Harnessing finite-size effects to gauge aging in the $2D$ Ising model

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Structure

Introduction to aging

Theory and application to concrete examples

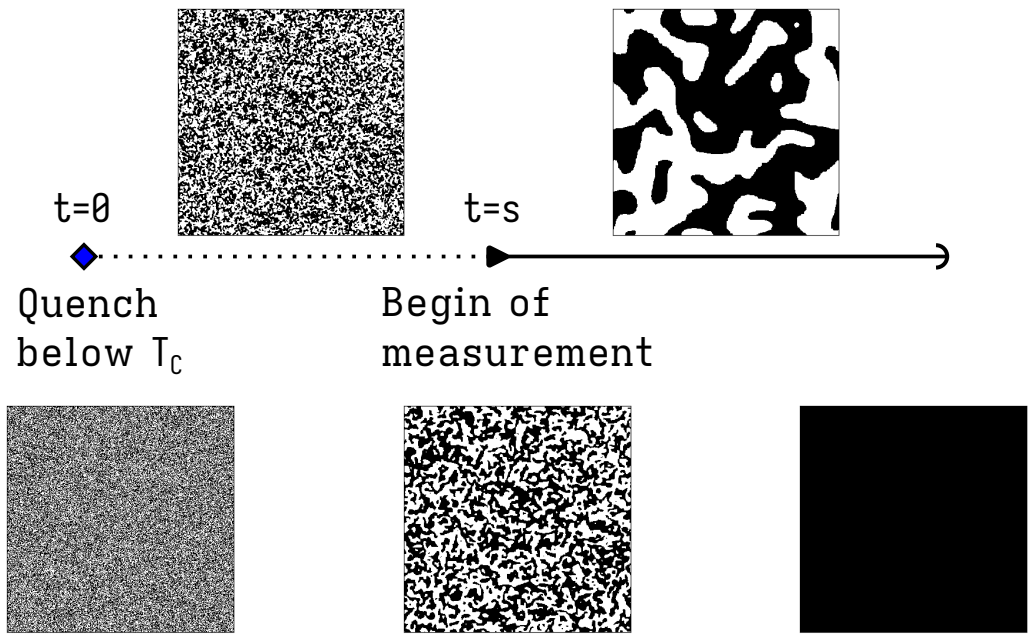
Results

Conclusion

Introduction to aging

Physical aging

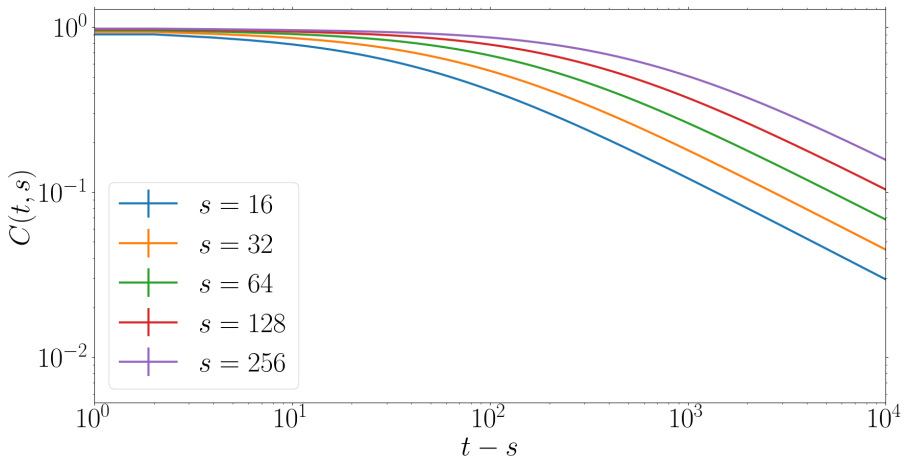
- Change of properties in materials over time
- Out-of-equilibrium system with slow relaxation

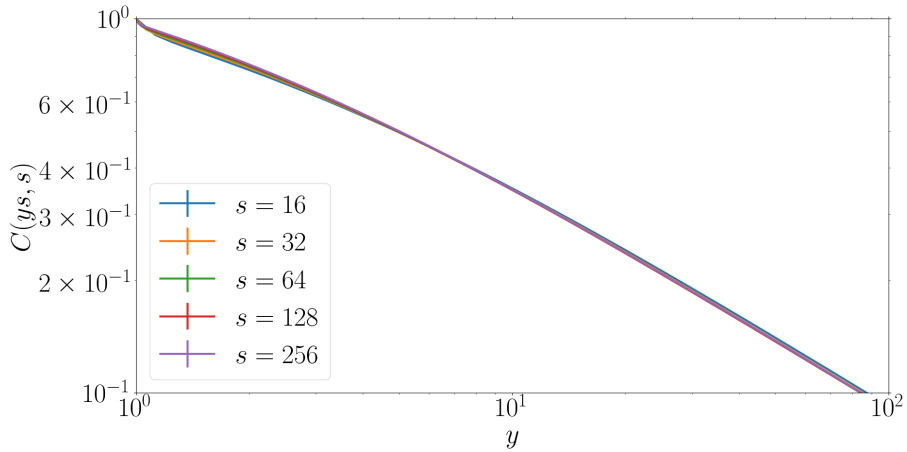


- Phase-ordering kinetics
- Characteristic length scale $\ell(t) \sim t^{\frac{1}{z}}$

- Observables depending on both - **observation time** t and **waiting time** $s > t$
- Here: **Unconnected two-time autocorrelation function**

