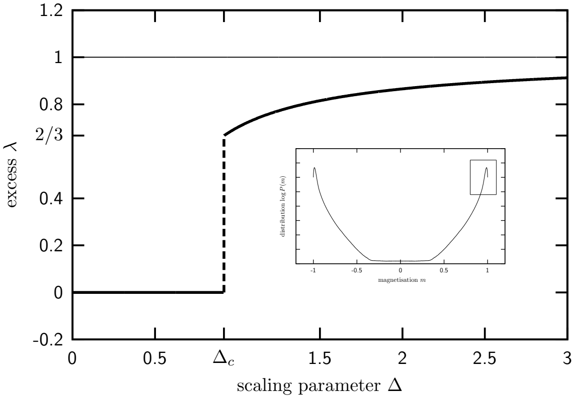

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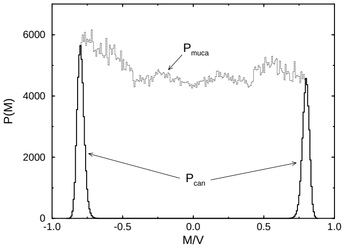
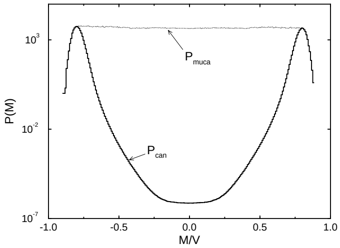
Numerical Studies

Suppressed two-phase region: use multicanonical type of simulation in magnetisation





Clear NON-random-walk behaviour observed !

Neuhaus & Hager, J. Stat. Phys. **116** (2003) 47

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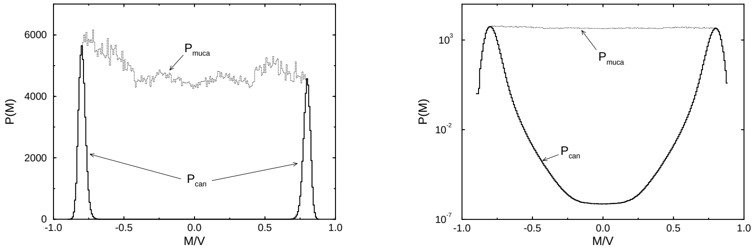

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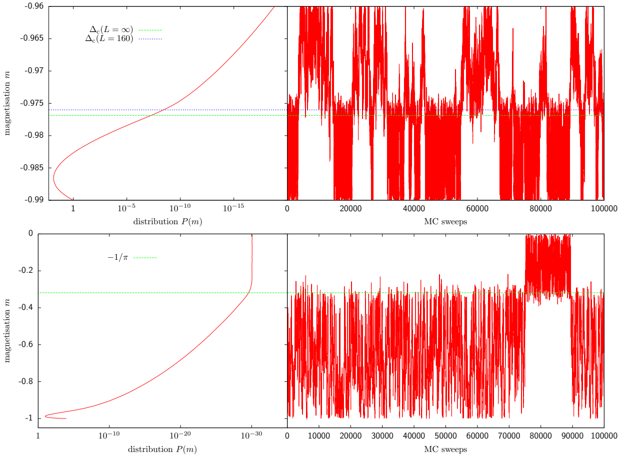
Reason: Two "hidden" barriers along transition trajectory



evaporation/
condensation

droplet/strip

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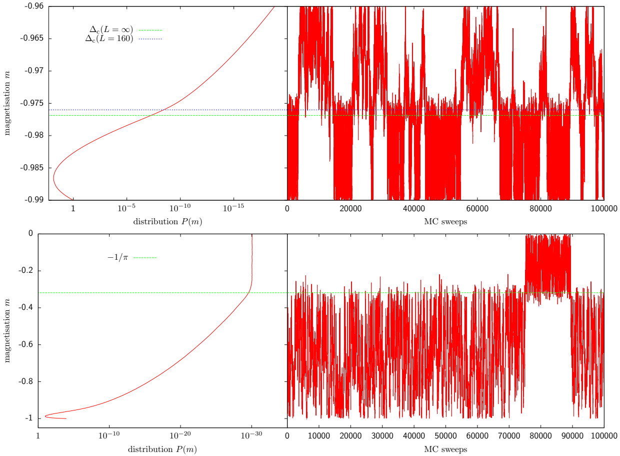


