Analysis of the Mpemba effect in magnetic systems

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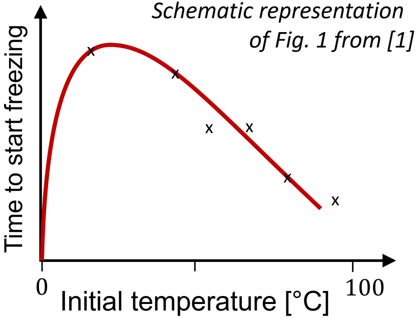
Mpemba Effect



[1] Mpemba, E.B. and Osborn, D.G. (1969) Phys. Educ. 4:172

Mpemba and Osborne (1969)

- Two equally prepared water samples with different $T_s > 0°$C
- Bring in contact with a bath of temperature below $0°$C (temperature quench)
- Counterintuitive effect:
  hotter sample freezes faster than colder sample
- Required condition: phase transition

Mpemba Effect

- Various investigations on this topic[2]
- No satisfactory general explanation to date
- Possible relevant effects
  - Evaporation, convection, supercooling, dissolved gases, . . .

Observed in various other systems[3]

- Granular fluid
- Magnetoresistance manganites
- Carbon nanotube resistors
- Spin glasses
- **Ising model**[4] / Potts model
- . . .

[2] Burridge, H.C. and Linden, P.F. (2016) *Sci. Rep.* 6:37665
[3] Kumar, A. (2022) *Anomalous Relaxation in Colloidal Systems* Springer
[4] Vadakkayil, N. and Das, K. (2021) *PCCP* 23:11186

Mpemba-Effect in Ising model

Is there a Mpemba effect in the coarsening of the 2D Ising model?

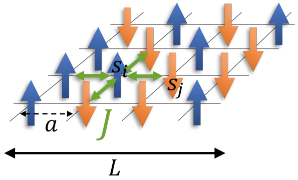
Agenda:

1. Introduction to 2D Ising model
2. Simulation setup of quench process and observables
3. Analysis, results and discussion
4. Summary

2D Ising model

- Ising model with nearest-neighbor interaction strength J

$$H(\sigma) = -J \sum_{\langle i,j \rangle} s_i\, s_j \qquad \text{with } s_i = \pm 1$$

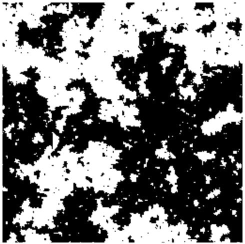


2D square lattice with lattice sites i, lattice constant $a = 1$, $J = 1$, and system size L

- Order parameter is magnetization M

$$M(\sigma) = \sum_i s_i$$

with phase transition at $T_\text{c} = \frac{2}{\ln(1+\sqrt{2})} = 2.26919$



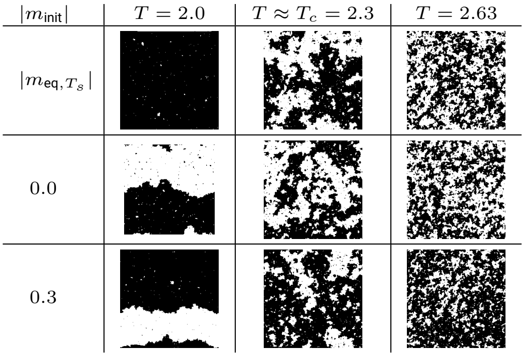
Spin configuration: $L = 256, T = 2.3$

Simulation setup of quench process

Protocol for quench process:

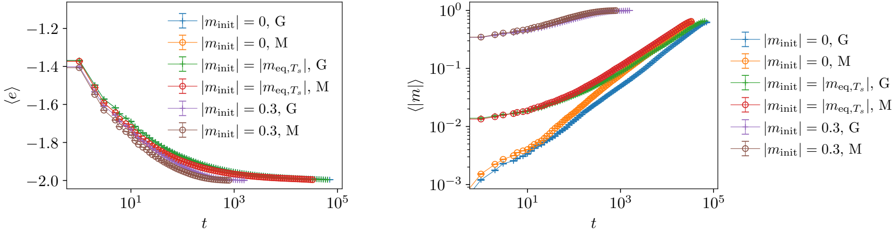
- Initialization: Random spins or fixed given magnetization
- Equilibration: Monte Carlo dynamics (Metropolis, Glauber, Kawaski) at start temperature T_s with $T_s < T_c$ and $T_s > T_c$
- Instantaneous quench: set temperature to $T_q < T_c$ and $T_q < T_s$
- Relaxation: Monte Carlo dynamics (Metropolis, Glauber) at T_q

