Partition Function Zeros of the Frustrated J_1-J_2 Ising Model on the Honeycomb Lattice

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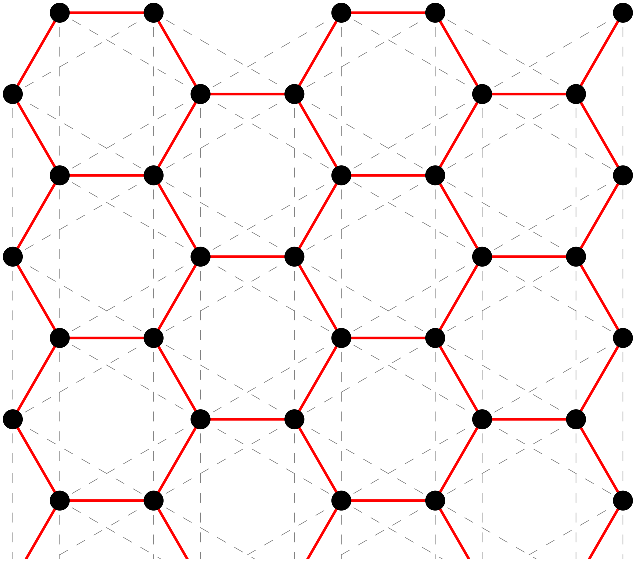
Contents

Model



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$$(J_1 > 0, J_2 < 0, \sigma_i \in \{-1, 1\})$$

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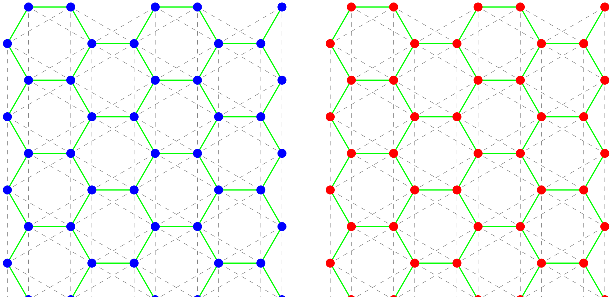

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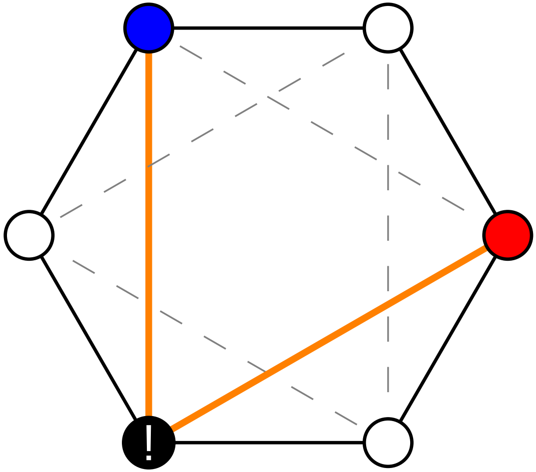

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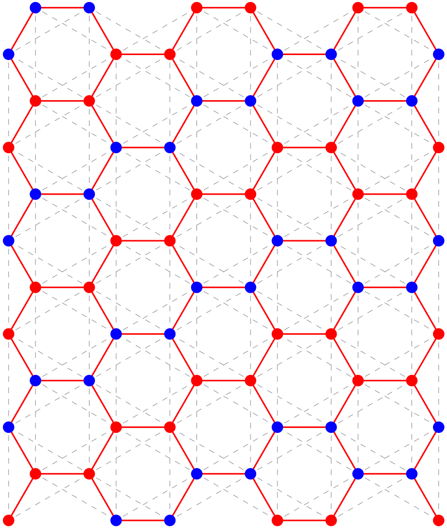

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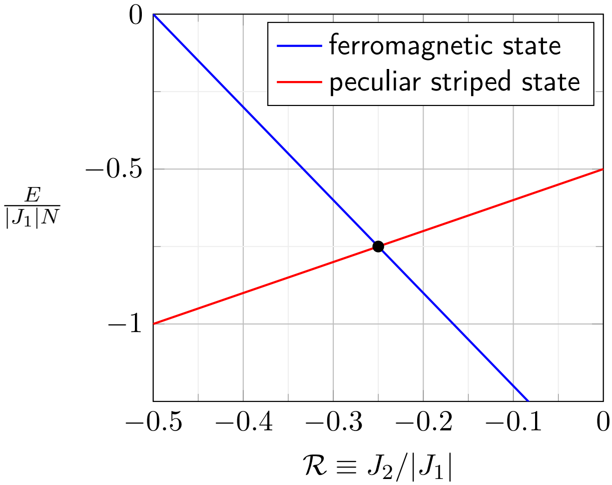

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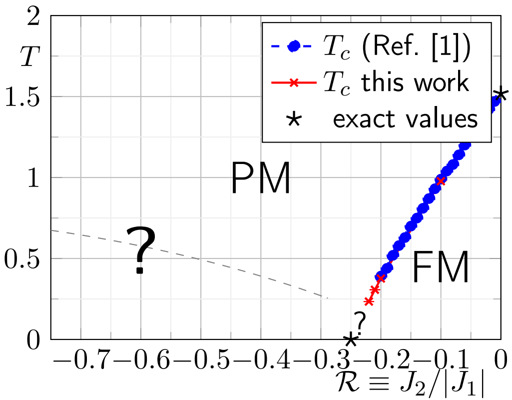

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$$(J_1 > 0, J_2 < 0, \sigma_i \in \{-1, 1\})$$

- For $\mathcal{R} \equiv J_2/|J_1| < -0.25$ ground-state entropy per *row* finite; existence and nature of phase transition (PT) unclear
- At $\mathcal{R} = -0.25$ the ground-state entropy per spin finite, and no PT expected.
- For $\mathcal{R} > -0.25$ an order-disorder transition [2][3] exists at a non-zero temperature that (except for a small unclear window $R \in (-0.25, -0.2)$) is in the **Ising universality class**[1].

[1] M. Žukovič, Phys. Lett. A **404**, 127405 (2021)
[2] A. Bobák, T. Lučivjanský, M. Žukovič, M. Borovský and T. Balcerzak, Phys. Lett. A **380**, 2693 (2016)
[3] M. Schmidt and P.F. Godoy, J. Magn. Magn. Mater. **537**, 168151 (2021)

'Traditional' finite-size scaling (FSS)

Critical exponents

- $\xi \propto |1 - T/T_c|^{-\nu}$
- $m \propto (1 - T/T_c)^{\beta} \quad (T < T_c)$
- $\chi \propto |1 - T/T_c|^{-\gamma}$
- ...

For finite system sizes L

- finite system $\Rightarrow \xi$ cannot diverge $\Rightarrow \xi \simeq L$
- $|1 - T/T_c| \propto \xi^{-1/\nu} \longrightarrow L^{-1/\nu}$
- $m \propto L^{-\beta/\nu} \quad (T < T_c)$
- $\chi \propto L^{\gamma/\nu}$
- ...

Relations used here

$$\mathrm{dln}|m| \equiv \frac{\partial}{\partial\beta} \ln\langle|M|\rangle = \frac{\langle|M|\mathcal{H}\rangle}{\langle|M|\rangle} - \langle\mathcal{H}\rangle \propto L^{-1/\nu}$$

$$\chi_L(\beta_c) = L^{-D}\beta_c\langle M^2\rangle_{\beta_c} \propto L^{\gamma/\nu}$$

Partition function zeros I

- Hamiltonian

$$\mathcal{H}(\{\sigma_i\}) = -J_1 \sum_{\langle ij \rangle} \sigma_i \sigma_j - J_2 \sum_{[ik]} \sigma_i \sigma_k - h \sum_i \sigma_i \equiv -J_1 \Sigma_1 - J_2 \Sigma_2 - hM$$

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$$\mathcal{Z}(\beta, h) = \sum_{\{\sigma_i\}} e^{-\beta \mathcal{H}(\{\sigma_i\})} = \sum_{\Sigma_1} \sum_{\Sigma_2} \sum_{M} \Omega(\Sigma_1, \Sigma_2, M) e^{\beta J_1 \Sigma_1 + \beta J_2 \Sigma_2 + \beta h M}$$

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- Free energy $F = -\ln \mathcal{Z}/\beta$ $\Rightarrow$ non-analytic if $\boxed{\mathcal{Z} = 0}$ $\Rightarrow$ phase transition

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- Free energy $F = -\ln \mathcal{Z}/\beta$ $\Rightarrow$ non-analytic if $\boxed{\mathcal{Z} = 0}$ $\Rightarrow$ phase transition
- But for finite systems

$$\mathcal{Z}(\beta, h) \neq 0 \; \forall (\beta, h) \in \mathbb{R}^2$$

"Free energy is analytic for finite systems." "No phase transitions in finite systems."