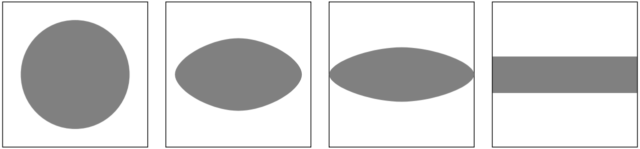
evaporation/ condensation

droplet/strip

Droplet/strip barrier rather well understood in 2D:

- strip: interface length $= 2L$
- circular droplet: Same length for radius $R = L/\pi$, area $= L^2/\pi$
- $\#$ overturned spins $= L^2/\pi$, hence (assuming isotropic interface tension)
- barrier located at about $m = m_0/\pi$

But $2R = \frac{2}{\pi}L < L$:



Leung & Zia, J. Phys. A **23** (1990) 4593

MC Simulations: Equilibrium Droplet Formation

Three goals:

- Test analytical prediction for the thermodynamic limit
- Investigate finite-size corrections
- Study lattice universality

Simulation strategy:

- fix the total excess v_L
- v_L together with the “known constants” m_0, χ, τ_W yields $\Delta(m_0, \chi, \tau_W, v_L)$.
- “micro-magnetical” simulation at:

$$M = -m_0 v_L + m_0(V - v_L) \quad \Rightarrow \quad M = m_0 V \left(1 - 2\frac{v_L}{V}\right)$$

- measure λ ($\simeq$ relative size of largest droplet)

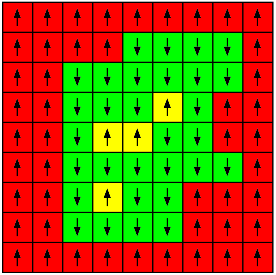
Algorithm:

- Kawasaki dynamics ($M = \text{const.}$)
- measure

$$\lambda = v_{\mathrm{d}}/v_L \ ,$$

the largest droplet size v_{d} (i.e., second largest cluster), by using the Hoshen-Kopelman algorithm

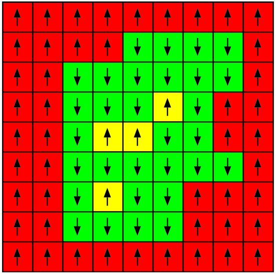
Difficulty: v_{d} is the area of the second largest cluster
$\Rightarrow$ What is inside and what is outside?



Idea: The Hoshen-Kopelman algorithm assigns to every cluster a unique number ⇒ interface between spins of the largest and second largest cluster

Droplet algorithm:

- do Hoshen-Kopelman
- for every new cluster, mark positions of spins belonging to that cluster
- starting from a spin inside the second largest cluster, apply “flood-fill”
- flood-fill stops only at spins belonging to the largest cluster



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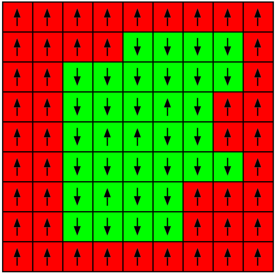
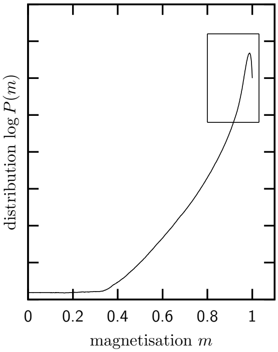
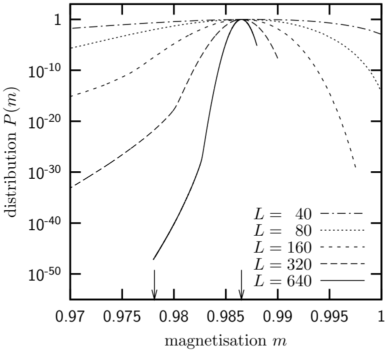


Outline

Square lattice NN Ising model ($T = 1.5 \approx 0.66 T_c$)