$$\boxed{C(t,s) = \langle \sigma(\vec{r},t) \cdot \sigma(\vec{r},s) \rangle}$$



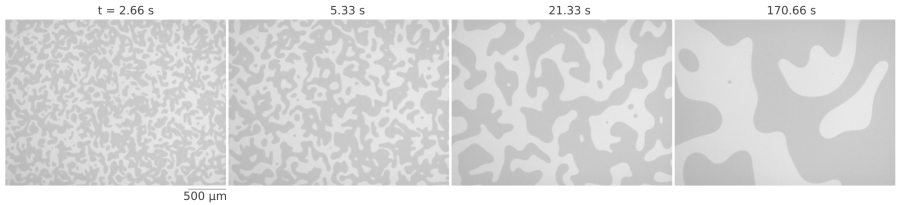


$$C(t,s) \sim \left(\frac{t}{s}\right)^{-\frac{\lambda_C}{z}}$$

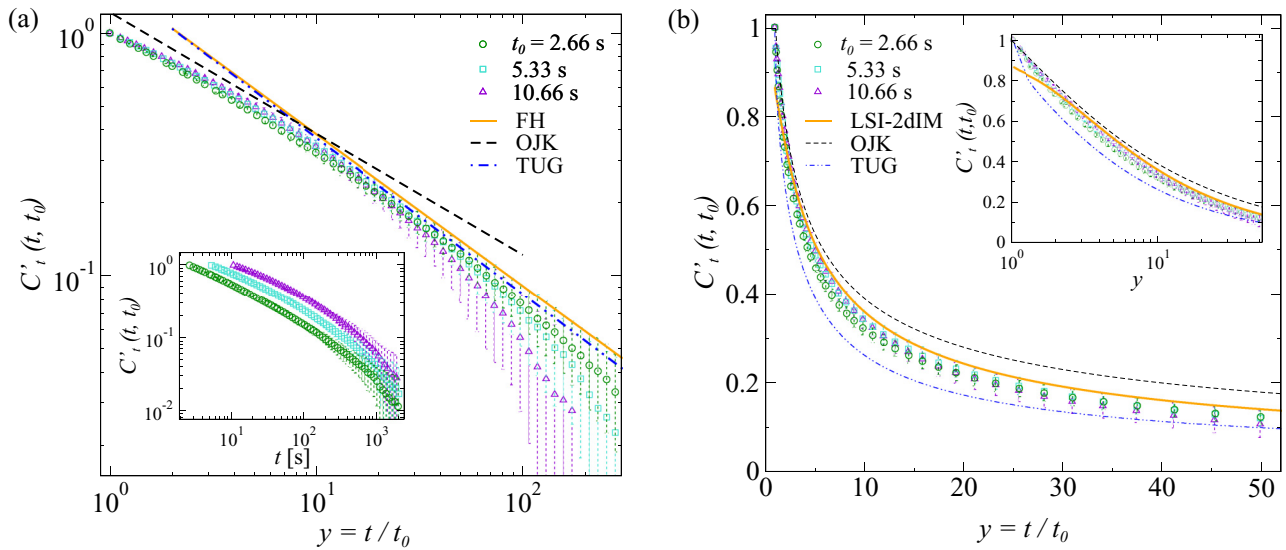
Three hallmarks of aging

1. Slow relaxation
2. Broken time-translational invariance
3. Scaling behavior

Experimental examples

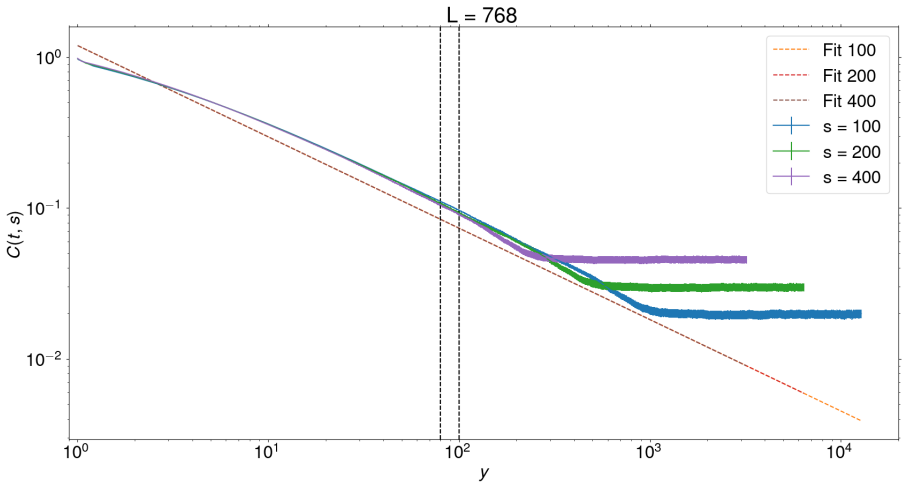


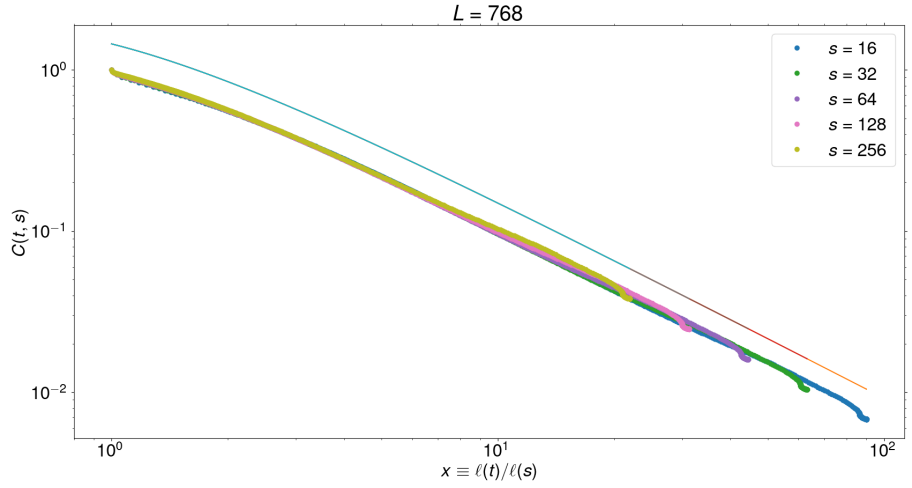
Aging in liquid crystals (reproduced from[1])



[1] Renan A. L. Almeida and Kazumasa A. Takeuchi. "Phase-Ordering Kinetics in the Allen-Cahn (Model A) Class: Universal Aspects Elucidated by Electrically Induced Transition in Liquid Crystals." In: *Phys. Rev. E* 104.5 (2021), p. 054103. DOI: 10.1103/PhysRevE.104.054103.

Current estimates





Direct measurement of λ/z

$$C(t,s) \sim \left(\frac{\ell(t)}{\ell(s)}\right)^{-\lambda}$$

- Theoretical ansatzes:
  - Fisher and Huse: $\lambda \leq 1.25$
  - Mazenko et al.: $\lambda \approx 1.2887$
- Simulations:
  - Lorenz et al.: $\lambda \approx 1.24(2)$
  - Midya et al.: $\lambda \approx 1.32(4)$
- ...

Here

Provide a new method of measuring aging in lattice systems via finite size effects

Theory

Heuristic derivation

- for large y: $C(t,s) = f_C(y) \sim y^{-\lambda/z} = \left(\frac{t}{s}\right)^{-\lambda/z} \sim \left(\frac{\ell(t)}{\ell(s)}\right)^{-\lambda}$
- With characteristic length scale $\ell(t) \sim t^{1/z}$ in the $2D$ Ising model with nearest-neighbor interactions
- In *finite lattices*, the domains cannot outgrow the lattice itself, limiting $\ell(t) \to L$
- Thus: $C(t,s) \to \left(\frac{L}{s^{1/z}}\right)^{-\lambda}$

Specifically

$C_\infty \sim s^{\frac{\lambda}{z}}$ with $L = \text{const.}$ and $C_\infty \sim L^{-\lambda}$ with $s = \text{const.}$

Model and simulation

Model

- $2D$ Ising model with nearest neighbor interaction and periodic boundary conditions
- $H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$ with spins $\sigma_i = \pm 1$ and ferromagnetic interaction $J = 1$
- Kinetic Monte Carlo (n-fold way) since $T < T_C$

Basic setup of non-equilibrium simulation

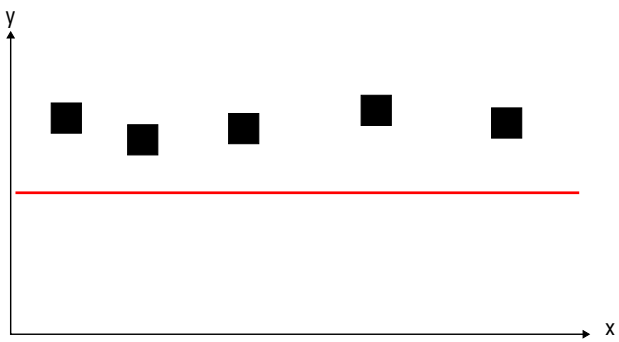
1. Initialize system with random spins ($T = \infty$)
2. Quench to $T < T_C$ (*here:* $t = 0$)
3. Advance simulation by local update
4. For every waiting time $s > t$: Snapshot current state of the lattice
5. Calculate $C(t, s)$