Partition function zeros II

Idea

Allow $(\beta, h) \in \mathbb{C}^2$ and study how complex roots approach real axes as $L \to \infty$

Fisher zeros	Lee-Yang zeros
• Solve $\mathcal{Z}(\beta_k, h = 0) = 0$ for β_k • 'critical' zeros scale as $$\Im(\beta_k) \propto L^{-y_t}$$ $$\Re(\beta_k) - \beta_c \propto L^{-y_t}$$ $$y_t = 1/\nu$$	• Solve $\mathcal{Z}(\beta, h_k) = 0$ for h_k (β fixed) • LY circle theorem: $\Re(h_k) = 0$ • for $\beta < \beta_c$: $\Im(h_k) \neq 0$ as $L \to \infty$ • for $\beta \geq \beta_c$: $\Im(h_k) \xrightarrow{L\to\infty} 0$ • for $\beta = \beta_c$: 'critical' zeros $\Im(h_k) \propto L^{-y_h}$ $$y_h = \frac{\beta\delta}{\nu} = \frac{\beta+\gamma}{\nu} = d - \frac{\beta}{\nu}$$

Fisher zeros of the non-frustrated Ising model

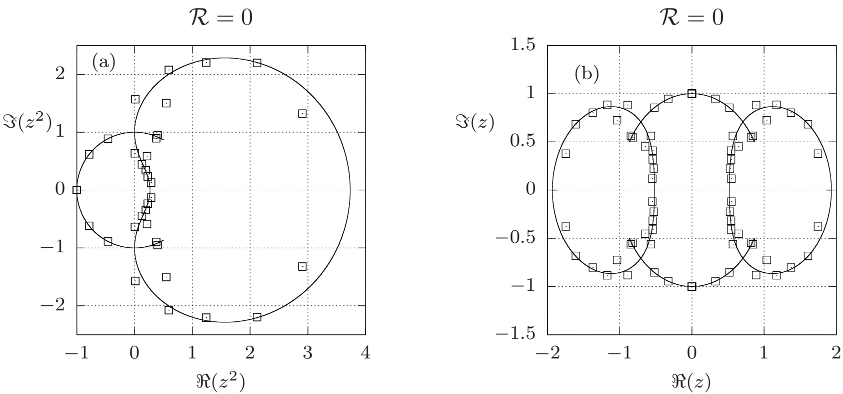

Figure: Fisher zeros in the complex temperature planes (a) $z^2 = e^{-2\beta J_1}$ and (b) $z = e^{-\beta J_1}$ for $\mathcal{R} = 0$. Points denote our data for $L = 4$ obtained by exact enumeration. The solid lines are the exact zeros for $L \to \infty$ [4][5].

[4] V. Matveev and R. Shrock, J. Phys. A **29**, 803 (1996)

[5] S.Y. Kim, C.O. Hwang and J.M. Kim, *Nucl. Phys. B* **805**, 441 (2008)

How to measure complex partition function zeros?

- Simulations with complex β & h

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WL MUCA **PA +MHR** **exact enumeration** analytically

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obtain: WL, MUCA, **PA +MHR**, **exact enumeration**, analytically

find:
- analytically
- polynomial root-finding
  $\Rightarrow$ all zeros
- non-polynomial root-finding
  $\Rightarrow$ leading zero(s)

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- here: different approach[6] not requiring DOS

[6] C. Flindt and J.P. Garrahan, Phys. Rev. Lett. **110**, 050601 (2013)

Cumulant method

- Factorize partition function by its roots, q_k:

$$\mathcal{Z}(q) = \tilde{\mathcal{Z}}(q)\prod_k (1 - q/q_k)$$

($\tilde{\mathcal{Z}}(q) = \mathcal{Z}(0)e^{cq}$, $(\Phi, q) = (E, -\beta)$ for F zeros and $(\Phi, q) = (M, \beta h)$ for LY zeros)

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- Solve approximation for q_0[6]:

$$\begin{pmatrix} 2\,\Re(q_0 - q) \\ |q_0 - q|^2 \end{pmatrix} \approx \begin{pmatrix} 1 & -\frac{\mu_n^{(+)}}{n} \\ 1 & -\frac{\mu_{n+1}^{(+)}}{n+1} \end{pmatrix}^{-1} \begin{pmatrix} (n-1)\mu_n^{(-)} \\ n\,\mu_{n+1}^{(-)} \end{pmatrix} \qquad \mu_n^{(\pm)} \equiv \langle\langle \Phi^{n\pm 1} \rangle\rangle / \langle\langle \Phi^n \rangle\rangle$$

[6] C. Flindt and J.P. Garrahan, Phys. Rev. Lett. **110**, 050601 (2013)

Solving for all Fisher zeros

Figure: Fisher zeros in the (transformed) complex temperature $z = e^{-\beta J_1}$ plane for $L = 4$ as $\mathcal{R}$ is varied from 0 to -1. The red circles highlight the Fisher zeros closest to the positive real axis.

Solving for all Fisher zeros

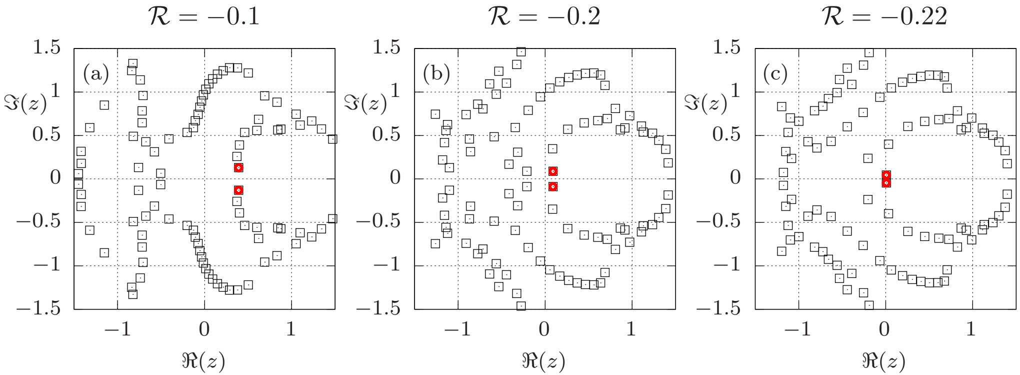


Figure: Fisher zeros in the (transformed) complex temperature $z = e^{-\beta J_1}$ plane for $L = 4$ and (a) $\mathcal{R} = -0.1$, (b) $\mathcal{R} = -0.2$, and (c) $\mathcal{R} = -0.22$. The red circles highlight the Fisher zeros closest to the positive real axis.

Direct vs. cumulant method: PA+MHR

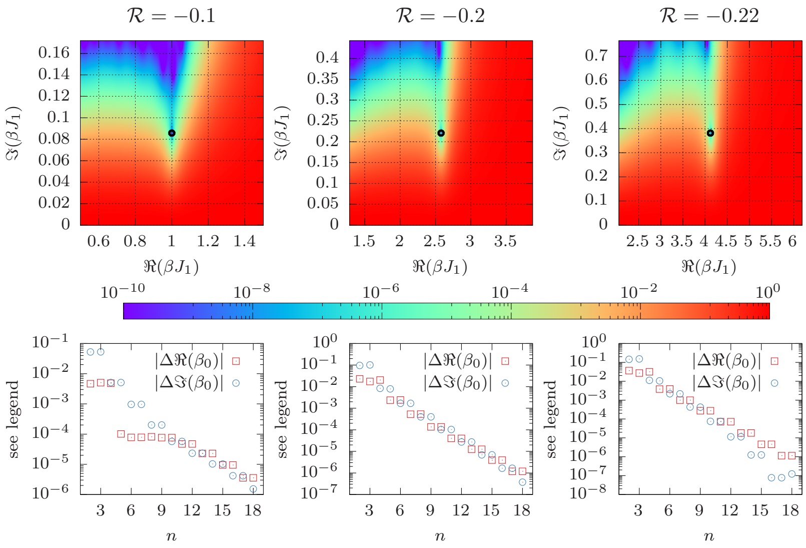
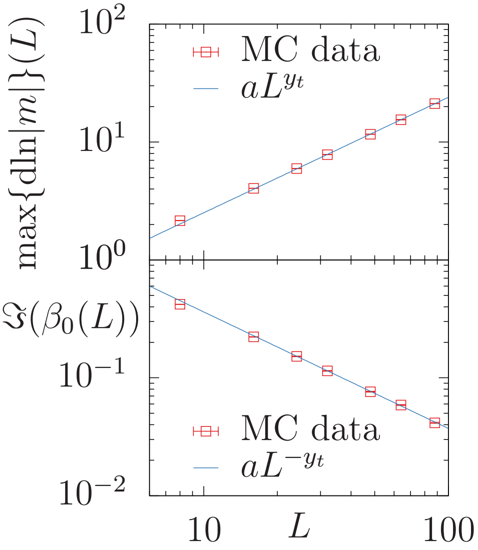


Figure: Same as before but for $L = 16$, and using multi-histogram reweighted PA simulation data instead of exact enumeration.