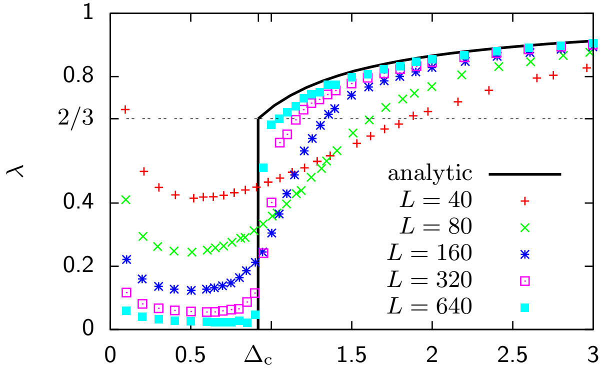
m range between arrows scanned with Kawasaki dynamics

Square lattice NN Ising model

- $m_0(\beta) = \left(1 - \sinh^{-4}(2\beta)\right)^{1/8}$
- $\chi(\beta) = \beta \sum_{i=0}^{n} c_i u^{2i}$ with $u = 1/(2\sinh(2\beta))$
  with $c = \{0, 0, 4, 16, 104, 416, 2224, 8896, 43840, 175296, 825648, 3300480, 15101920, \ldots\}$ up to order 323 (last term at $T = 1.5$: 10^{-158}). 2008–10: order 2000 ...
- $\tau_W(\beta) = 2\sqrt{W}$ with
  $W = \frac{4}{\beta^2} \int_0^{\beta\sigma_0} dx \cosh^{-1}\left[\frac{\cosh^2(2\beta)}{\sinh(2\beta)} - \cosh(x)\right]$
  and $\sigma_0 = 2 + \ln[\tanh(\beta)]/\beta$ the tension of an (1,0) interface.

Note: At $T = 1.5 \approx 0.66 T_c$, assuming isotropy:
$\tau_W \approx 2\sqrt{\pi\sigma_0} = 4.219$; exact $\tau_W = 4.245$ (0.6% difference).

Square lattice NN Ising model ($T/T_c \approx 0.66$)

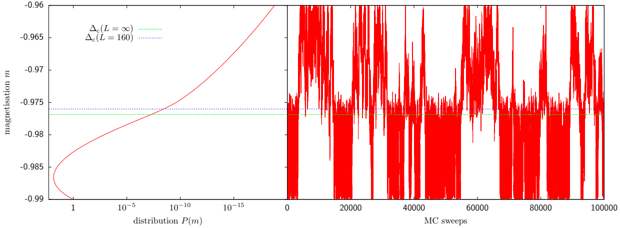


$$\Delta = 2\frac{m_0^2}{\chi\tau_W}\frac{v_L^{3/2}}{L^2}$$

Nußbaumer, Bittner, Neuhaus & WJ, Europhys. Lett. **75** (2006) 716

Square lattice NN Ising model

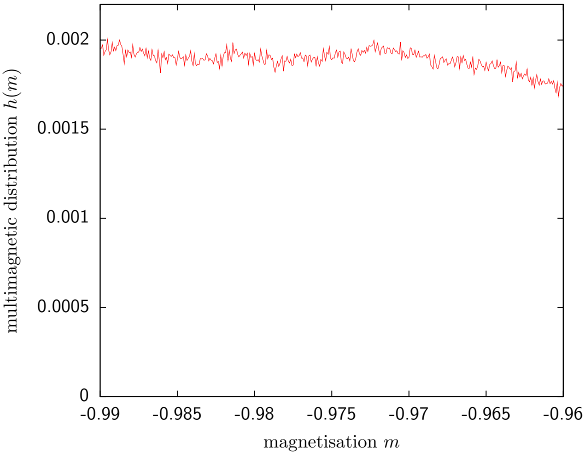
Numerical problem: “Hidden” barrier is reflected in simulations