Measurement and analysis

1. Extract C_∞ from plateau in $C(ys, s)$
2. Form Jackknife blocks containing all initializations but one
3. Perform fit for each Jackknife block
4. Repeat procedure for each constant parameters s or L
5. Correlation-weighted average over all constant parameters

Note

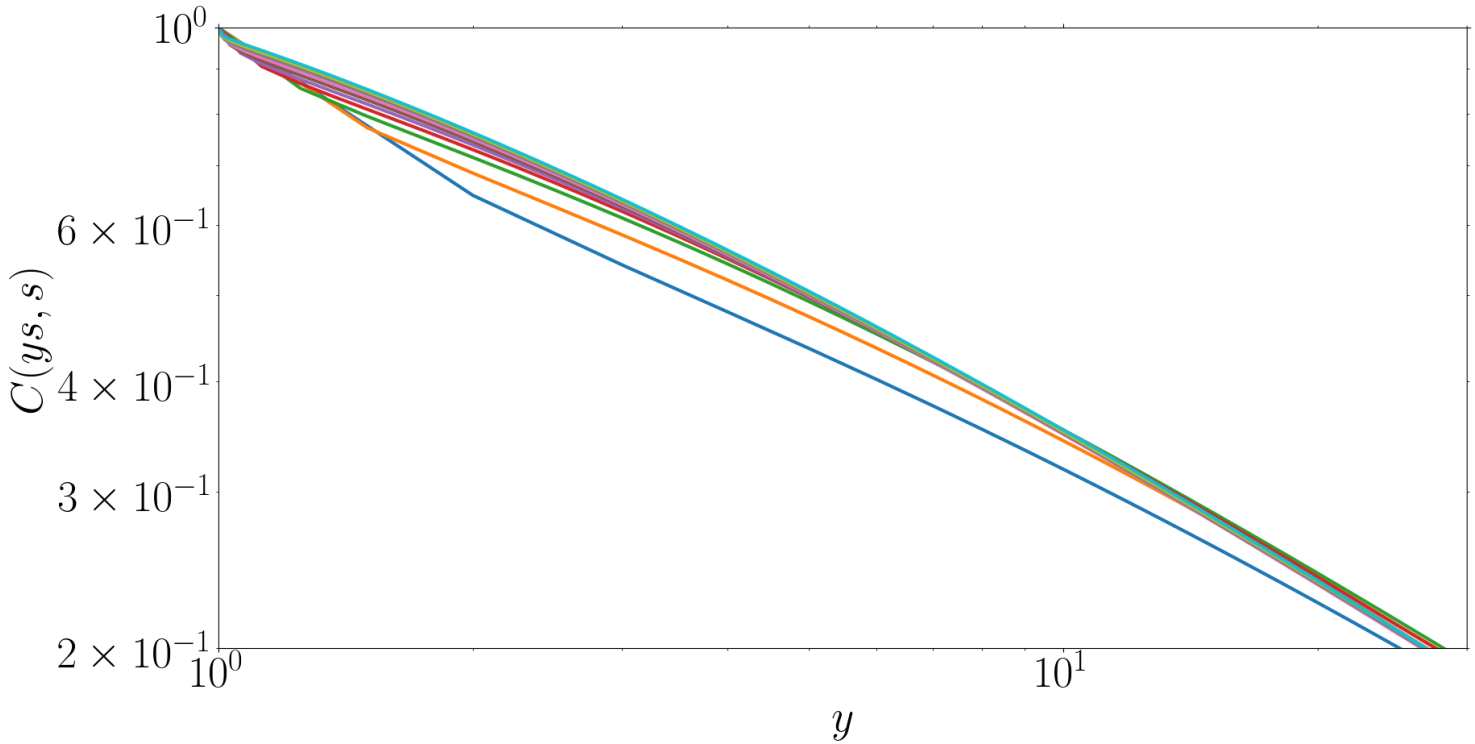
Highly correlated estimates can yield counterintuitive results



Gauging and eliminating systematic errors

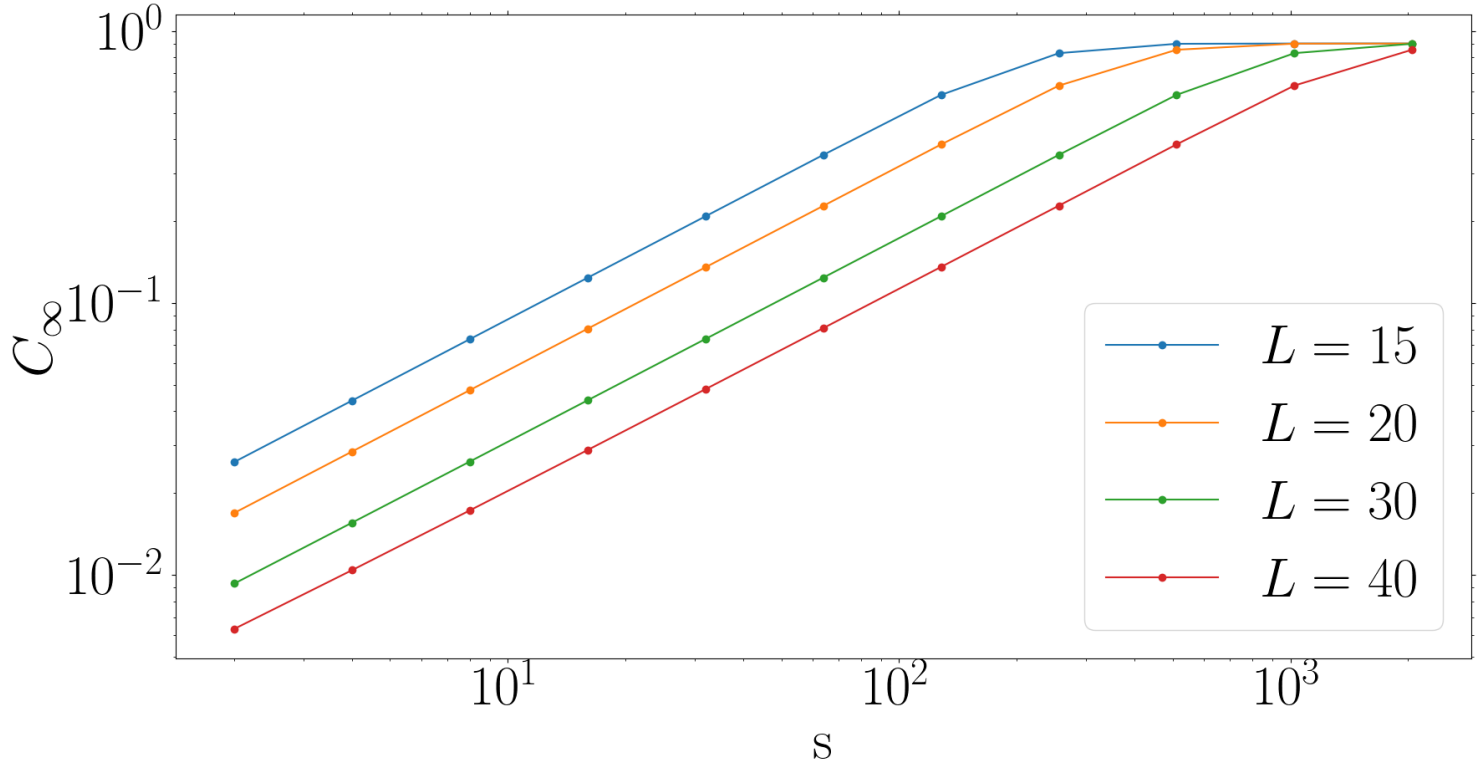
(1) Lower bound of s: Via microscopic timescale τ_{micro} Necessary for scaling argument $C(t,s) = f_C(y) \sim y^{-\lambda/z}$