Typical configurations after equilibration process:



Observables

1. Energy per spin $\langle e \rangle$ (N ...realizations): $$\langle e \rangle = \frac{1}{N} \sum_{\sigma} \frac{H(\sigma)}{L^2}$$
2. (Absolute) magnetization per spin $\langle |m| \rangle$: $$\langle |m| \rangle = \frac{1}{N} \sum_{\sigma} \frac{|M(\sigma)|}{L^2}$$



Example:
$L = 512$,
$T_s = 2.5, T_q = 0$,
Glauber dyn. (G),
Metropolis dyn. (M)

$\Rightarrow$ Results for Glauber dynamics are shown subsequently.

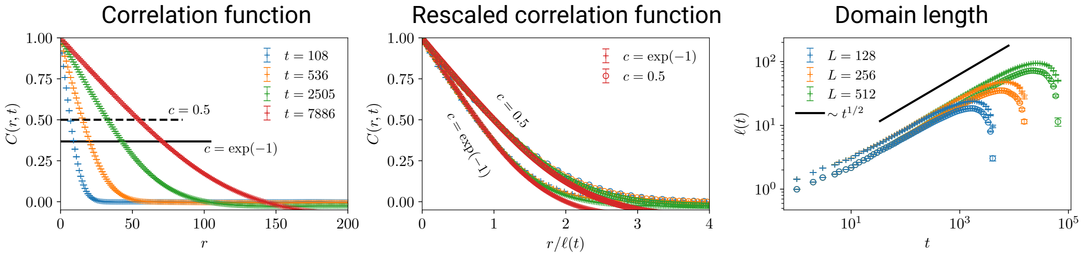
Observables for quench process

1. Energy per spin $\langle e \rangle$ (N ...realizations):
$$\langle e \rangle = \frac{1}{N} \sum_{\sigma} \frac{H(\sigma)}{L^2}$$
2. (Absolute) magnetization per spin $\langle |m| \rangle$:
$$\langle |m| \rangle = \frac{1}{N} \sum_{\sigma} \frac{|M(\sigma)|}{L^2}$$
3. Average domain length $\ell(t)$ with asymptotic scaling (Allen-Cahn-growth):
$$\ell(t) \sim t^{\alpha}, t = 1/2 \quad \leftrightarrow \quad C(r,t) = \hat{C}(r/\ell(t))$$
4. Two-point autocorrelation function $C(r,t)$:
$$C(r,t) = \langle s_i \, s_j \rangle - \langle s_i \rangle \langle s_j \rangle \quad \text{with } r = |\vec{i} - \vec{j}|$$

Determining domain growth

Quenching of system leads to coarsening of spin domains, i.e. growth of $\ell(t)$

- Extraction of $\ell(t)$ from $C(r,t) = c$
- Rescaling of $C(r,t)$ leads to data collapse
- Asymptotic scaling: $\ell(t) \sim t^{\alpha}$ with $\alpha = 1/2$ (and here finite size effect)
- Example: Glauber Dyn., $L = 512$, $T_s = 3.03$, $T_q = 0.0$, $|m_{\text{init}}| = 0$



$\Rightarrow$ Results for $c = 0.5$ are shown subsequently.

Mpemba Effect?