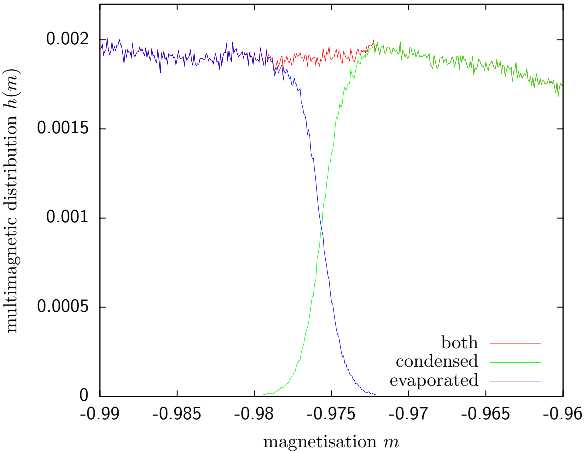
evaporation/
condensation

Similar “hidden droplet barriers” in spin glasses?

Evaporation/condensation barrier:

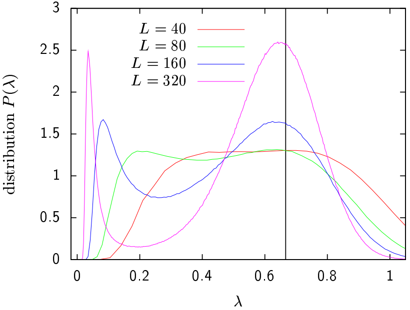


Evaporation/condensation barrier:



Square lattice NN Ising model

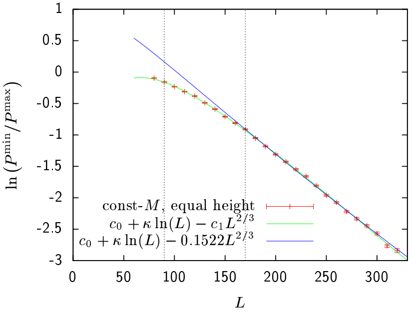
Distribution of fraction $\lambda = v_\mathrm{d}/v_L$ for Δ close to Δ_c

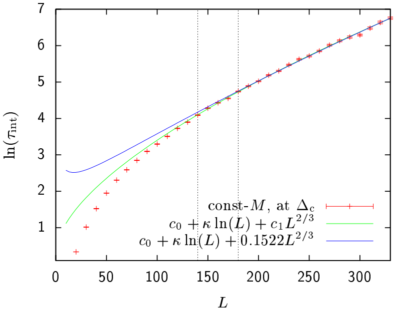


⇒ Clear coexistence signal !

Square lattice NN Ising model

Free-energy barrier resp. autocorrelation time scaling with system size





Theory: $\beta \Delta F \approx 0.1522\, L^{2/3}$ (at $T = 1.5$)

Nußbaumer, Bittner & WJ, Prog. Theor. Phys. Suppl. **184** (2010) 400

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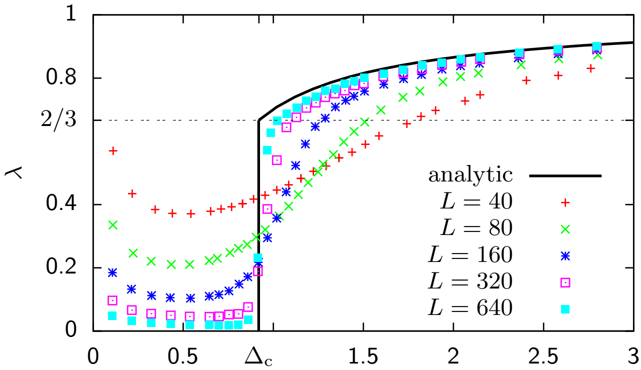
   - Triangular lattice Ising model
   - Square lattice NNN Ising model