- $t, s, t-s \gg \tau_{\text{micro}}$



(2) Upper bound of s and lower bound of L: Via deviations from finite-size scaling

- Condition: $\frac{L^2}{s} \gg 1$
- Stems from demand that $\ell(s) \sim s^{1/z}$
- Effectively: $L \gg \ell(s)$
- Necessary, as system would equilibrate too quickly otherwise



(3) Upper bound of L:

- For finite systems: $\frac{t}{L^z}$ large enough
- Systems under study must be fully equilibrated
- Difficult for low temperatures owing to metastable states - **stripes**

- At low $T > 0$: lifetime $\tau \sim L^3 \cdot e^{\frac{4J}{k_B T}}$ for **all** metastable states

Difficulty

Inhomogeneity in the number of striped states between L
$\Longrightarrow$ **Plateau heights** $C_\infty(s, L)$ **hardly comparable**

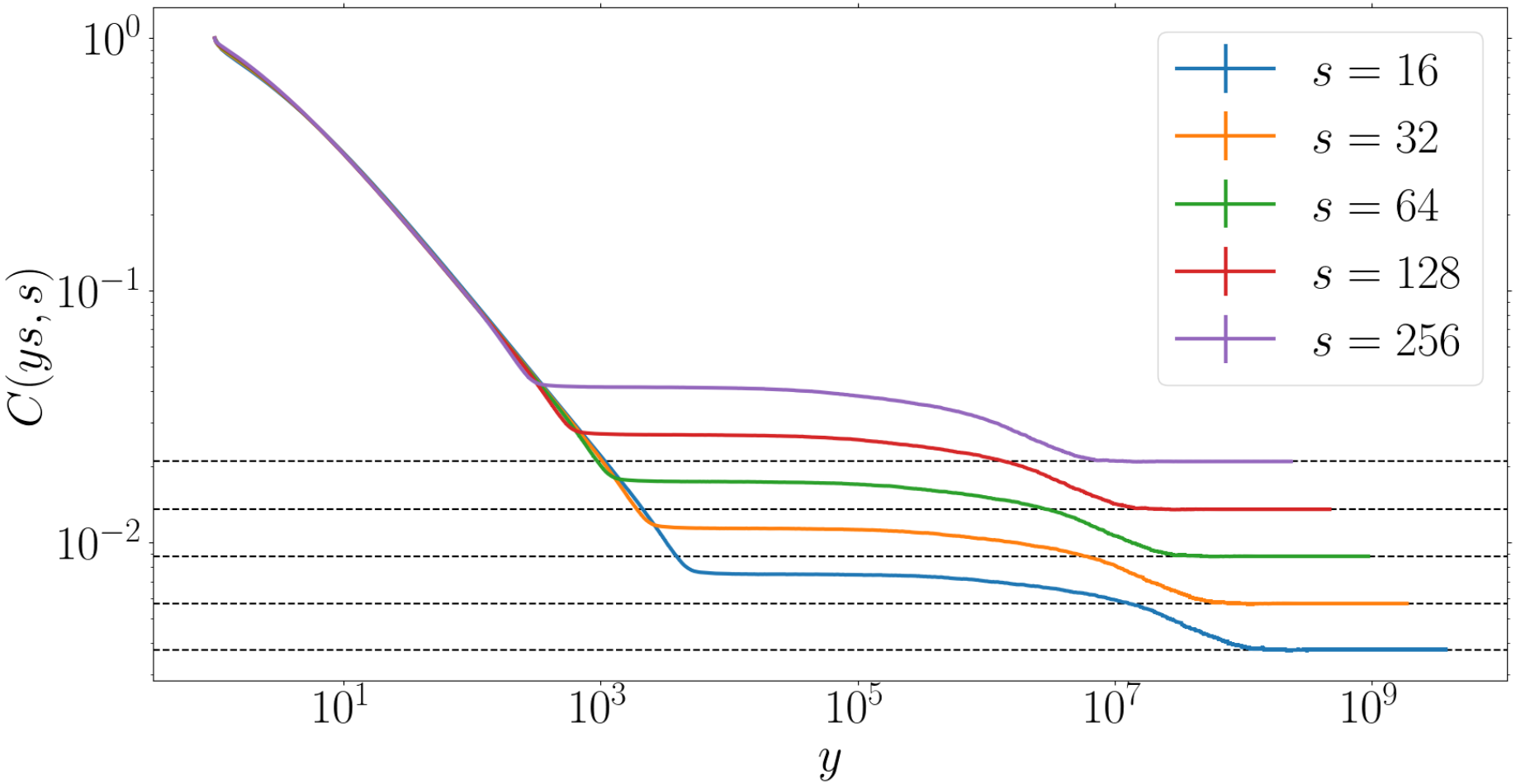
Question

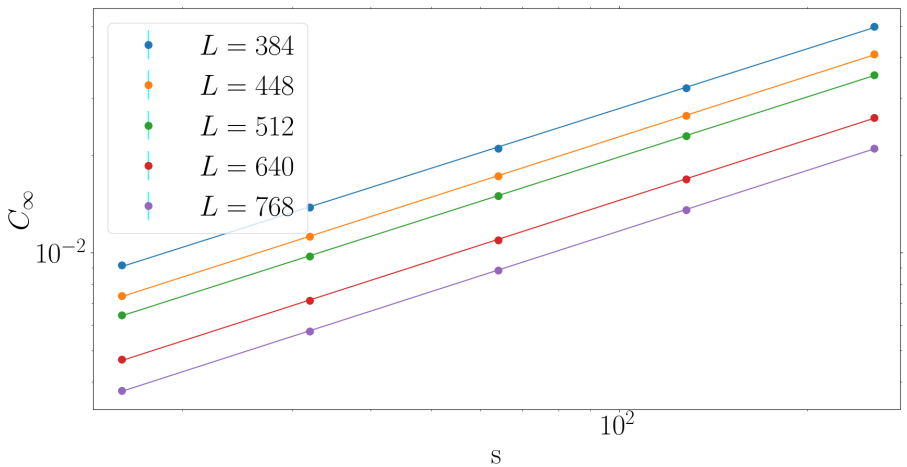
How can metastable states be dealt with?