FSS fit example ($\mathcal{R} = -0.2$)



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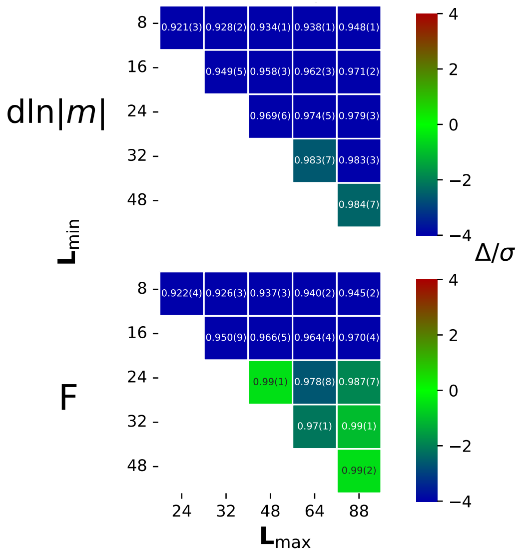
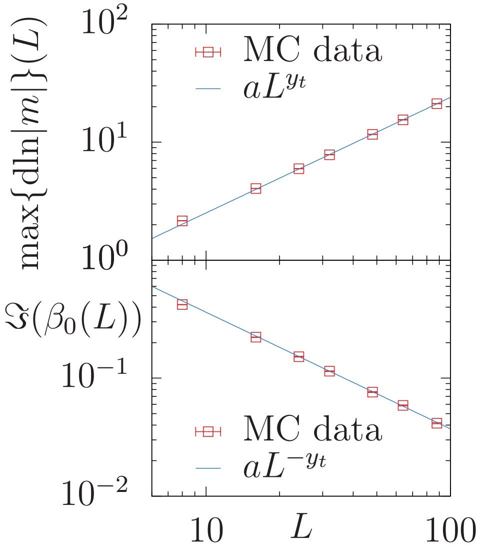
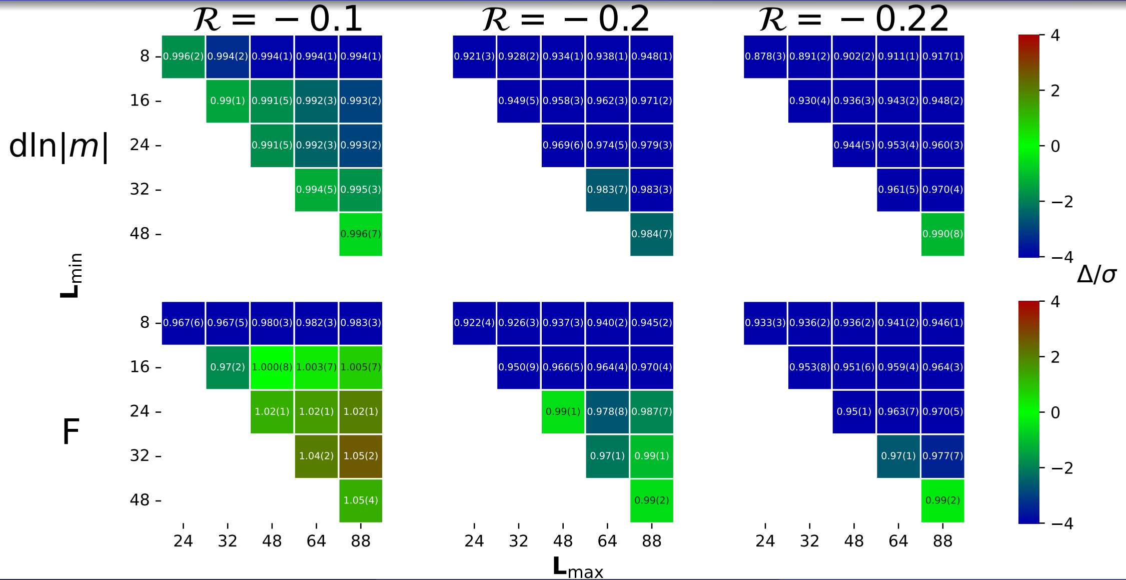
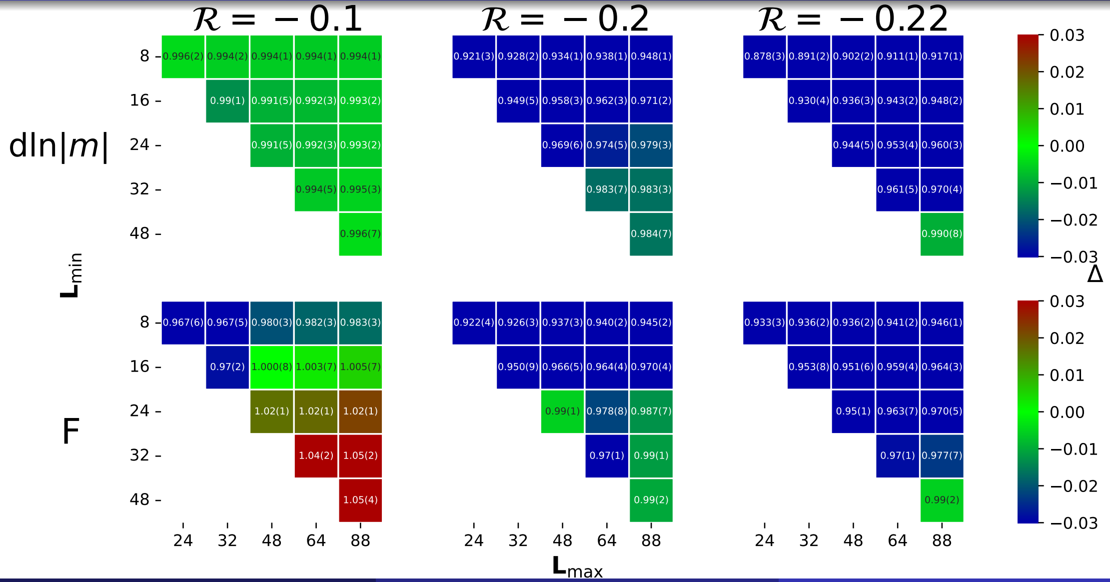




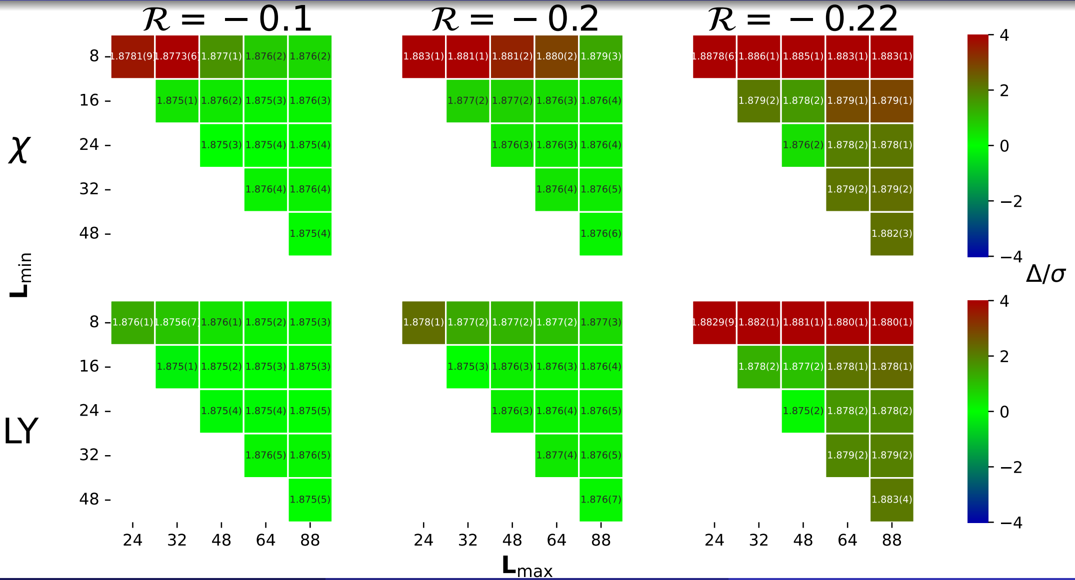
Temperature exponent y_t (color relative)