Question of interest:

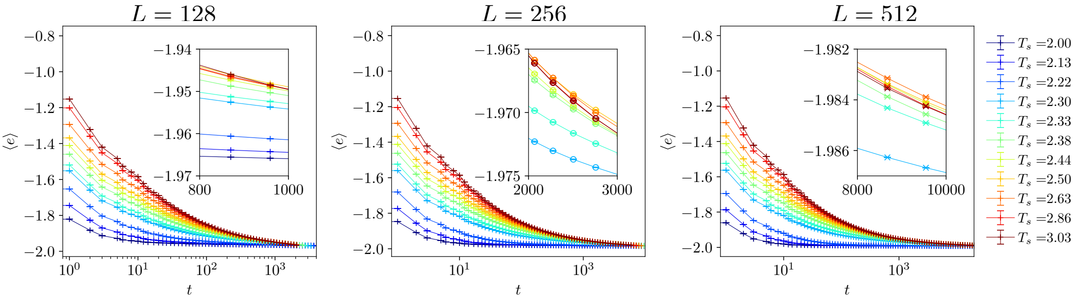
- What is observed when comparing different initial T_s over time?
- Does it persist over different length scales?
- How does the initial magnetization influence the process?

Simulation parameters shown:

- System sizes: $L = 128, 256, 512$
- Starting temperatures: $T_s = 2.0, \ldots, 2.3, \ldots 3.03$
- Quench temperature: $T_q = 0$
- Initial magnetization: $|m_{\text{init}}| = 0., 0.1$ and $|m_{\text{init}}| = |m_{\text{eq},T_s}|$
- Dynamics: Glauber (G) with single spin flip
- Realizations $N = 200$ per each combination

Mpemba effect? Scenario with $T_q = 0$ and $|m_{\text{init}}| = 0$

Energy per spin for different system sizes



- Crossing of $\langle e \rangle$-curves for $T_s > 2.4 \rightarrow$ Mpemba effect $\rightarrow$ Consistent with Vadakkayil and Das[4]

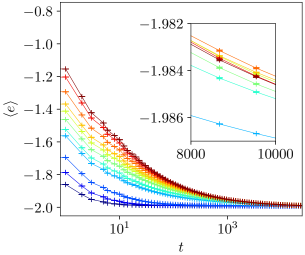
  [4] Vadakkayil, N. and Das, K. (2021) *PCCP* 23:11186
- Not all temperature combinations show a crossing $\rightarrow$ Does it depend on system size?

Observation of Mpemba effect for energy! What happens for other observables?

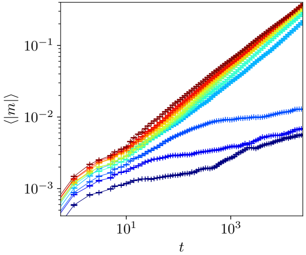
Mpemba effect? Scenario with $T_q = 0$ and $|m_{\text{init}}| = 0$

Different observables over t for $L = 512$

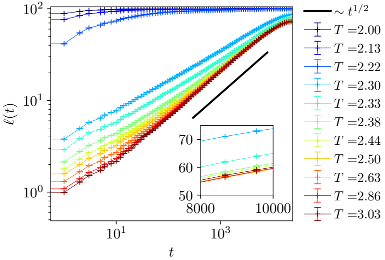
energy per spin



magnetization per spin



Domain length

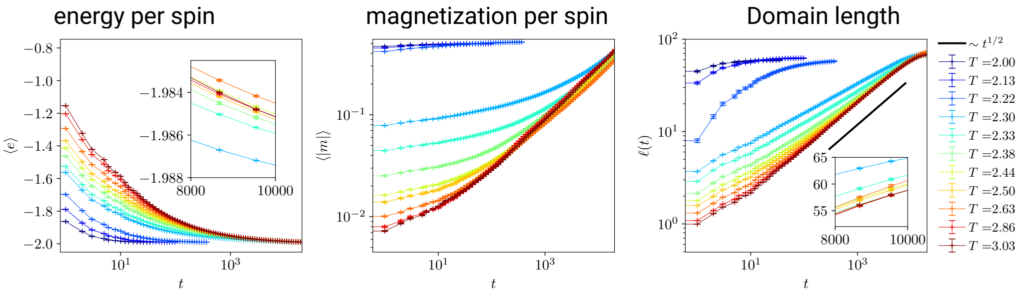


- The higher T_s the faster $\langle|m|\rangle$ increases $\rightarrow$ effect due to the constrain $|m_{\text{init}}|$
- Only for higher T_s $\ell(t) \approx t^{1/2}$ $\rightarrow$ crossings of $\ell(t)$ existent but larger L for analysis necessary

How does the fixed initial $|m|$ influence the Mpemba effect?