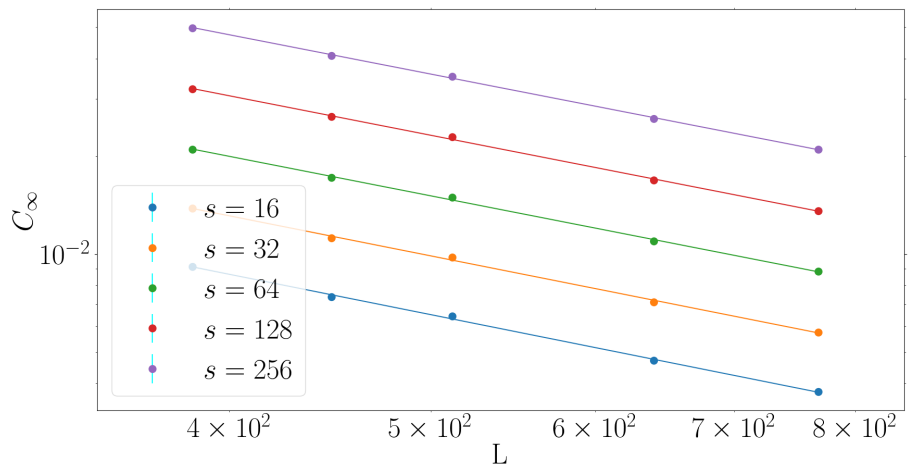
Full equilibration

Parameters:

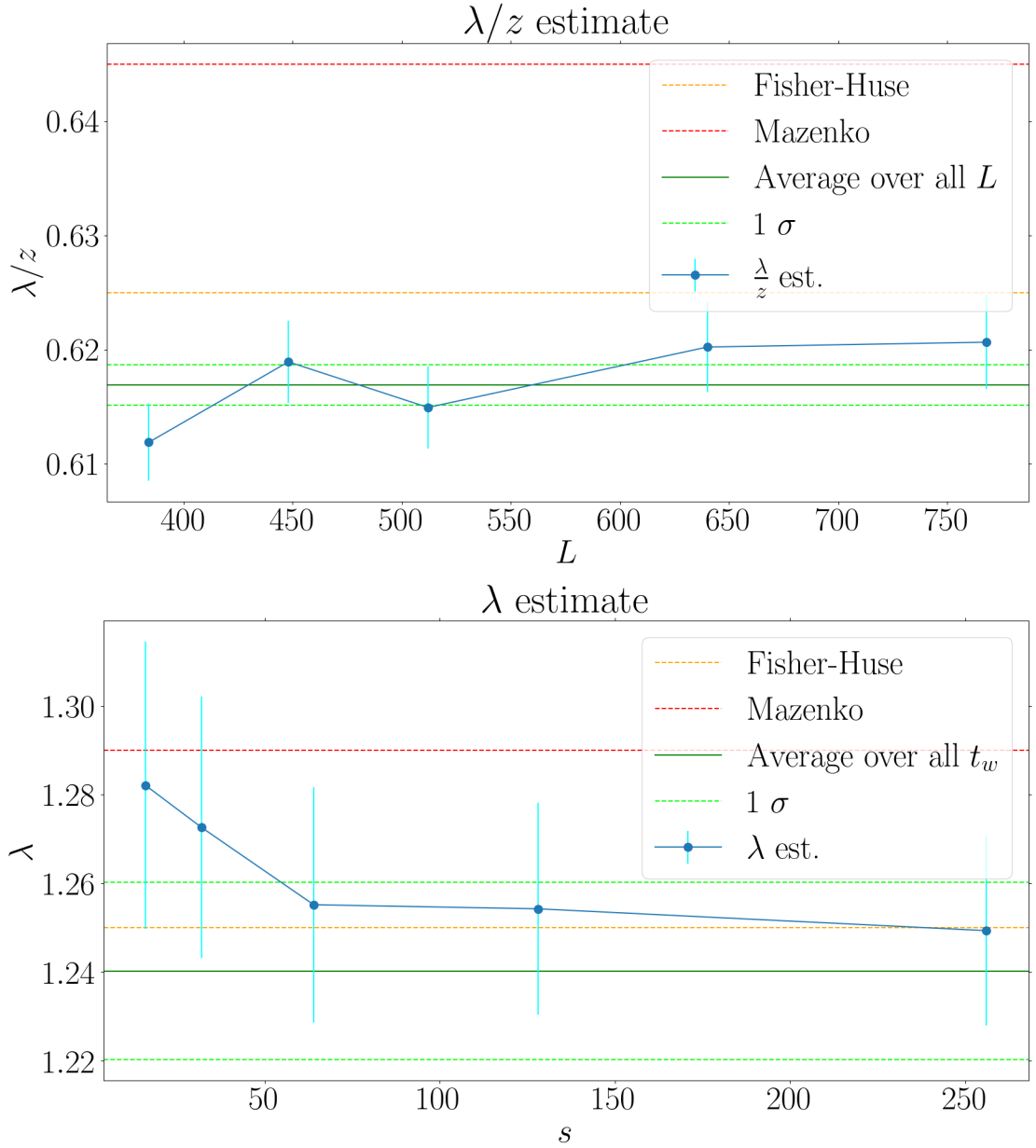
- Temperature $T = 0.2\, T_C$
- Number of distinct initializations: $25\,600$
- waiting times: $s \in \{16, 32, \ldots, 256\}$
- length: $L \in \{384, 448, 512, 640, 768\}$


10^0
10^{-1}
10^{-2}
$C(ys, s)$
10^1
10^3
10^5
10^7
10^9
y
$s = 16$
$s = 32$
$s = 64$
$s = 128$
$s = 256$