Temperature exponent y_t (color absolute)



Field exponent y_h (color relative)



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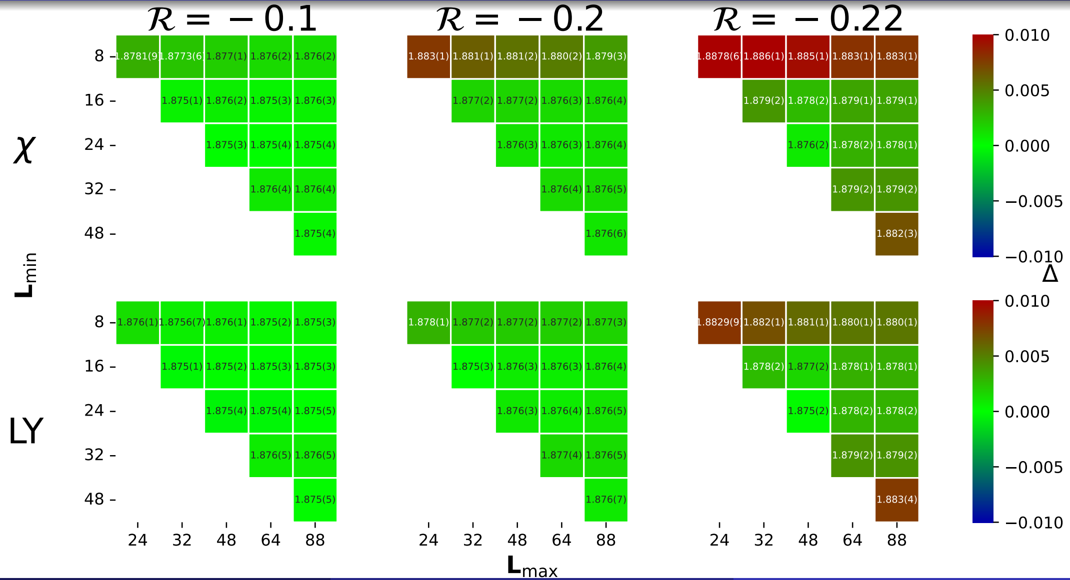
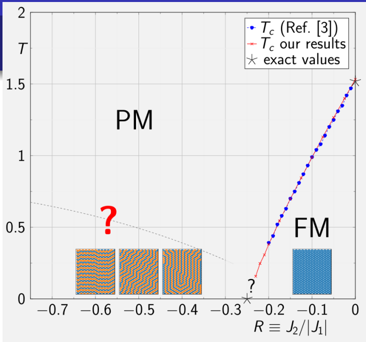


Summary & Outlook



Summary

- Model in Ising universality class at least until $\mathcal{R} = -0.22$
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  but: different correction amplitudes $\Rightarrow$ useful to study both
  $\Rightarrow$ computing resources focussed on low Ts at which the system is very hard to equilibrate

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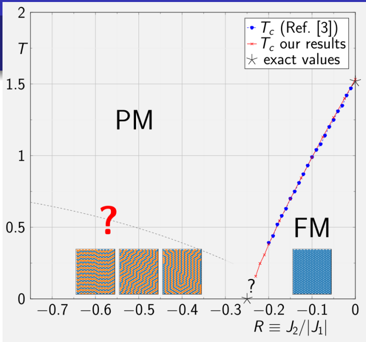

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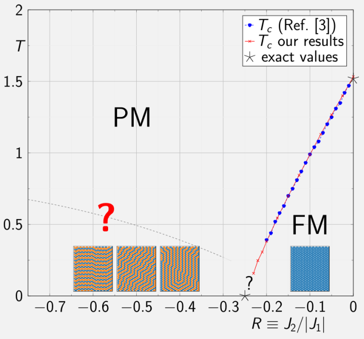

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Outlook (work in progress)

- FSS closer to $\mathcal{R} = -0.25$
- Strongly frustrated regime $\mathcal{R} < -0.25$

Thank you for your attention.

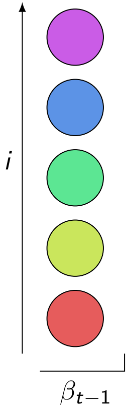
Questions?

6 Backup slides

- Population Annealing (PA)
- GPU implementation
- $L = 4$ checks
- Checks for larger system sizes
- Regime of strong antiferromagnetic next-nearest neighbor interactions

Population Annealing [7]

[7]K. Hukushima and Y. Iba, AIP Conf. Proc. **690**, 200 (2003)



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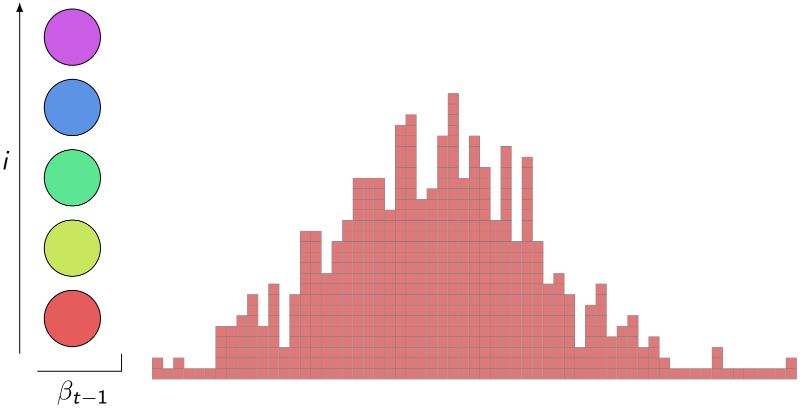
$R = 500, \beta_{t-1} = 0.7$



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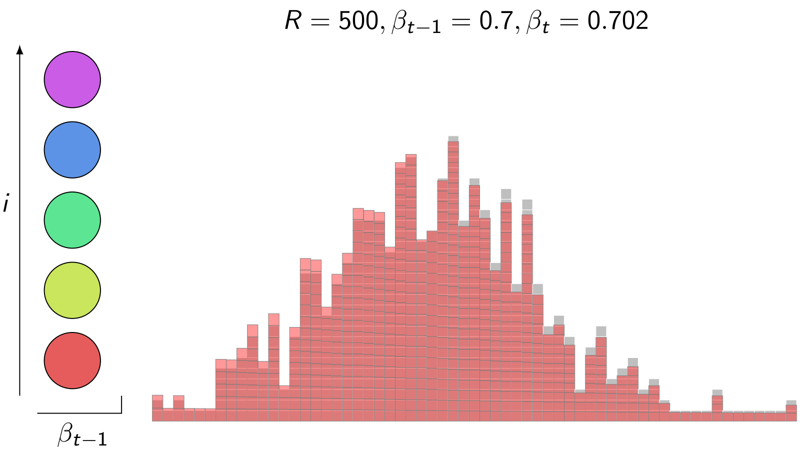

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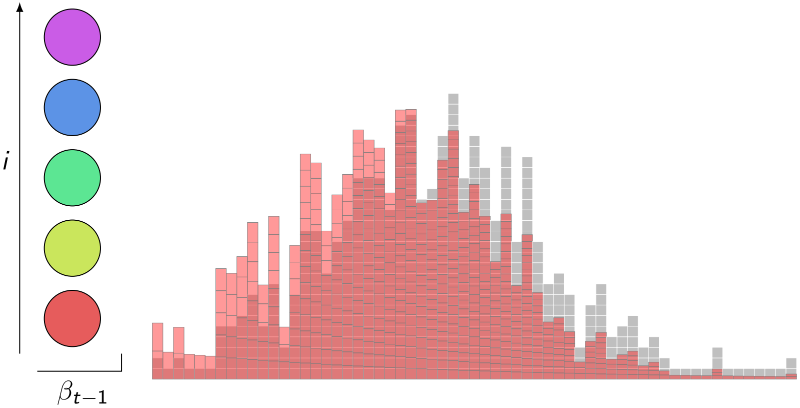
[7]K. Hukushima and Y. Iba, AIP Conf. Proc. **690**, 200 (2003)