Mpemba effect? Scenario with $T_q = 0$ and $|m_{\text{init}}| = |m_{\text{eq},T_s}|$

Different observables over t for $L = 512$ at equilibrated $|m_{\text{init}}|$



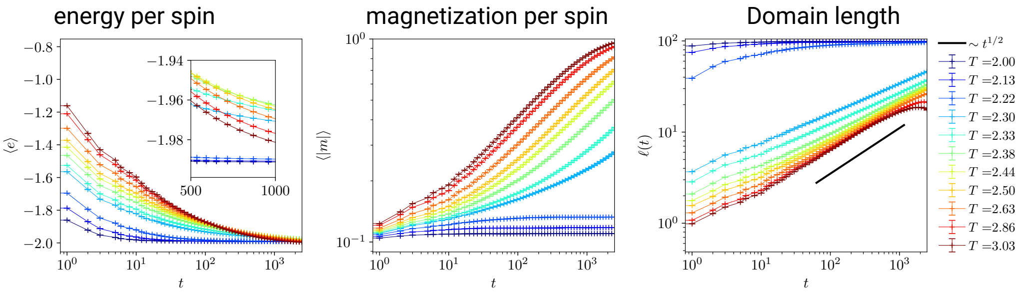
- $T_s = 2.63$ shows "slowest" cooling and different order of crossing → Mpemba effect to some extent
- Different initial time behavior of $\langle |m| \rangle$ but same long time behavior
- Idea from Lu and Raz[5]: Energy barriers in the energy landscape hinder the fast cooling for lower T_s while quenching

[5] Lu, Z. and Raz, O. (2017) *PNAS* 114(20):11186

Do the different $|m_{init}|$ influence the coarsening? What happens for a fixed $|m_{\text{init}}| > 0.0$?

Mpemba effect? Scenario with $T_q = 0$ and $|m_{\text{init}}| = 0.1$

Different observables over t for $L = 512$

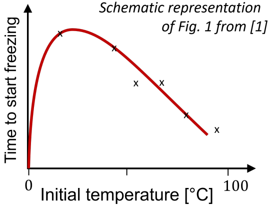


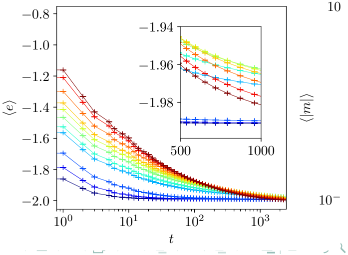
- Inversion of all $\langle e \rangle$ curves for earlier times $\rightarrow$ Clear Mpemba effect
- Magnetization of higher T_s grows faster
- Similar behavior of $\ell(t)$

Clear observation of Mpemba effect for small initial magnetization!

Summary

- Mpemba effect for the 2D Ising model:
  - ✓ for different length scales
  - ✓ for different update dynamics
  - ✓ for different initial magnetization
  - ✗ for all initial temperature
- First Take Home Message:
  - Phase transition is required
  - Initial magnetization plays a crucial role
- Outlook:
  - Detailed analysis of intermediate domain growth exponent and finite size scaling.
  - Investigation of influence of energy barriers and metastable state on quench process.



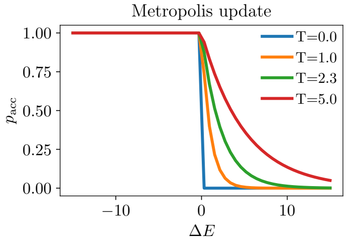


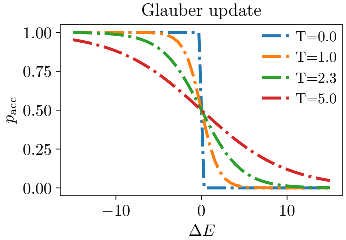
Summary

2D Ising model - Spin dynamics

Monte Carlo (MC) methods for spin dynamics at T:

- Choose a (random) site i
- Determine energy difference $\Delta E = H(\sigma) - H(\sigma')$ if spin s_i would be flipped
- Accept new configuration σ' with probability p_{acc}
  1. Metropolis update: $p_{\text{acc}} = \min\left(1, \exp\left(-\frac{\Delta E}{k_{\text{B}}T}\right)\right)$
  2. Glauber update: $p_{\text{acc}} = \frac{1}{1+\exp\left(\frac{\Delta E}{k_{\text{B}}T}\right)}$
- Repeat all steps L^2 times
  $\Rightarrow$ One Monte Carlo sweep (MCS)





2D Ising model - Spin dynamics

Monte Carlo methods for spin dynamics at T:

- Choose a (ra)one/two sites i
  1. a random site i (Random)
  2. the next site i in a list (Typewriter)
  3. choose two random sites i, j (Kawasaki)
- Determine energy difference $\Delta E = H(\sigma) - H(\sigma')$
  - if spin s_i would be flipped
  - if spins s_i and s_j would be swapped
- Accept new configuration σ' with probability p_{acc}
  1. Metropolis update: $p_{\text{acc}} = \min\left(1, \exp\left(-\frac{\Delta E}{k_B T}\right)\right)$
  2. Glauber update: $p_{\text{acc}} = \frac{1}{1+\exp\left(\frac{\Delta E}{k_B T}\right)}$
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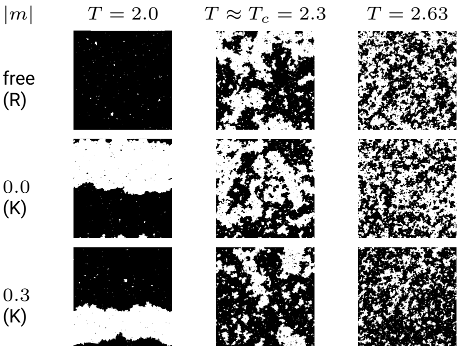


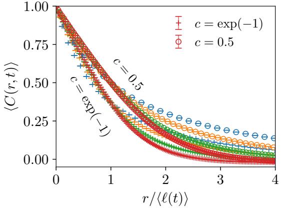
2D Ising model - Equilibration

- (L, t_{eq}): $(128,)$, $(256,)$, $(512,)$

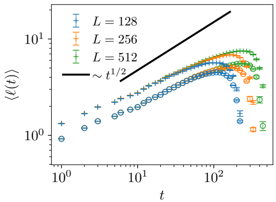
Analysis of domain growth

- Choice of c does not alter power law scaling of $\ell(t)$
  $\rightarrow c = 0.5$
- Metropolis and Glauber update lead to a similar overall behavior $\ell(t)$
  $\rightarrow$ Glauber dynamics
- Initial $T_s < 2.4$ (close to T_c) lead to deviations of $\hat{C}(r,t)$ at short time scales
- An initial $\langle|m|\rangle > 0$ leads to "faster" dynamics, thus larger system sizes are needed

