Macroscopic degeneracy influences the finite-size scaling at first-order phase transitions

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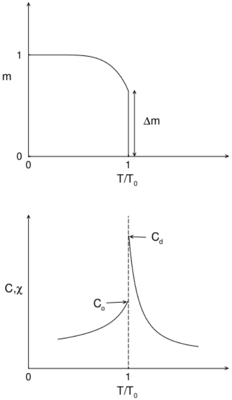
(Leipzig)

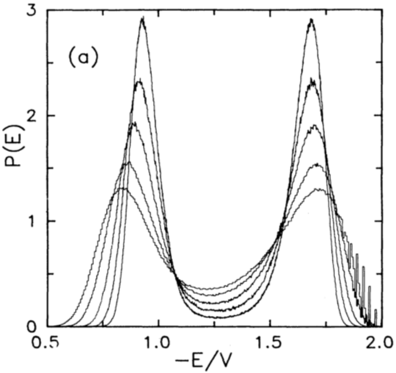
First-order phase transitions are ubiquitous in nature

(driven by temperature)

(driven by field)

First-order phase transitions

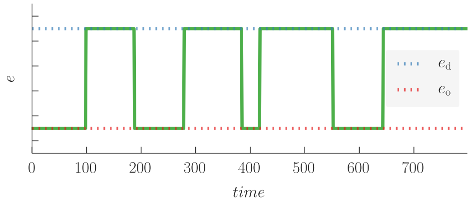




(a) W. Janke, Phys Rev. B **47** (1993) 14757

Standard finite-size scaling

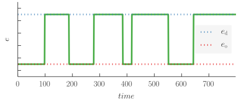
"phase coexistence" idealized for a finite-system close to the transition point $\beta^\infty = 1/k_B T^\infty$



- time fraction W_o in ordered phase with energy $\hat{e}_\mathrm{o}$
- time fraction W_d in disorderd phase with energy $\hat{e}_\mathrm{d}$
- energy moments $\langle e^n \rangle = W_\mathrm{o}\hat{e}_\mathrm{o}^n + (1 - W_\mathrm{o})\hat{e}_\mathrm{d}^n$
- specific heat

  $$C_V(\beta, V) = -\beta^2 \partial e(\beta, V)/\partial\beta = V\beta^2 \left(\langle e^2 \rangle - \langle e \rangle^2 \right)$$

Standard finite-size scaling



- specific heat

$$C_V(\beta, V) = V\beta^2 W_o(1 - W_o)\Delta\hat{e}^2$$

- maximum value at $W_o = W_d = 0.5$ and position $\beta^{C_V^{\max}}(V)$

$$C_V^{\max}(V) = V(\beta^\infty \Delta\hat{e}/2)^2 \propto V$$

Standard finite-size scaling

ratio of time fractions are connected to probabilities of the states

$$W_{\rm o}/W_{\rm d} \simeq q e^{-V\beta\hat{f}_{\rm o}}/e^{-\beta V\hat{f}_{\rm d}}$$

(up to exponentially small corrections)
expansion of the logarithm for $W_{\rm o} = W_{\rm d}$,

$$0 = \ln(W_{\rm o}/W_{\rm d}) \simeq \ln q + V\beta(\hat{f}_{\rm d} - \hat{f}_{\rm o})$$

$$\beta^{\rm eqw} = \beta^{C_V^{\rm max}}(V) = \beta^{\infty} - \frac{\ln q}{V\Delta\hat{e}} + \ldots$$

and analogously for $B(\beta) = 1 - \frac{\langle e^4\rangle}{3\langle e^2\rangle^2}$

$$\beta^{B^{\rm min}}(V) = \beta^{\infty} - \frac{\ln(q\hat{e}_{\rm o}^2/\hat{e}_{\rm d}^2)}{V\Delta\hat{e}} + \ldots$$

Gonihedric model

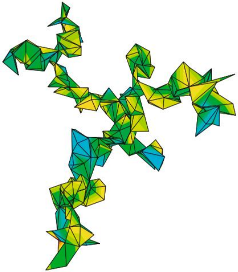


Fig. 7.1. A typical collapsed triangulated surface resulting from a simulation of the Gaussian Hamiltonian in (7.1)

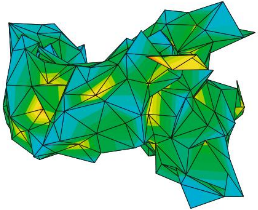


Fig. 7.2. A typical uncollapsed triangulated surface resulting from a simulation of the Gaussian plus extrinsic curvature Hamiltonian in (7.2) with $\lambda = 1.1$

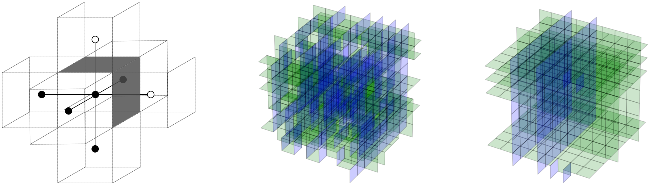
D. A. Johnston, A. Lipowski, and R. P. K. C. Malmini, in *Rugged Free Energy Landscape,s*, Vol. 736 of *Lecture Notes in Physics, Berlin Springer Verlag*, edited by W. Janke (2008), pp. 173–199.