$R = 500, \beta_{t-1} = 0.7, \beta_t = 0.71$



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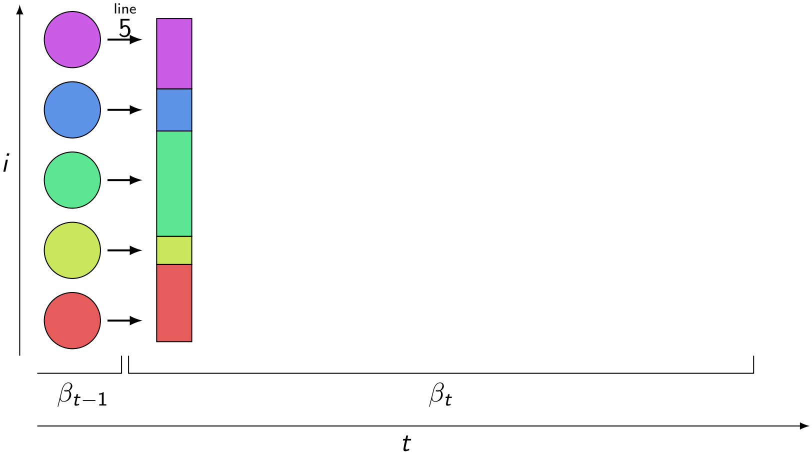

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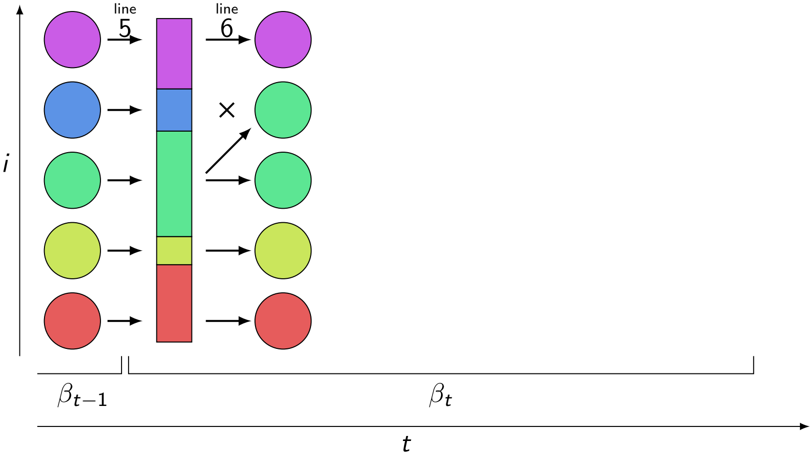

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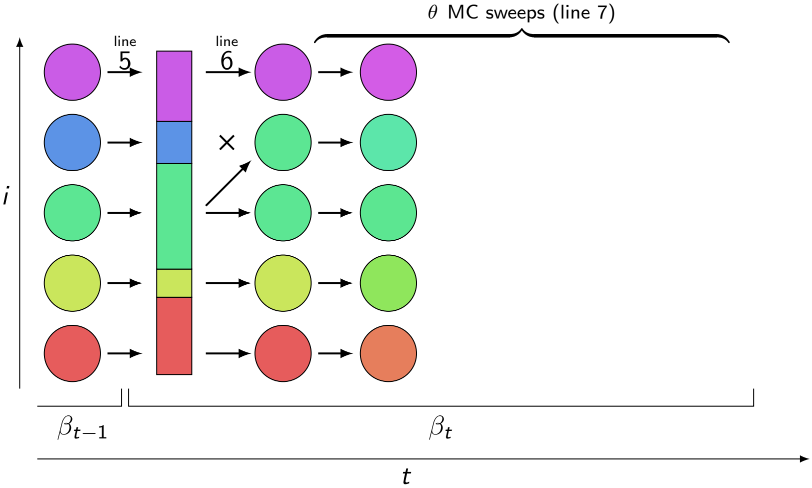

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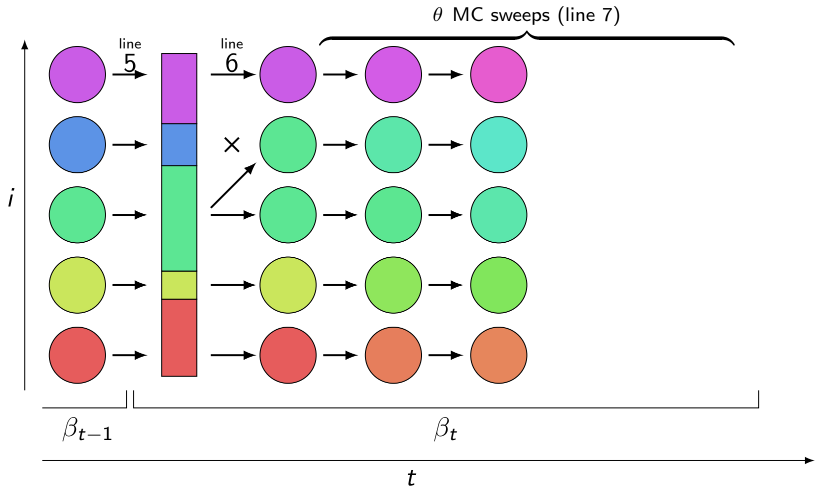

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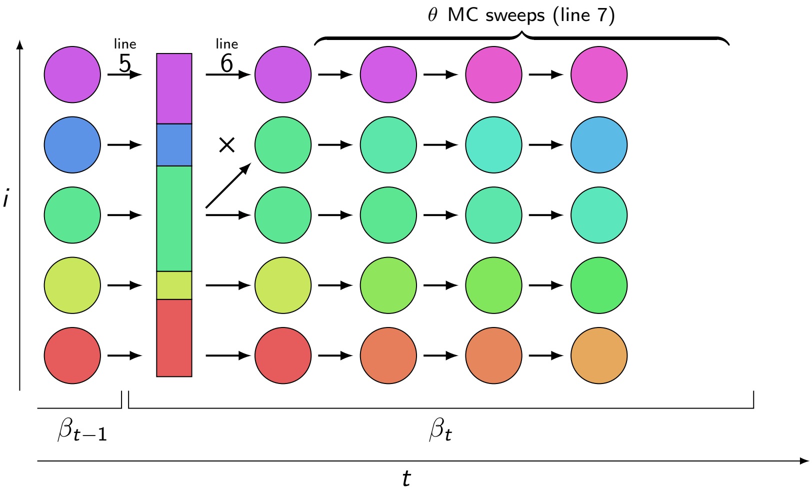

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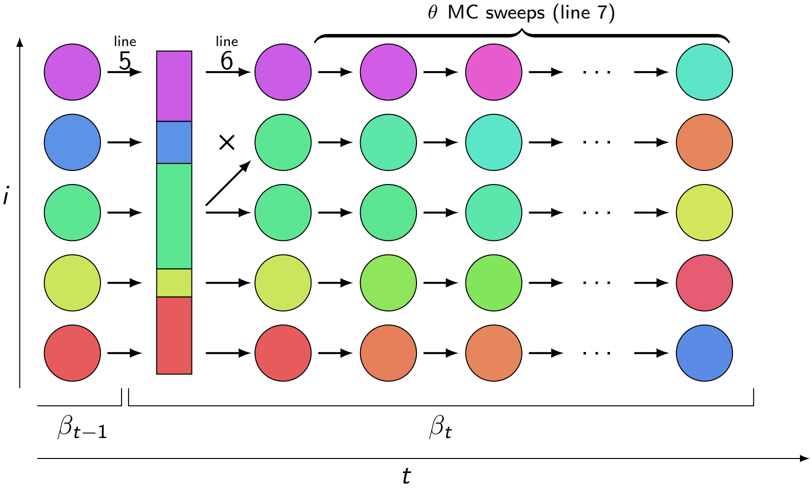

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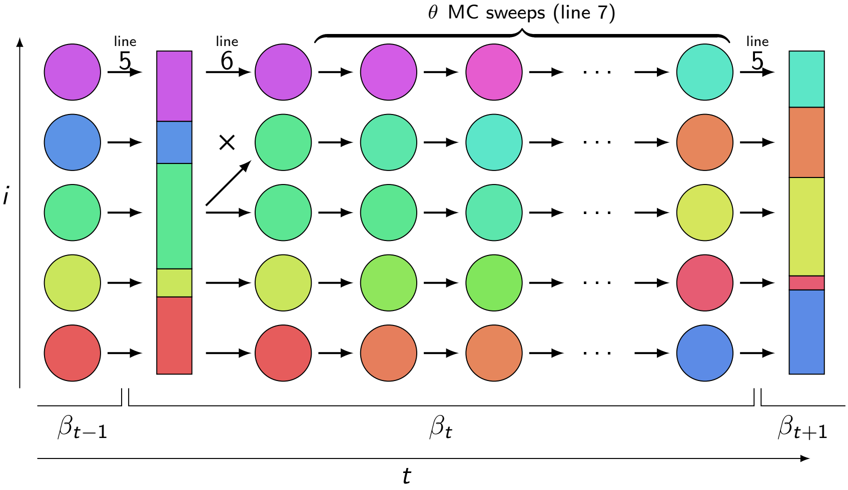