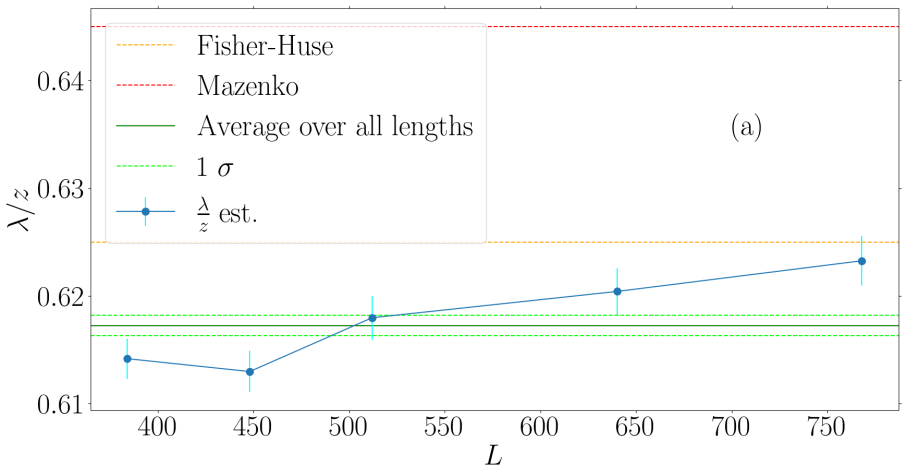

$L = 384$
$L = 448$
$L = 512$
$L = 640$
$L = 768$
C_∞
10^{-2}
10^2
s

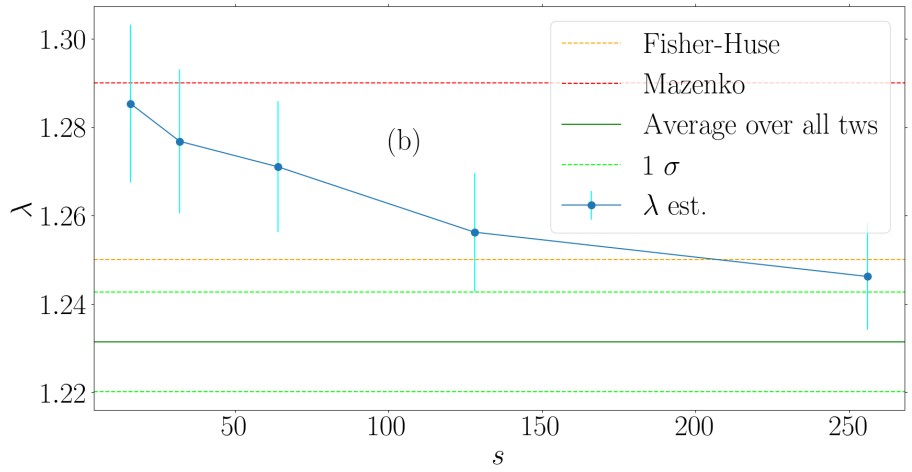

$s = 16$
$s = 32$
$s = 64$
$s = 128$
$s = 256$
C_∞
10^{-2}
4×10^2
5×10^2
6×10^2
7×10^2
8×10^2
L

Full equilibration



Plain estimate at $T = 0.1 T_C$



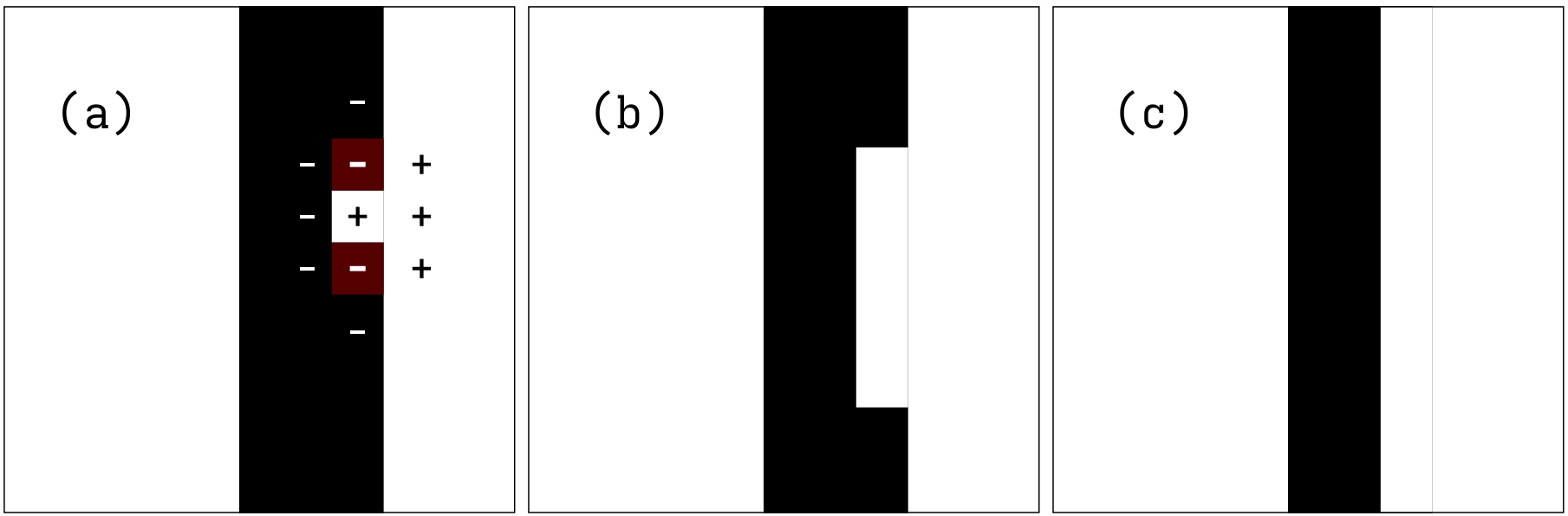


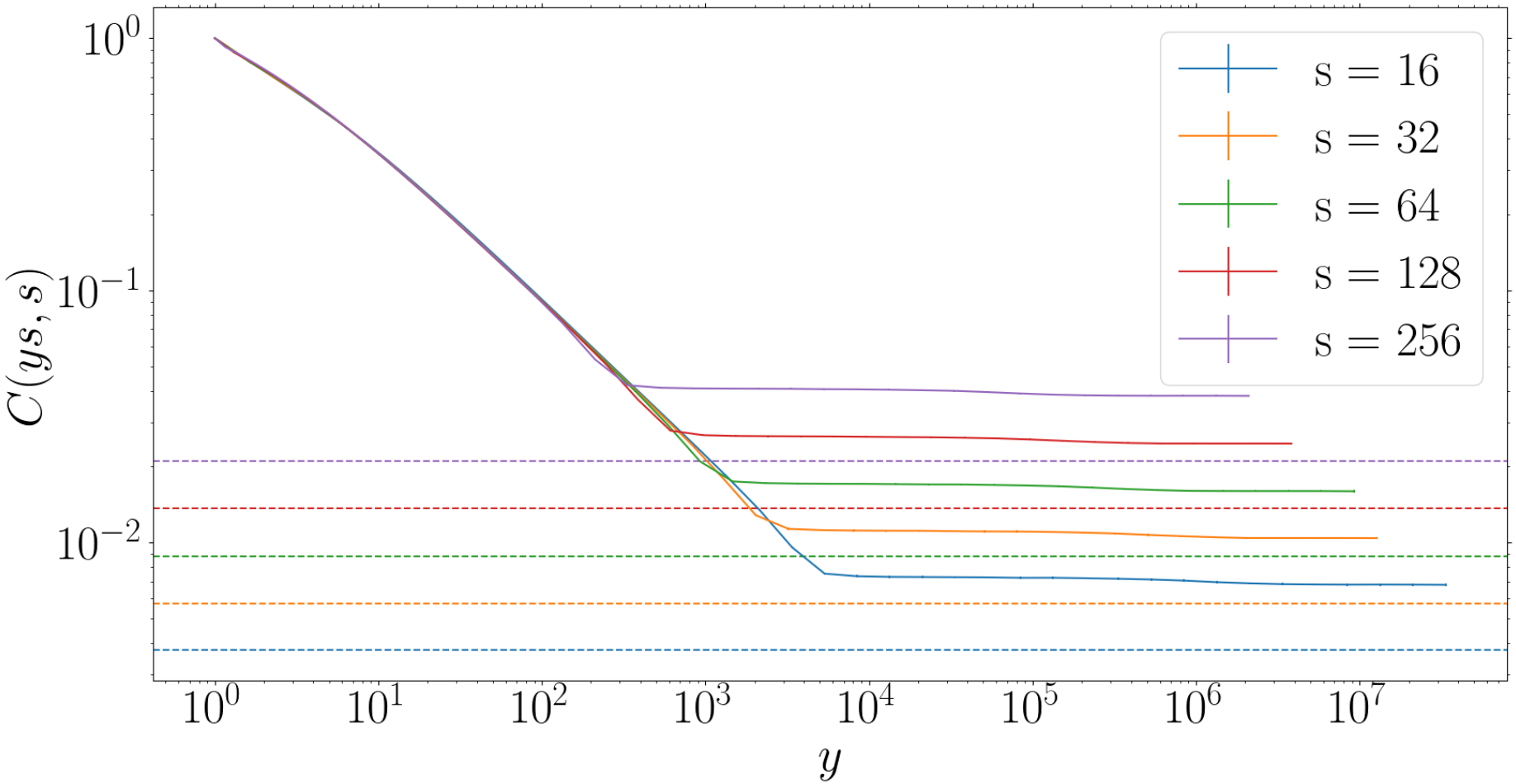
Metastable states as premature finite-size effects