Gonihedric model

- Hamiltonian for classical Ising spins in 3d-lattices

$$\mathcal{H} = -2\kappa \sum_{\langle i,j \rangle} \sigma_i \sigma_j + \frac{\kappa}{2} \sum_{\langle\langle i,j \rangle\rangle} \sigma_i \sigma_j - \frac{1-\kappa}{2} \sum_{[i,j,k,l]} \sigma_i \sigma_j \sigma_k \sigma_l$$

  - prefactors fine-tuned for vanishing contribution of the *area*, but edges and self-intersections
  - self-avoidance parameter κ



Gonihedric model

$$\mathcal{H} = -\frac{1}{2} \sum_{[i,j,k,l]} \sigma_i \sigma_j \sigma_k \sigma_l$$

earlier inverse transition temperature estimates

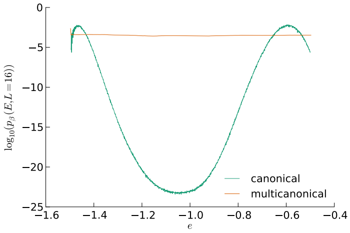
method	mean field		Monte Carlo	
year	1996	1996 pbc	2004 fixed bc.	2011 pbc, dual
β^∞	0.325	0.50(1)	0.54757(63)	0.510(2)

- Inconsistent transition temperatures due to
  - fixed vs. periodic boundary conditions?
  - representations not matching?
  - *spoiler* neither!

Multicanonical simulations

$$Z_{\mathrm{can}} = \sum_{\{\sigma\}} e^{-\beta E(\{\sigma\})} = \sum_{E} \Omega(E) e^{-\beta E}$$

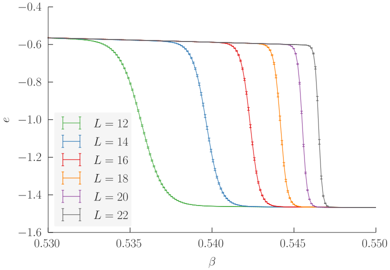
$$Z_{\mathrm{muca}} = \sum_{\{\sigma\}} W\left(E\left(\{\sigma\}\right)\right) = \sum_{E} \Omega(E) W(E)$$

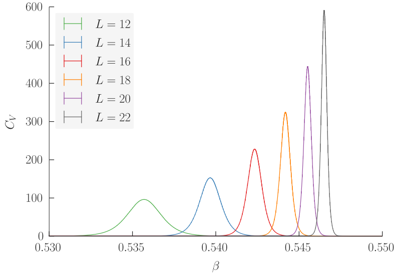


weights via simple iteration:

$$W^{(n+1)}(E) = W^{(n)}(E)/H^{(n)}(E)$$

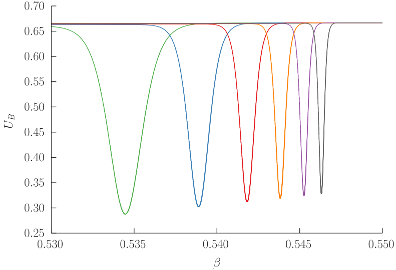
or via more sophisticated, accumulative approach





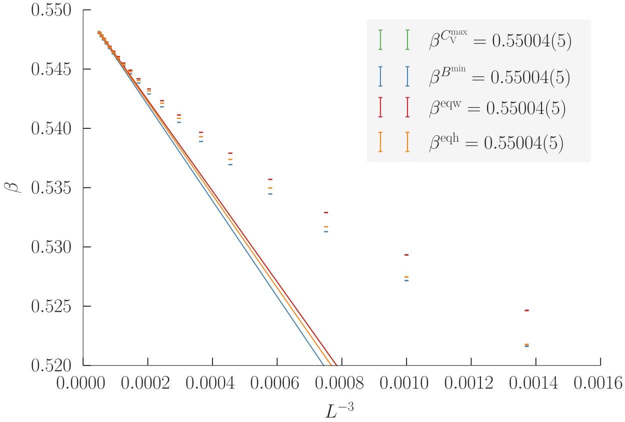
$$C_V = V\beta^2 \left(\langle e^2 \rangle - \langle e \rangle^2 \right)$$