Population Annealing (formal)

Algorithm Standard Population Annealing algorithm[7]

1: $t \leftarrow 0$
2: Initialize population of R independent replicas at β_0
3: **while** $\beta_{t+1} < \beta_{\max}$ **do**
4: $t \leftarrow t + 1$
5: Calculate **Boltzmann weights** w_i of the replicas at β_t
6: **if** $t \equiv 0 (\mathrm{mod}\ M)$ then **resample** population according to weights (on avg. $\tau_i = Rw_i$ copies of replica i)
7: **Monte Carlo update** of the replicas (θ MC sweeps at β_t)
8: **Measure** observables $\mathcal{O}$
9: **end while**

rediscovered by Machta seven years later[8]

[7] Hukushima, K. and Iba, Y., AIP Conf. Proc. **690**, 200–206 (2003), p. 7.
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    Monte Carlo update of the replicas (θ MC sweeps at β_t)
    Measure observables $\mathcal{O}$
end while

Parameters

- population size R
- annealing schedule β_k
- # of MC updates at each temperature step
- resampling interval M (usually $= 1$)
- resampling method
- **equilibration method**

rediscovered by Machta seven years later[8]

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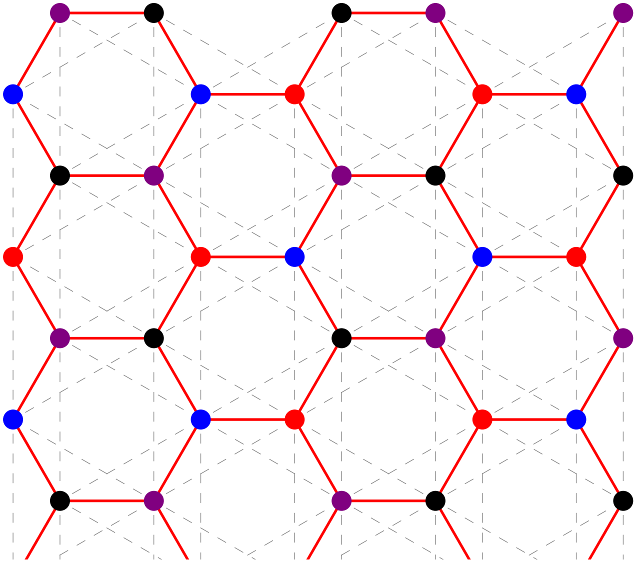
GPU implementation



$$H = -J_1 \sum_{\langle ij \rangle} \sigma_i \sigma_j - J_2 \sum_{[ik]} \sigma_i \sigma_k$$

$$(J_1 > 0, J_2 < 0)$$

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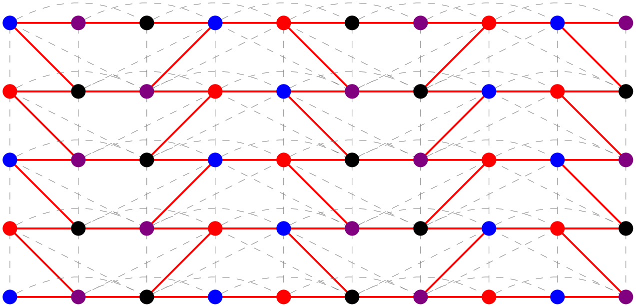

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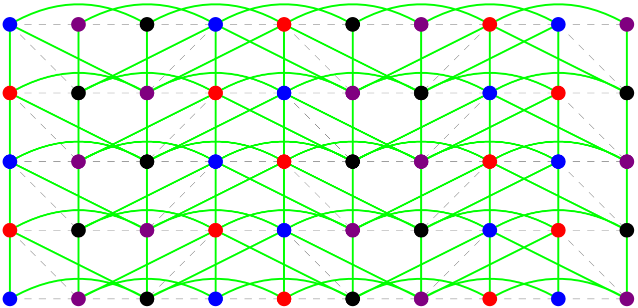

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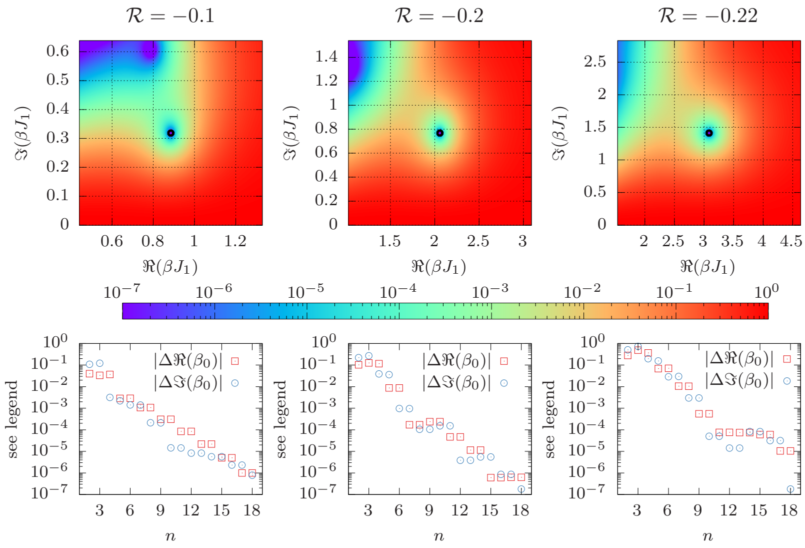
Cumulant method: Fisher zeros

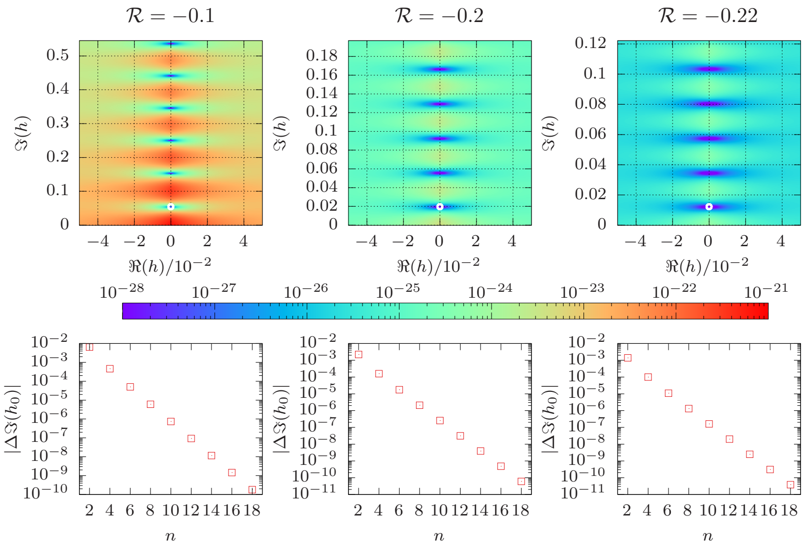


Top row: Heat maps of $|Z(\Re(\beta), \Im(\beta))|$ for $\mathcal{R} \in \{-0.1, -0.2, -0.22\}$ (centered around leading zero).

$$Z(\Re(\beta), \Im(\beta)) \equiv \frac{\mathcal{Z}(\Re(\beta) + i\Im(\beta), h = 0)}{\mathcal{Z}(\Re(\beta), h = 0)}$$

Bottom row: Differences $\Delta\Re(\beta_0)$ and $\Delta\Im(\beta_0)$, comparing the direct method with the cumulant method.

Cumulant method: Lee-Yang zeros



Top row: Heat maps of $|Z_{\beta_c}(\Re(h), \Im(h))|$ for $\mathcal{R} \in \{-0.1, -0.2, -0.22\}$ (centered around leading zero).

$$Z_\beta(\Re(h), \Im(h)) \equiv \frac{\mathcal{Z}(\beta, \Re(h) + i\Im(h))}{\mathcal{Z}(\beta, \Re(h))}$$

Bottom row: Difference difference in $\Im(h_0)$ comparing the direct method with the cumulant method.