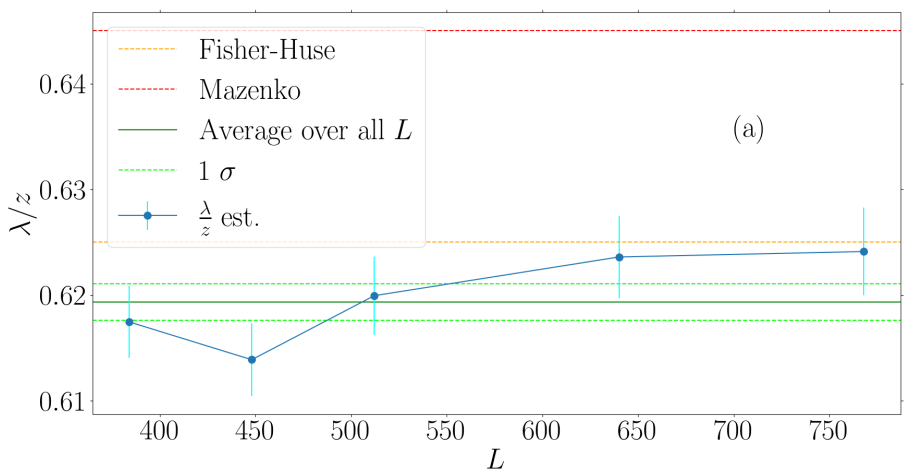
- Estimates fully compatible
- $C(ys, s) \sim \left(\frac{L - w(L)}{s^{1/z}}\right)^{-\lambda}$
- $\frac{C_\infty}{L^{-\lambda}} \sim \left(1 - \frac{w(L)}{L}\right)$
- Diagonal stripes must evaporate beforehand

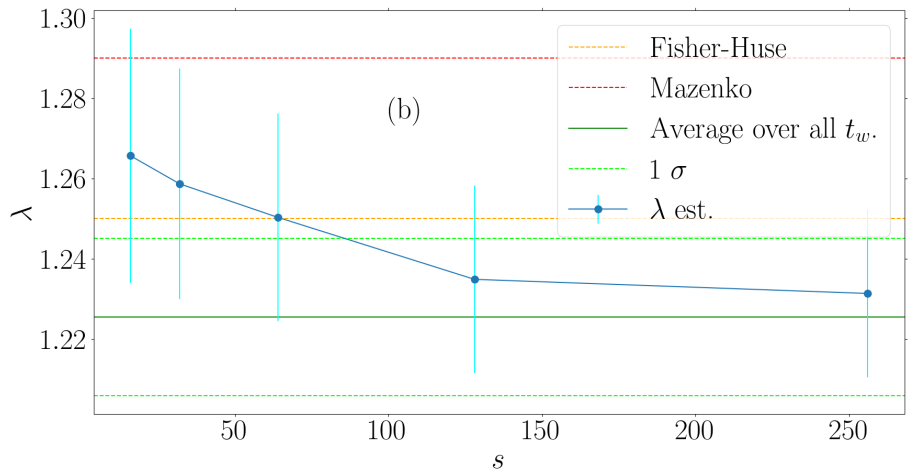
Statistically equilibrate stripes

- $T = 0.1\ T_C$
- Based on probability that majority phase dominates
- Only works, since **even** stripes can be described as columns of $1D$ random walks
- $\Longrightarrow$ Revisit metastable states and randomly assign a fully-aligned state via $p_{\text{minor}} \approx \frac{w}{L}$




$C(ys, s)$
y
s = 16
s = 32
s = 64
s = 128
s = 256


Fisher-Huse
Mazenko
Average over all L
1 σ
$\frac{\lambda}{z}$ est.
(a)
λ/z
L


Fisher-Huse
Mazenko
Average over all t_w.
1 σ
λ est.
(b)
λ
s

Summary:

- Estimates are fully compatible to other variants
- Fate of metastable states can be estimated **without** full equilibration

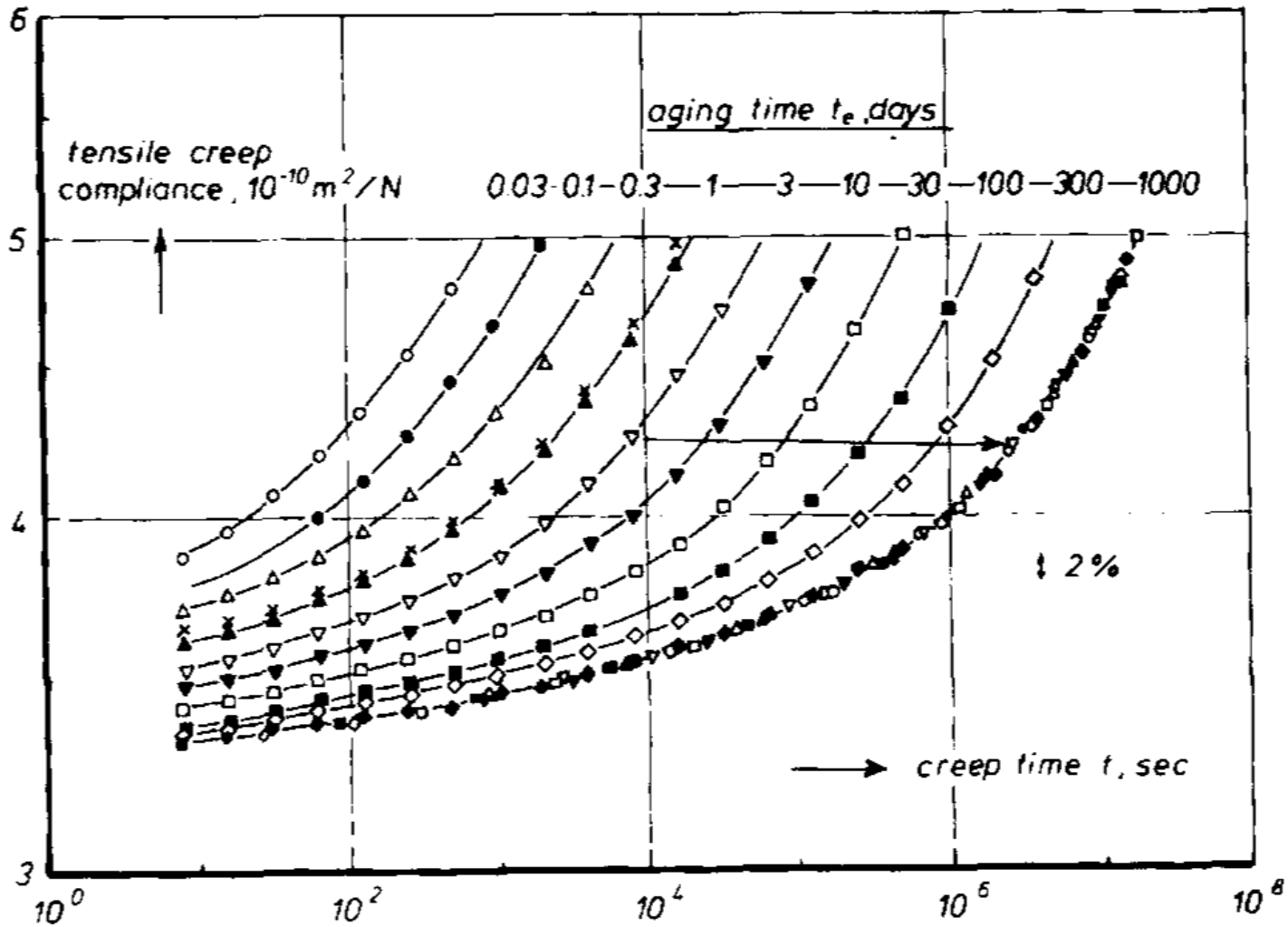
However: Only usable on very low temperatures with solely rectangular stripes