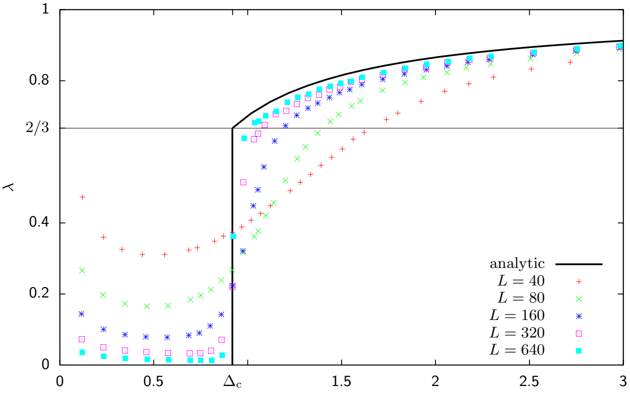
Triangular lattice Ising model ($T/T_c \approx 0.66$)



$$\Delta = 2\alpha \frac{m_0^2}{\chi \tau_W} \frac{v_L^{3/2}}{L^2}$$

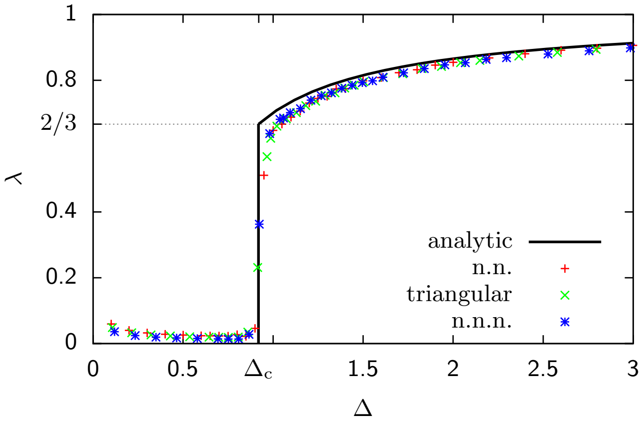
Outline

Square lattice NNN Ising model ($T/T_c \approx 0.66$)



$$\Delta = 2\frac{m_0^2}{\chi \tau_W}\frac{v_L^{3/2}}{L^2}$$

Check lattice universality ($L = 640$, $T/T_c \approx 0.66$)



Summary

- Analytical predictions for the asymptotic behaviour of the evaporation/condensation transition of the 2D square lattice NN Ising model confirmed numerically
- Finite-size corrections investigated
- Universality tested by studying triangular lattice and square lattice NNN Ising models

Nußbaumer, Bittner, Neuhaus & WJ, Europhys. Lett. **75** (2006) 716; Nußbaumer, Bittner & WJ, Phys. Rev. E **77** (2008) 041109; Prog. Theor. Phys. Suppl. **184** (2010) 400

Acknowledgements

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- EU–RTN Network “ENRAGE”
- Graduate School “BuildMoNa”
- Computer time NIC, Forschungszentrum Jülich

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See you there ?

Oops – wait another minute,
it's football time

Footballphysics

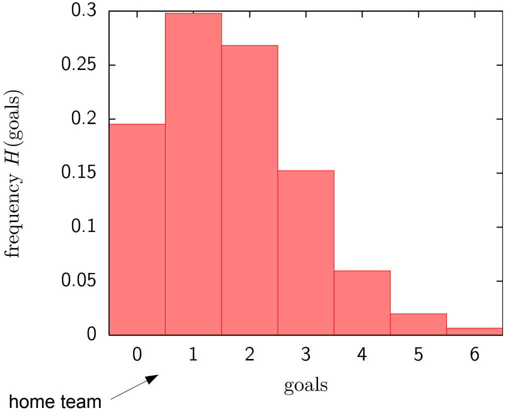
How probable is the next goal in soccer?

or

Football fever: goal distributions and non-Gaussian statistics

A “typical” result:

1. Fußball-Bundesliga
2004/05 (Germany)



Goals	Matches
0	153
1	189
2	148
3	77
4	26
5	6
6	5

Question: what kind of distribution is this?

Simplest possible idea:

Goals are scored with a constant probability (in time)!

The scores of the home and the away team don't influence each other!

N number of time steps (?)

p probability to score a goal during one time step

goals

Binomial distribution

$$P_{N,p}(k) = \binom{N}{k} p^k (1-p)^{N-k}$$

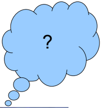
$$N\,p = \lambda \rightarrow p = \frac{\lambda}{N}$$

Poisson distribution

$$\lim_{N\rightarrow\infty} P_{N,p}(k) = P_\lambda(k) = \frac{\lambda^k}{k!} e^{-\lambda}$$

average number of goals: $\langle P_\lambda(k) \rangle_k = \lambda$

Maybe a model can help?