Cumulant method: Asymptotic approach - Fisher zeros

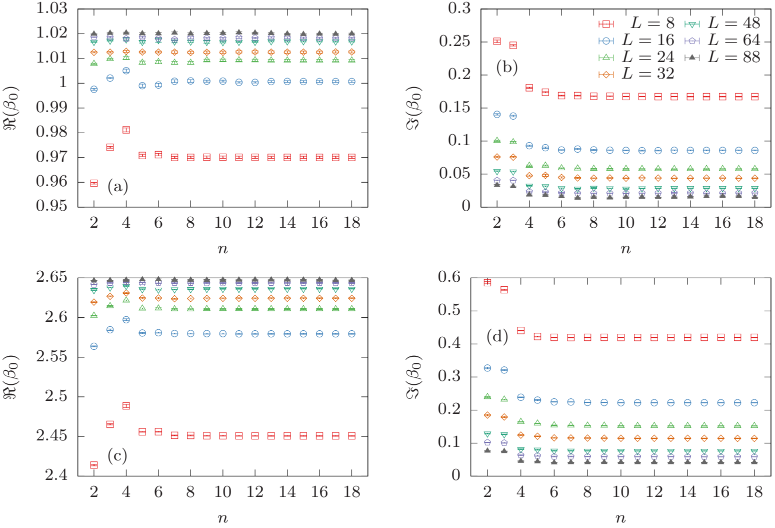


Figure: Real and imaginary part of the Fisher zeros β_0 obtained through the cumulant method as a function of n for different L. In (a) and (b) $\mathcal{R}=-0.1$, and in (c) and (d) $\mathcal{R}=-0.2$.

Cumulant method: Asymptotic approach - Lee-Yang zeros

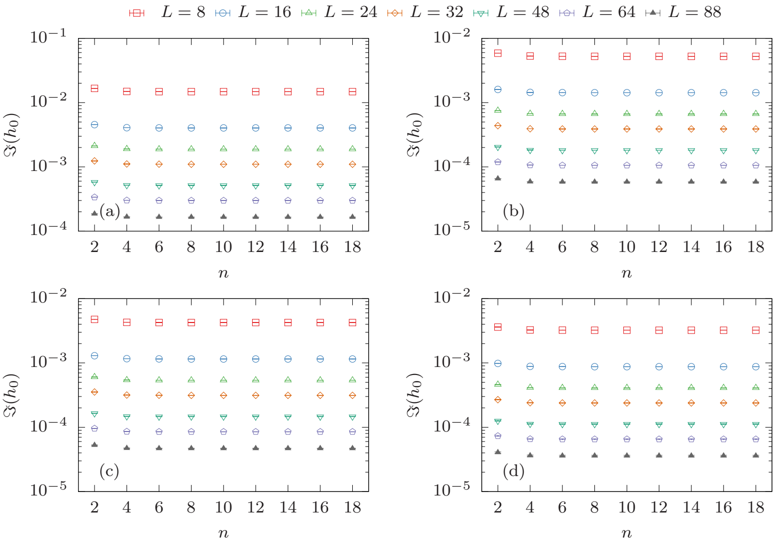


Figure: Imaginary part of the Lee-Yang zeros h_0 for different system sizes L and coupling strengths $\mathcal{R}$. (a) $\mathcal{R} = -0.1$, (b) $\mathcal{R} = -0.2$, (c) $\mathcal{R} = -0.21$, and (d) $\mathcal{R} = -0.22$.

Strong antiferromagnetic interactions

For $R < -0.25$ we know

- the **ground state** manifold is **largely degenerate** ($\sim 2^L$ ground states for a system with $L \times L$ hexagons)

[2]A. Bobák and T. Lučivjanský and M. Žukovič and M. Borovský and T. Balcerzak, Phys. Lett. A **380**, 2693 (2016)

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What is unknown for $R < -0.25$:

- order parameter of phase transition
- order of transition
- existence of phase transition

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Specific heat signals I

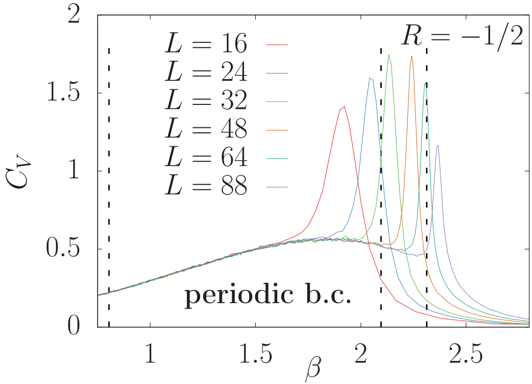
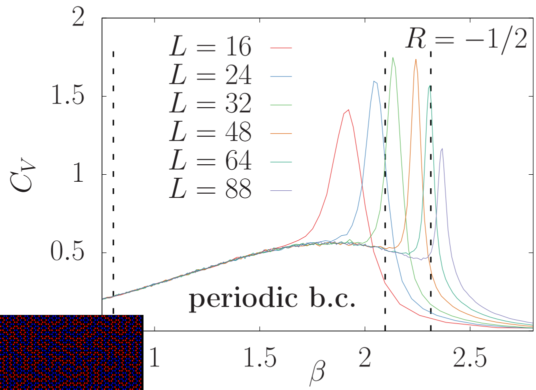
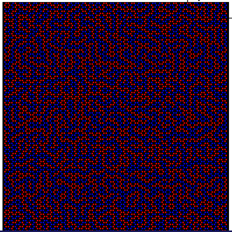


Figure: Specific heat for $R = -1/2$ using (a) periodic, and (b) free boundary conditions for different linear system sizes L.

Specific heat signals I





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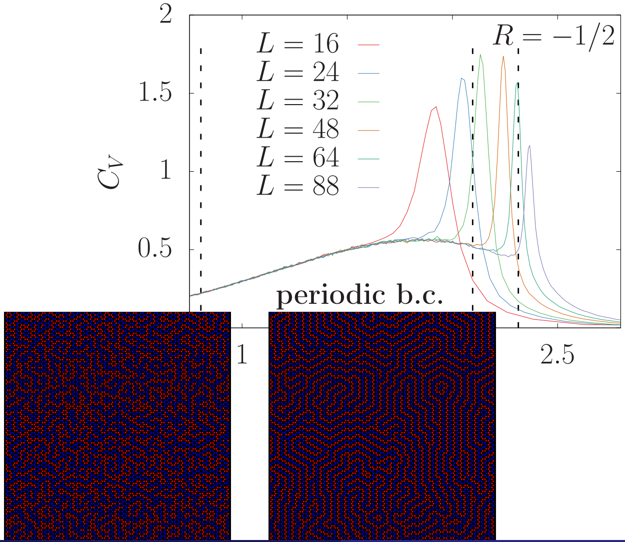

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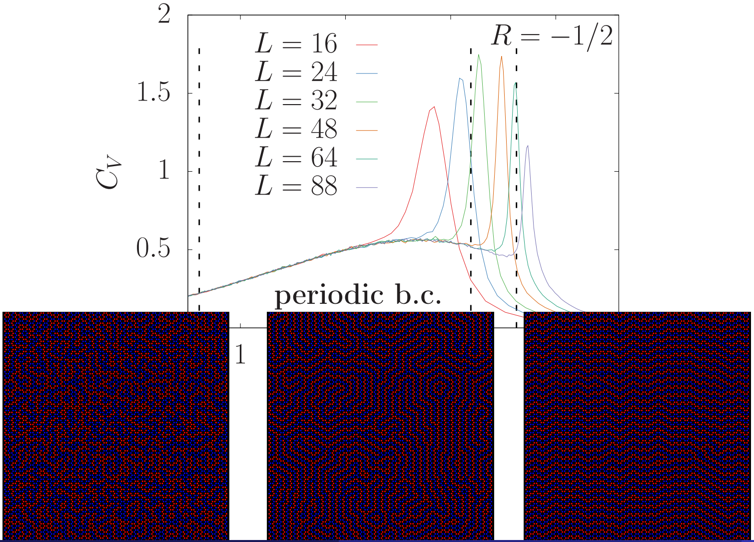

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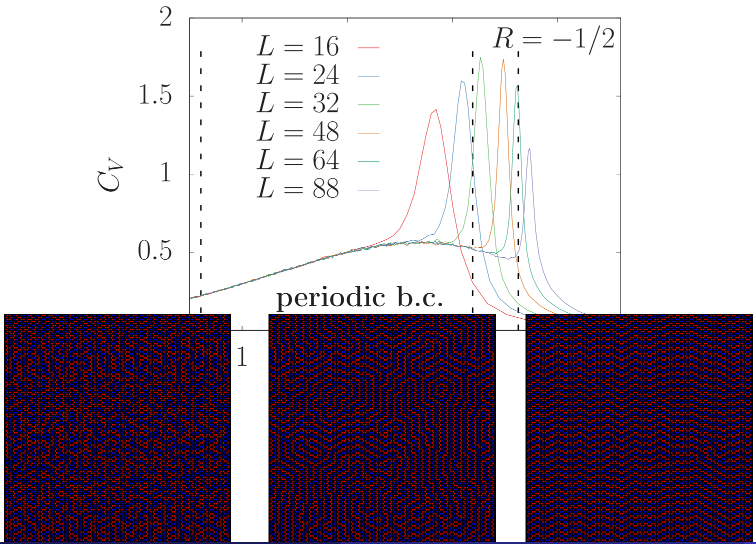

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What about different boundary conditions?