$T_s = 2.33$, $|m_{\text{init}}| = 0$

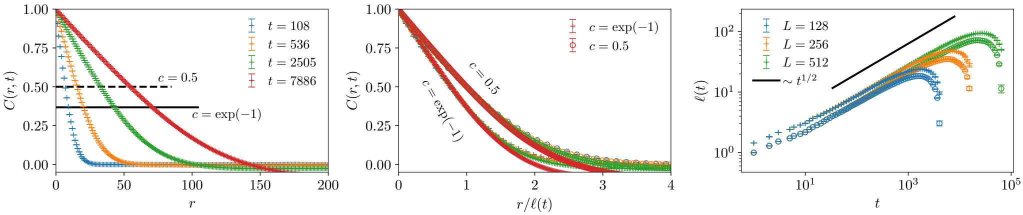


$T_s = 3.03$, $|m_{\text{init}}| = 0.3$



Analysis of domain growth

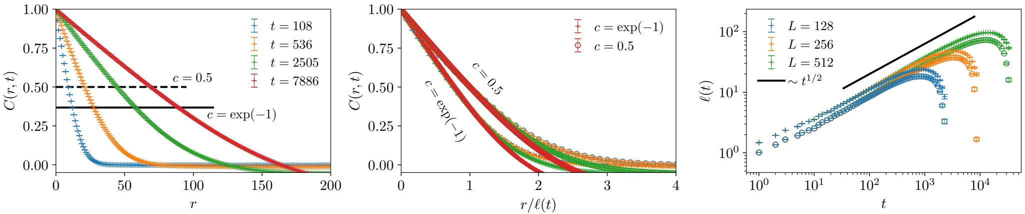
Example: Glauber Dyn., $L = 512$, $T_s = 3.03$, $T_q = 0.0$, $|m_{\text{init}}| = 0$



- Glauber or Metropolis dynamics does not change rescaling or exponential behavior but may shift times/lengths

Analysis of domain growth

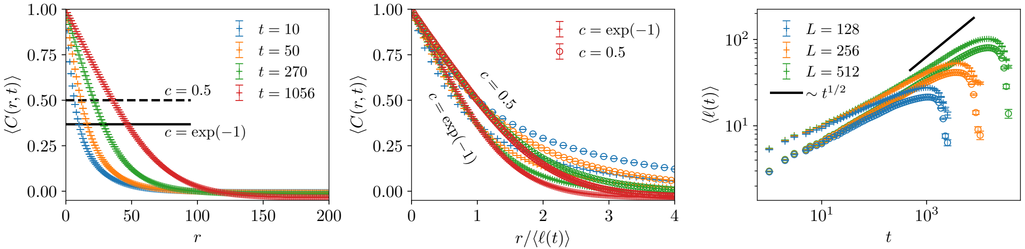
Example: Metropolis Dyn., $L = 512$, $T_s = 3.03$, $T_q = 0.0$, $|m_{\text{init}}| = 0$



- Glauber or Metropolis dynamics does not change rescaling or exponential behavior but may shift times/lengths

Analysis of domain growth

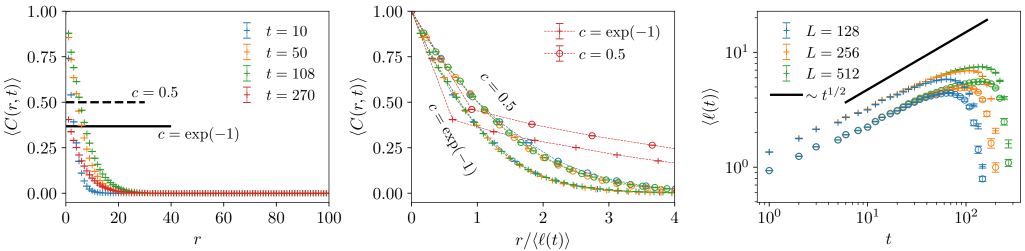
Example close to T_c: Metropolis Dyn., $L = 512$, $T_s = 2.33$, $T_q = 0.0$, $|m_{\text{init}}| = 0$



- CLose to T_c for short times clear deviations for $\hat{C}(r/\ell(t))$ and $\ell(t)$
- Asymptotic scalingof $\ell(t)$ not reached

Analysis of domain growth

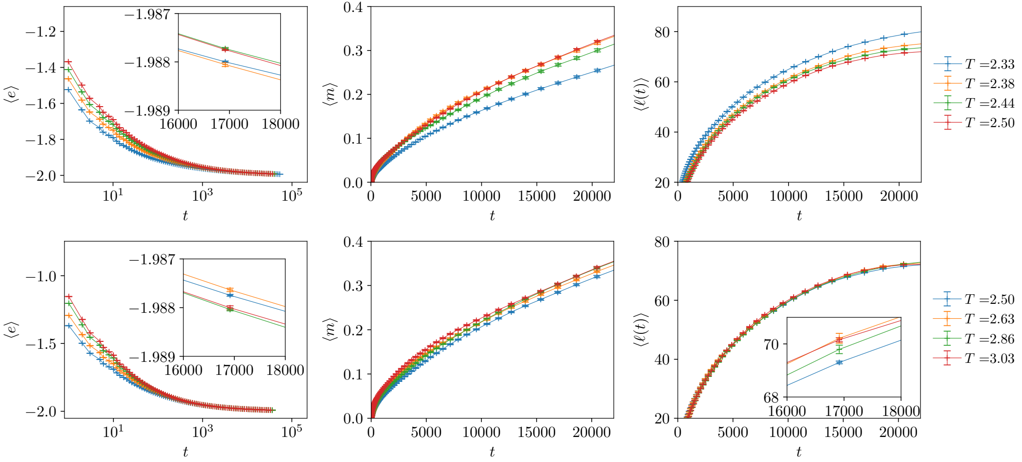
Example with larger inital $\langle |m| \rangle$: Metropolis Dyn., $L = 512$, $T_s = 3.03$, $T_q = 0.0$, $|m_{\text{init}}| = 0.3$