$$U_{\mathrm{B}} = 1 - \frac{\langle e^4 \rangle}{3 \langle e^2 \rangle^2}$$

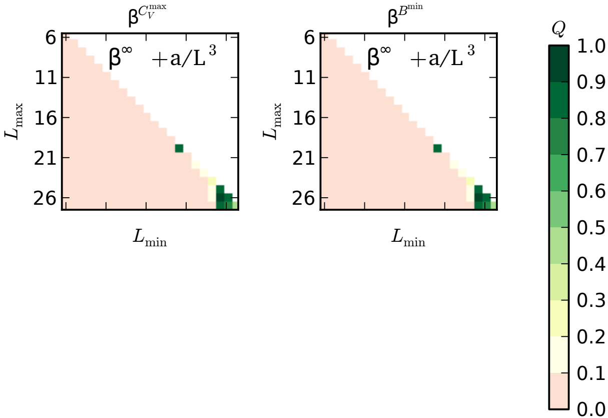


Standard scaling ansatz

$$\beta^{C_V^{\max}}(L) = \beta^{\infty} - \frac{\ln q}{\Delta \hat{e}} \frac{1}{L^3} + \dots; \quad \beta^{B^{\min}}(L) = \beta^{\infty} - \frac{\ln(q \hat{e}_{\mathrm{o}}^2 / \hat{e}_{\mathrm{d}}^2)}{\Delta \hat{e}} \frac{1}{L^3} + \dots$$

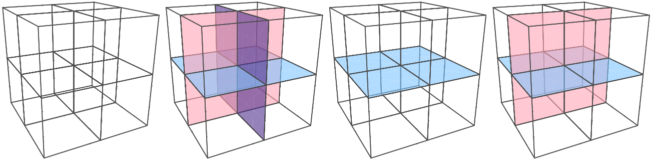


Standard scaling ansatz



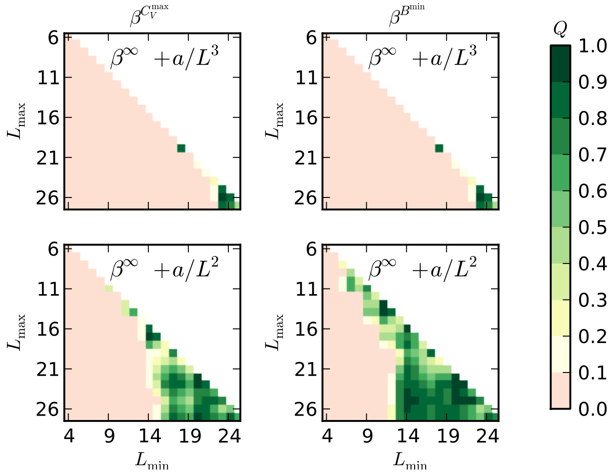
Interlude: zero temperature ground state

- span one of the following elementary cubes over the whole lattice



- whole planes can be flipped (each plane is either "on" or "off")
- $\Rightarrow$ degeneracy of $q = 2^{3L}$

Nonstandard-scaling ansatz



Nonstandard-scaling ansatz

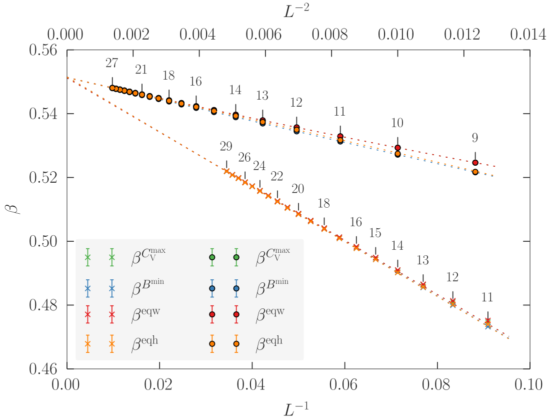
$$\beta^{C^{\max}}(L) = \beta^{\infty} - \frac{\ln 2^{3L}}{\Delta \hat{e}} \frac{1}{L^3} + \dots$$

$$= \beta^{\infty} - \frac{3 \ln 2}{\Delta \hat{e}} \frac{1}{L^2} + \mathcal{O}\left(L^{-4}\right)$$

$$\beta^{B^{\min}}(L) = \beta^{\infty} - \frac{\ln(2^{3L} \hat{e}_{\mathrm{o}}^2 / \hat{e}_{\mathrm{d}}^2)}{\Delta \hat{e}} \frac{1}{L^3} + \dots$$

$$= \beta^{\infty} - \frac{3 \ln 2}{\Delta \hat{e}} \frac{1}{L^2} + \frac{\ln(\hat{e}_{\mathrm{o}}^2 / \hat{e}_{\mathrm{d}}^2)}{\Delta \hat{e}} \frac{1}{L^3} + \mathcal{O}\left(L^{-4}\right),$$

Fitting results



$\beta^{\infty} = 0.551\,332(8)$ (periodic bc., with higher-order corrections)

$\beta^{\infty} = 0.551\,38(5)$ (fixed bc.)