Specific heat signals I

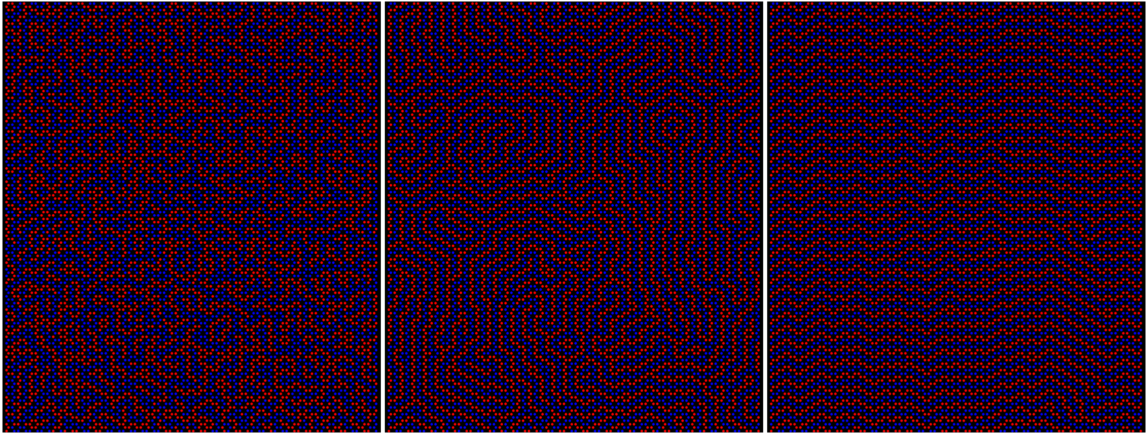
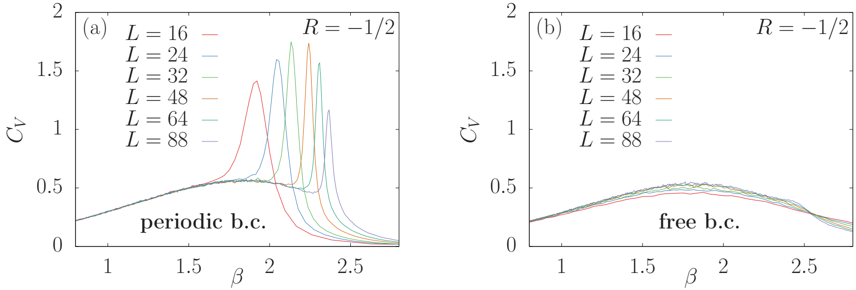


Figure: Equilibrium configurations for $L = 64$ for $\beta = 0.80, 2.09, 2.31$.

Specific heat signals II: What about different b.c.



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Specific heat signals: Summary

- sharp peaks in C_V for periodic b.c.s (pbc)
  - grows with system size (for small L) and becomes sharper
    $\Rightarrow$ **interpreted as sign of phase transition**
  - peak **absent** when using **free b.c.** (fbc)
    $\Rightarrow$ **peak irrelevant in the thermodynamic limit**

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    $\Rightarrow$ **interpreted as sign of phase transition**
  - peak **absent** when using **free b.c.** (fbc)
    $\Rightarrow$ **peak irrelevant in the thermodynamic limit**
- broad "background" peak
  - **no system size dependence** for pbc, and little for fbc $\Rightarrow$ expected to **remain in the thermodynamic limit**
  - reminiscent of spin glasses [7][8] $\Rightarrow$ check autocorrelation and two-time quantities

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Two-time spin-spin autocorrelator

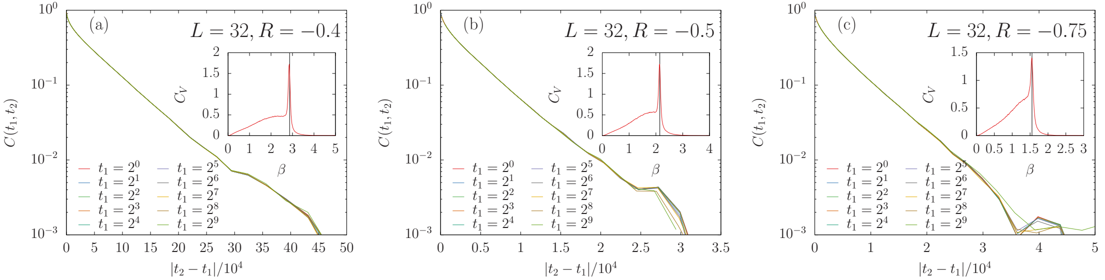

Figure: Two-time autocorrelation function $C(t_1, t_2)$ as a function of $|t_2 - t_1|$ for (a) $R = -0.4$, (b) $R = -0.5$, and (c) $R = -0.75$ at the temperature of the specific heat maximum. The collapse of the curves indicates time-translation invariance. The inset shows the specific heat, and the inverse temperature used for the main panel is indicated by a vertical line

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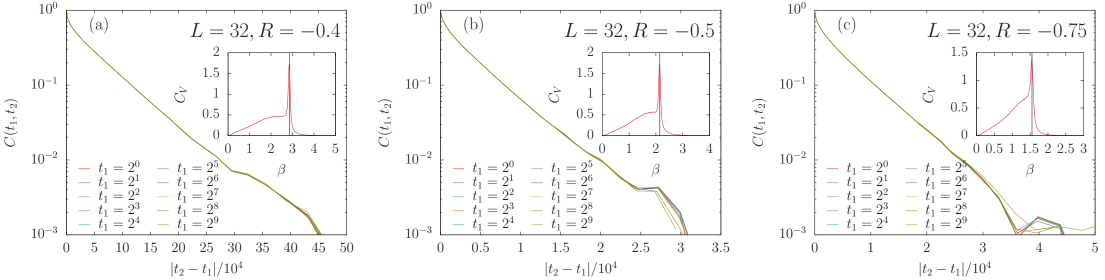

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- time-translation invariance of $C(t_1, t_2)$ is visible for all values of R studied
  $\Rightarrow$ **not consistent with glassy behavior!**

Exponential autocorrelation time

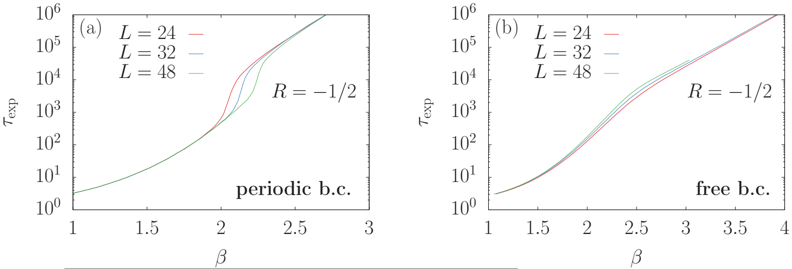

Figure: Exponential autocorrelation time for $R = -1/2$ using (a) periodic*, and (b) free boundary conditions for different linear system sizes L.

* The data in panel (a) was obtained by using random-site-flip dynamics and *not* with the GPU-optimized domain-decomposition dynamics.

- large autocorrelation times at low temperature ⇒ equilibration / sampling difficult

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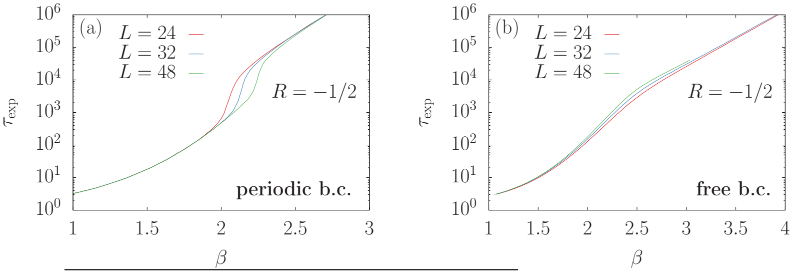

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- large autocorrelation times at low temperature ⇒ equilibration / sampling difficult
- **almost no system-size dependence** ⇒ further indication for the **absence of a phase transition**