Conclusion

- Development and honing of method to estimate exponents λ and z using deliberately small lattice sizes
- Mathematically simple structure allows spotting systematic errors, especially compared to direct fitting
- Role of metastable states in aging processes
- Things to keep in mind:
  - Only valid for specific s and L ranges
  - Simulations and experiments must be performed until equilibration, if possible
  - Demand for homogeneity between different L is obligatory and not always possible ($3D$ Ising, Potts model ?)

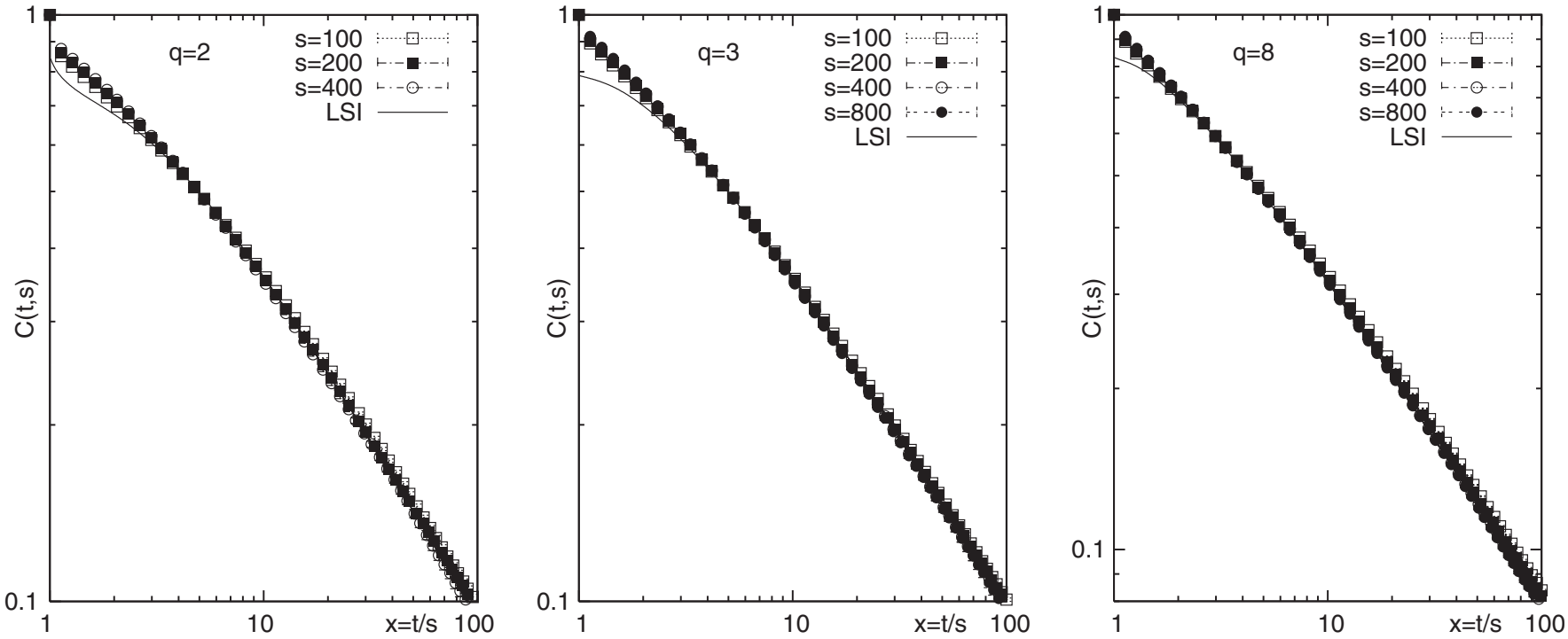
Thank you

Thank you for your attention!



Physical aging of PVC (reproduced from[2])

[2] L. C. E. Struik. "Physical Aging in Plastics and Other Glassy Materials." In: *Polymer Engineering & Sci* 17.3 (1977), pp. 165–173. DOI: 10.1002/pen.760170305.



Fit via local scale invariance (reproduced from[3])

[3] E Lorenz and W Janke. "Numerical Tests of Local Scale Invariance in Ageing Q-State Potts Models." In: *Europhys. Lett.* 77.1 (2007), p. 10003. DOI: 10.1209/0295-5075/77/10003.

Bibliography I

Almeida, Renan A. L. and Kazumasa A. Takeuchi. "Phase-Ordering Kinetics in the Allen-Cahn (Model A) Class: Universal Aspects Elucidated by Electrically Induced Transition in Liquid Crystals." In: *Phys. Rev. E* 104.5 (2021), p. 054103. DOI: 10.1103/PhysRevE.104.054103.

Henkel, Malte. "Non-Equilibrium Relaxations: Ageing and Finite-Size Effects." In: *Condens. Matter Phys.* 26.1 (2023), p. 13501. DOI: 10.5488/CMP.26.13501. arXiv: 2211.03657 [cond-mat, physics:hep-th, physics:math-ph].

— ."Generalised Time-Translation-Invariance in Simple Ageing." In: *hal-04377461* (2024).

Müller, Fabio et al. "Fast, Hierarchical, and Adaptive Algorithm for Metropolis Monte Carlo Simulations of Long-Range Interacting Systems." In: *Phys. Rev. X* 13.3 (2023), p. 031006. DOI: 10.1103/PhysRevX.13.031006.

Bibliography II

Struik, L. C. E. "Physical Aging in Plastics and Other Glassy Materials." In: *Polymer Engineering & Sci* 17.3 (1977), pp. 165–173. DOI: 10.1002/pen.760170305.

Low, Ze-Xian et al. "Gas Permeation Properties, Physical Aging, and Its Mitigation in High Free Volume Glassy Polymers." In: *Chem. Rev.* 118.12 (2018), pp. 5871–5911. DOI: 10.1021/acs.chemrev.7b00629.

Lorenz, E and W Janke. "Numerical Tests of Local Scale Invariance in Ageing Q-State Potts Models." In: *Europhys. Lett.* 77.1 (2007), p. 10003. DOI: 10.1209/0295-5075/77/10003.