Ingrediens:

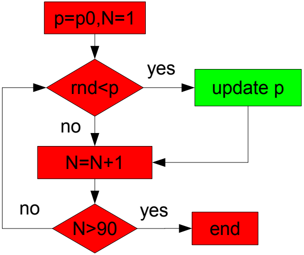
1. Starting probability
2. Probability to score a goal depends on the actual score

3 different updates if a goal is scored:

	home scores	away scores
model "A":	$p_h \leftarrow p_h + \kappa_h$	$p_a \leftarrow p_a + \kappa_h$
model "B":	$p_h \leftarrow p_h \cdot \kappa_h$	$p_a \leftarrow p_h \cdot \kappa_a$
model "C":	$p_h \leftarrow p_h \cdot \kappa_h$ $p_a \leftarrow p_a / \kappa_a$	$p_h \leftarrow p_h / \kappa_h$ $p_a \leftarrow p_a \cdot \kappa_a$

κ : additional movtivation "success succeeds"

Algorithm:



What distribution is described by model "A", "model B", ...

take recursion relation → transform in difference equation
→ perform continuum limit $N \to t$
→ transform in differential equation
→ solve differential equation using *p*(*n*)

(first three steps:) independent of a specific *p*(*n*)

Finally, for **model "A"**

$$P_{r,p}(n) = e^{-p_0 t} \frac{\Gamma(p_0/\kappa + n)}{n!\,\Gamma(p_0/\kappa)} \left(1 - e^{-\kappa t}\right)^n$$

compare

negative binomial distribution

$$P_{r,p}(n) = \frac{\Gamma(r + n)}{n!\,\Gamma(r)} p^n (1-p)^r$$

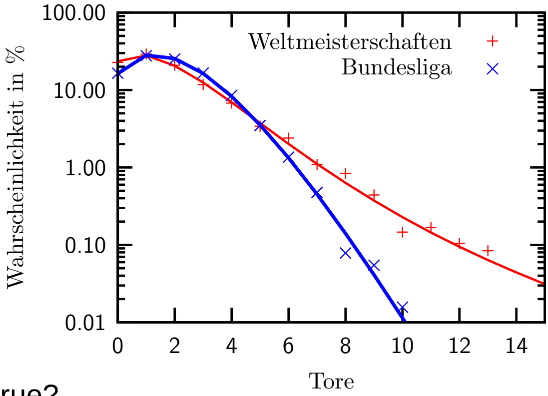
$$p = 1 - e^{-\kappa t} \qquad r = \frac{p_0}{\kappa}$$

No closed expressions for model "B" and model "C" so far!

The **negative binomial distribution** describes a **process** with:

- *n*+*r* Bernoulli trials (0,1)
- success probability *p*
- *n* times success
- *r* times failure
- last attempt is a failure

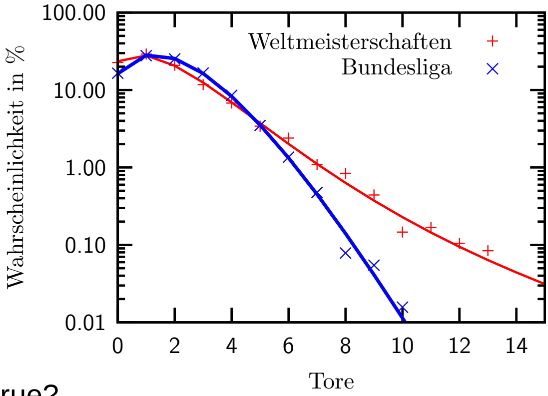
Bio-, Econo-, Sociophysics, . . . , **Footballphysics**



Is all that true?

Disclaimer: No NIC supercomputer (JUMP, JUBL,. . .) time was used
E. Bittner, A. Nußbaumer, M. Weigel & WJ, Eur. Phys. J. B **67** (2009) 459

Bio-, Econo-, Sociophysics, . . . , Footballphysics



Is all that true?

Watch the EURO2012 games and check yourself !!!

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