- Larger inital $\langle |m| \rangle$ leads to relative fast dynamics, thus larger system sizes needed
- Asymptotic scaling of $\ell(t)$ not reached

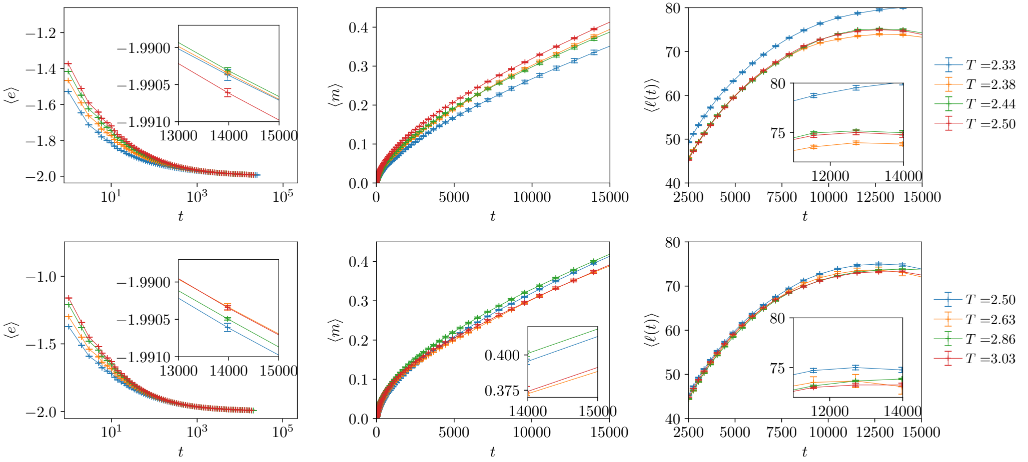
Mpemba effect? Scenario with $T_q = 0$ and $|m_{\text{init}}| = 0$

Observables: Glauber, $L = 512, m = 0$



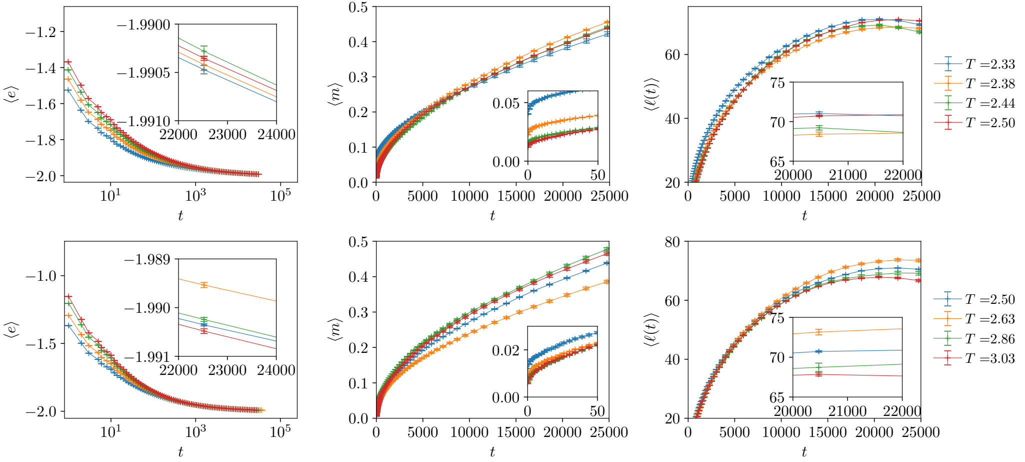
Mpemba effect? Scenario with $T_q = 0$ and $|m_{\text{init}}| = 0$