- transition temperatures from our multicanonical simulations and non-standard FSS:

  $\beta^{\infty} = 0.551\,332(8)$ (periodic bc.)

  $\beta^{\infty} = 0.551\,38(5)$ (fixed bc.)

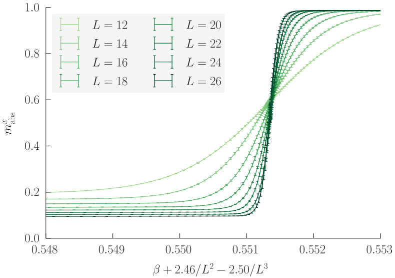
  $\beta^{\infty} = 0.551\,43(5)$ (dualization)

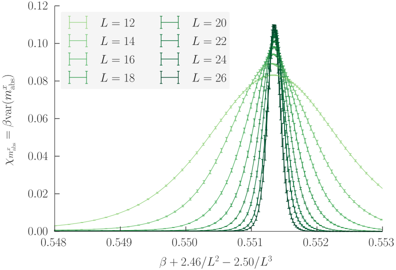
Earlier inverse transition temperatures for the plaquette-only gonihedric Ising model

method	mean field	Monte Carlo			
year	1996	1996	2004	2011	2011
		pbc	fixed bc.	pbc, dual	pbc, dual
β^{∞}	0.325	0.50(1)	0.54757(63)	0.510(2)	0.508(2)

Planar order parameters ("Fuki-Nuke")

$$M_x^{\mathrm{abs}} = \frac{1}{L} \sum_{\mathrm{yz-planes}} \left\langle \frac{1}{L^2} \left| \sum_{\text{single plane}} \sigma_i \sigma_{i+\hat{e}_x} \right| \right\rangle$$





Conclusion and Outlook

- exponential ("macroscopic") low-temperature degeneracy transmutes finite-size scaling corrections

$$1/V = 1/L^d \to 1/L^{d-1}$$

- potential other models with this property: antiferromagnetic FCC Ising models, spin ice systems, "orbital" compass model, ANNNI-model, ...

Thank you for your attention

M. Mueller, W. Janke, D. A. Johnston, Phys. Rev. Lett. **112**, 200601 (2014);

M. Mueller, D. A. Johnston, W. Janke, Nucl. Phys. B **888**, 214 (2014)

Consistency checks

input	$\Delta\hat{e}$	$\frac{3\ln(2)}{\Delta\hat{e}}$	$\frac{2\ln(\hat{e}_\mathrm{o}/\hat{e}_\mathrm{d})}{\Delta\hat{e}}$	$\frac{\ln(\hat{C}_\mathrm{d}/\hat{C}_\mathrm{o})}{2\Delta\hat{e}}$	$B^{\min}_{L\to\infty}$
fit on $C_V^{\max}(L)$	0.85130(7)	–	–	–	–
fit on $B^{\min}(L)$	–	–	–	–	0.34729(7)
fit on $\beta^{C_V^{\max}}(L)$	0.8771(14)	2.371(4)	–	–	–
fit on $\beta^{B^{\min}}(L)$	0.871(14)	2.39(4)	1.6(8)	–	–
fit on $\beta^{\mathrm{eqw}}(L)$	0.8770(14)	2.371(4)	–	–	–
fit on $\beta^{\mathrm{eqh}}(L)$	0.84(4)	2.47(11)	–	2.8(2.4)	–
fit on $\beta^{C_V^{\max}} - \beta^{B^{\min}}$	–	–	2.03469(7)	–	–
fit on $\beta^{C_V^{\max}} - \beta^{\mathrm{eqh}}$	–	–	–	0.892(14)	–
energy moments from simulations ...					
... multicanonical	0.85148(5)	2.44215(15)	2.03649(27)	0.9594(10)	0.347(4)
... canonical	0.850968(18)	2.44362(6)	2.03625(6)	0.9591(16)	0.34723(9)

- strong hysteresis, seen in the dual model
- multicanonical simulations nicely interpolate between the branches, yielding more accurate transition temperatures