Observables: Metropolis, $L = 512, m = 0$



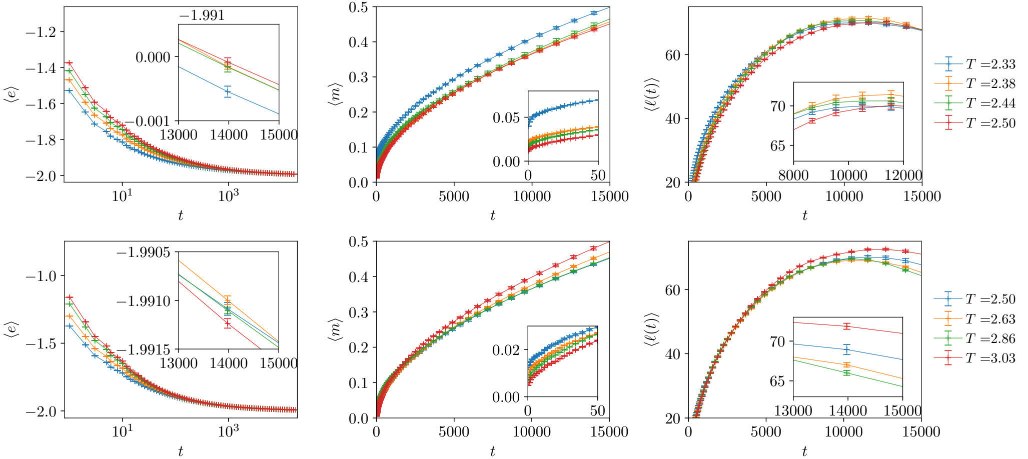
Mpemba effect? Scenario with $T_q = 0$ and $|m_{\text{init}}| \neq 0$

Observables: Glauber, $L = 512, m \neq 0$



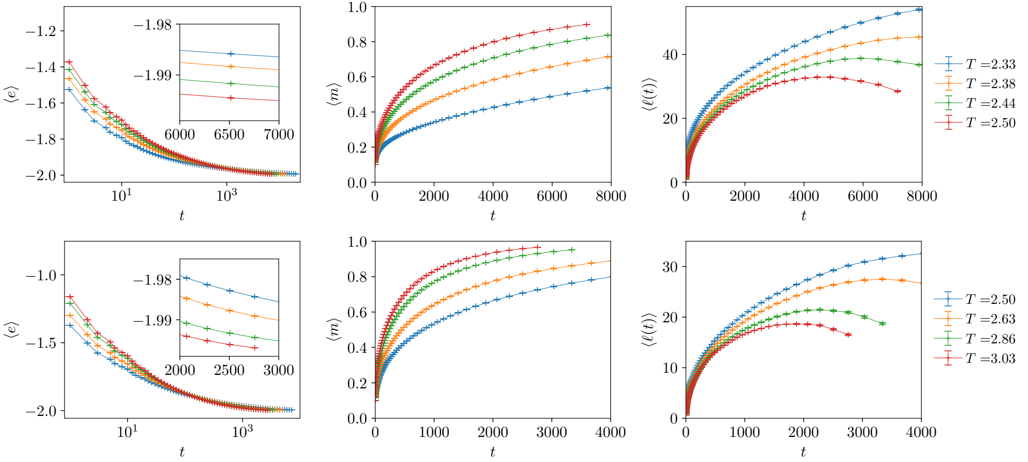
Mpemba effect? Scenario with $T_q = 0$ and $|m_{\text{init}}| \neq 0$

Observables: Metropolis, $L = 512, m \neq 0$



Mpemba effect? Scenario with $T_q = 0$ and $|m_{\text{init}}| = 0.1$

Observables: Glauber, $L = 512, m = 0.1$



Mpemba effect? Scenario with $T_q = 0$ and $|m_{\text{init}}| = 0.1$

Observables: Metropolis, $L = 512, m = 0.1$