University of Trento

Numerical Implementation of the Spherical Model

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Overview

01

INTRODUCTION

Problem statement:

- No one simulated the spherical model before
- I wanted to apply Monte Carlo methods on this model

Process:

- Analytical solutions
- Simulation setup
- Results and problems

Challenges:

- High simulation times
- Best optimisation of the code
- Good algorithm to lower Monte Carlo cycles
- Memory management

02

THE SPHERICAL MODEL

The spherical model generalises the Ising model by allowing spins to take continuous values, constrained by a global condition:

$$\sum_{i}^{N} \sigma_i^2 = N$$

$$\sigma_i \in \Re$$

$$\mathbf{H} = -J \sum_{\text{n.n.}(i,j)} \sigma_i \sigma_j - H \sum_i \sigma_i$$

02

THE SPHERICAL MODEL

The spherical model generalises the Ising model by allowing spins to take continuous values, constrained by a global condition:

$$\sum_{i}^{N} \sigma_i^2 = N$$

$$\sigma_i \in \Re$$

PROS

- Analytically solvable for all dimensions and all temperatures
- Exactly solvable also with a field

CONS

- Risks of not being a physical model
- Defects of a continuum model: at absolute zero, the entropy is infinite and the specific heat non zero

02

THE SPHERICAL MODEL

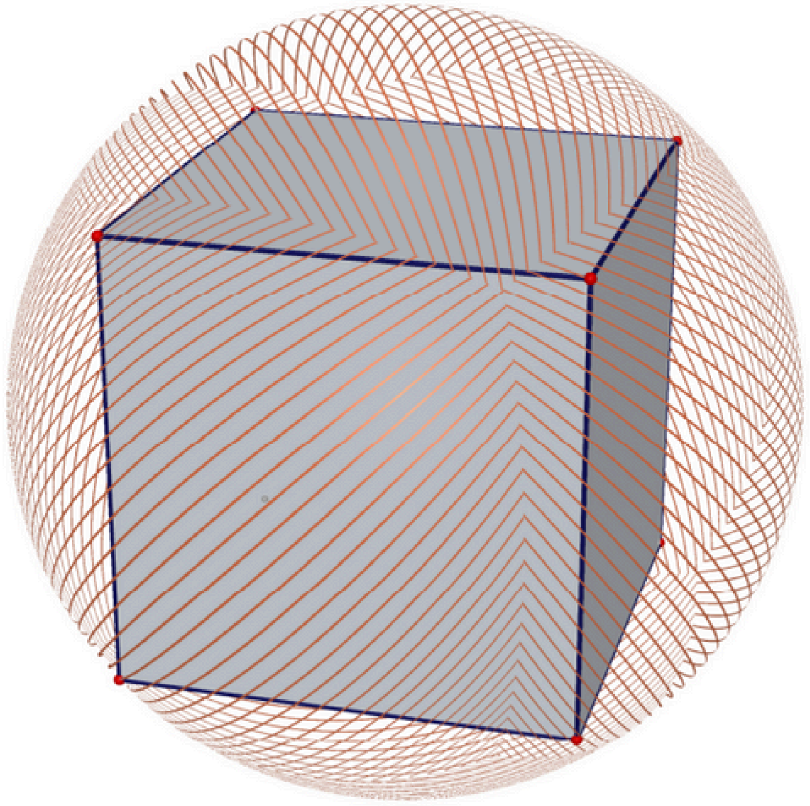
ISING

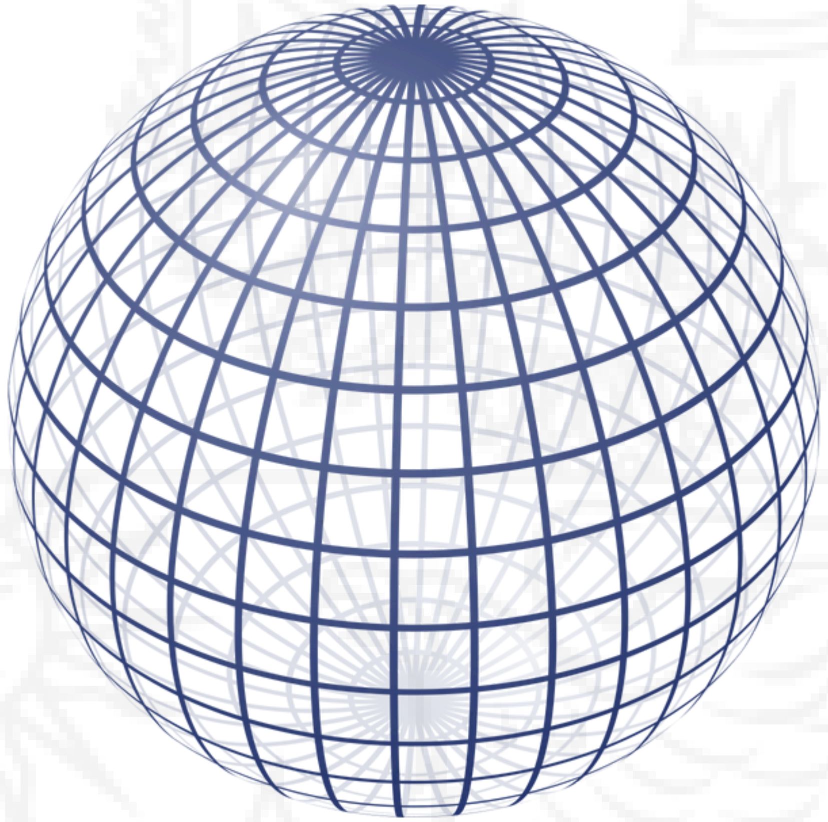
$$\sigma_i \in \{-1, +1\}$$

SPHERICAL

$$\sigma_i \in \Re$$

$$\sum_i^N \sigma_i^2 = N$$





02

THE SPHERICAL MODEL

The internal energy normalised to number of spins:

$$u_- = \frac{1}{2}k_B T - Jd, \qquad \text{for } T < T_c,$$

$$u_+ = \frac{1}{2}k_B T - Jd - Jz_0, \qquad \text{for } T > T_c.$$

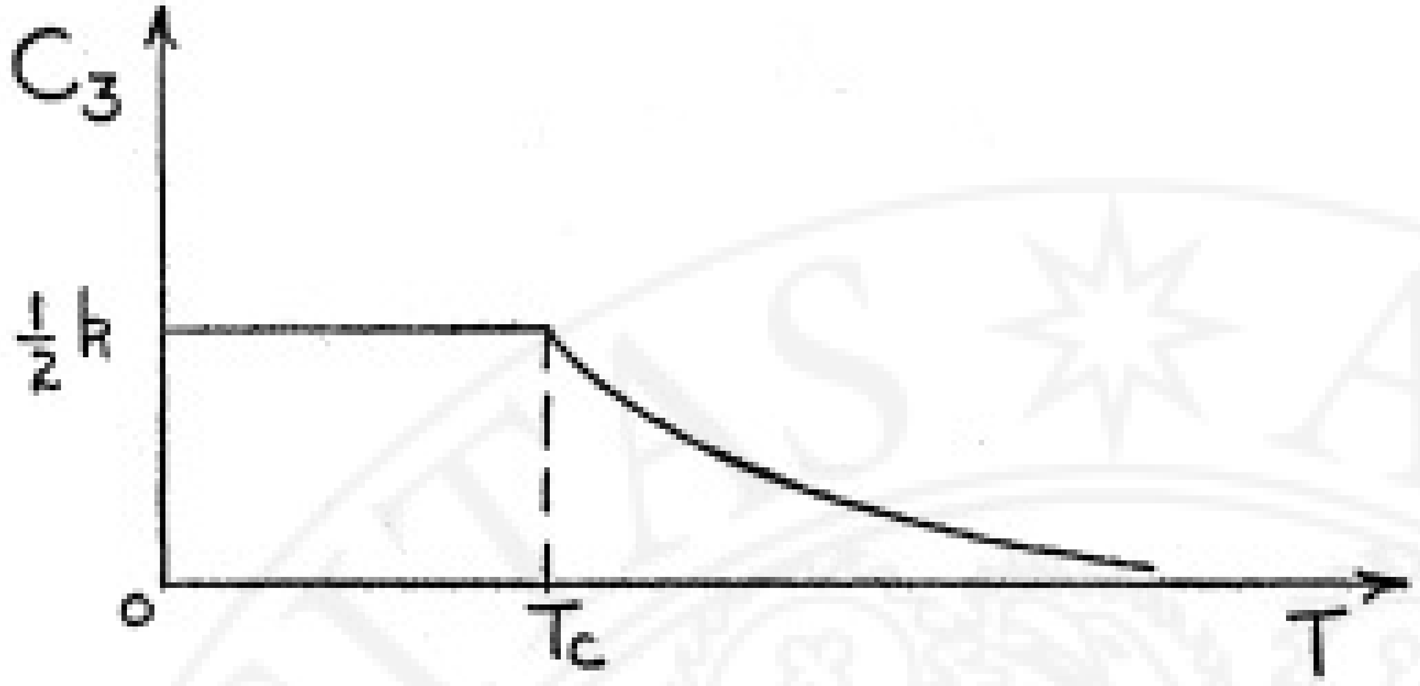
Magnetisation normalised to number of spins:

$$M = \text{sgn}(H)\left(1 - \frac{T}{T_c}\right)^{1/2}, \qquad \text{for } T < T_c,$$

$$M = 0, \qquad \text{for } T > T_c,$$

02 THE SPHERICAL MODEL

Specific heat normalised to number of spins:



constant for $T < T_C$

Susceptibility normalised to number of spins:

diverges for $T = T_C$

03

IMPLEMENTATION IN C++

INTERACTION MATRIX

The matrix is cyclic to represent the Periodic Boundaries Condition and symmetric

$$c_{L^{k-1}+1} = c_{N-L^{k-1}+1} = 1,$$
$$k = 1, 2, \ldots, d$$

$$\begin{pmatrix} c_1 & c_2 & c_3 & \ldots & c_{N-1} & c_N \\ c_N & c_1 & c_2 & \ldots & c_{N-2} & c_{N-1} \\ c_{N-1} & c_N & c_1 & \ldots & c_{N-3} & c_{N-2} \\ . & . & . & \ldots & . & . \\ . & . & . & \ldots & . & . \\ c_2 & c_3 & c_4 & \ldots & c_N & c_1 \end{pmatrix}$$

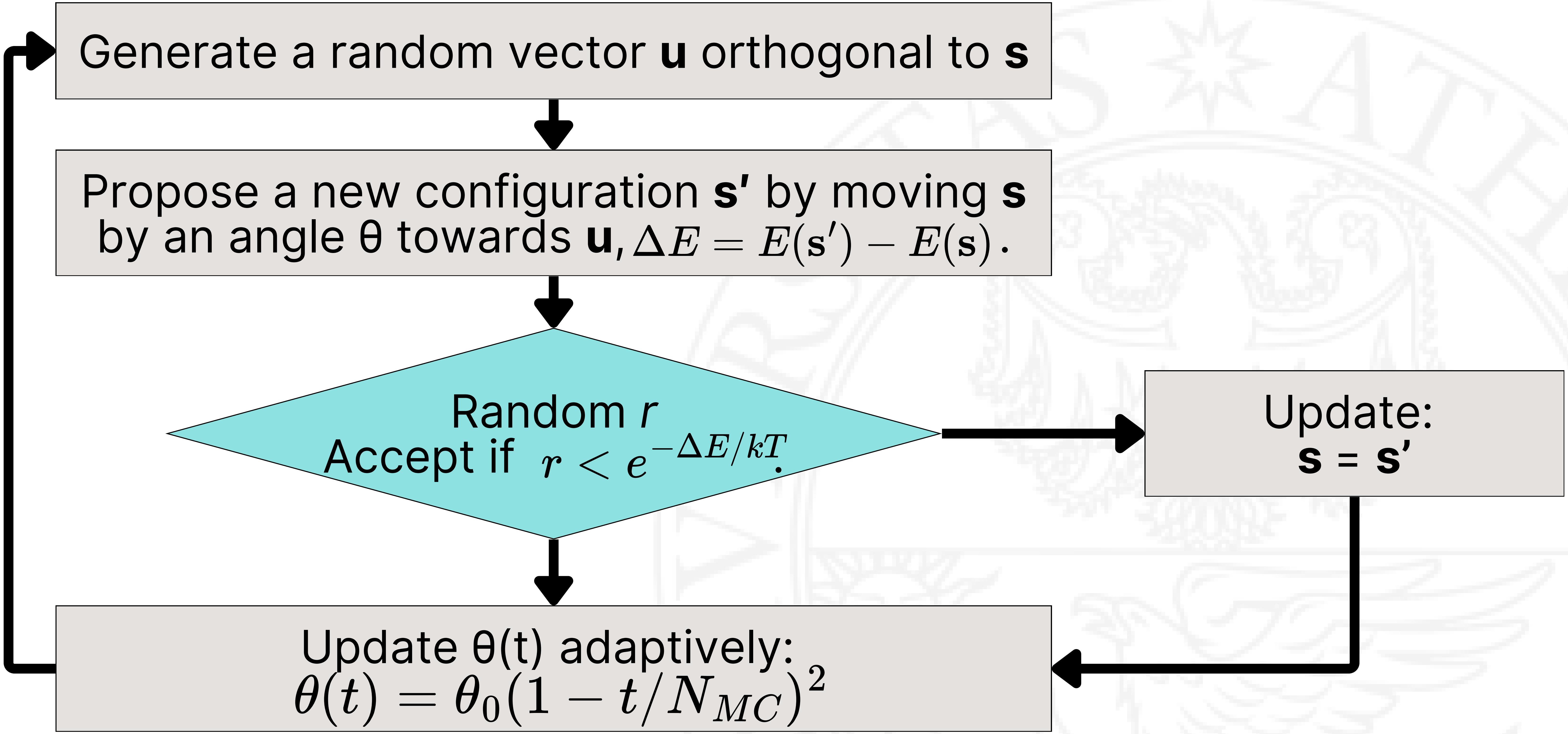
To compute the interaction energy we perform the operation:

$$\bar{\sigma}^t M \bar{\sigma}$$

03

IMPLEMENTATION IN C++

METROPOLIS ALGORITHM

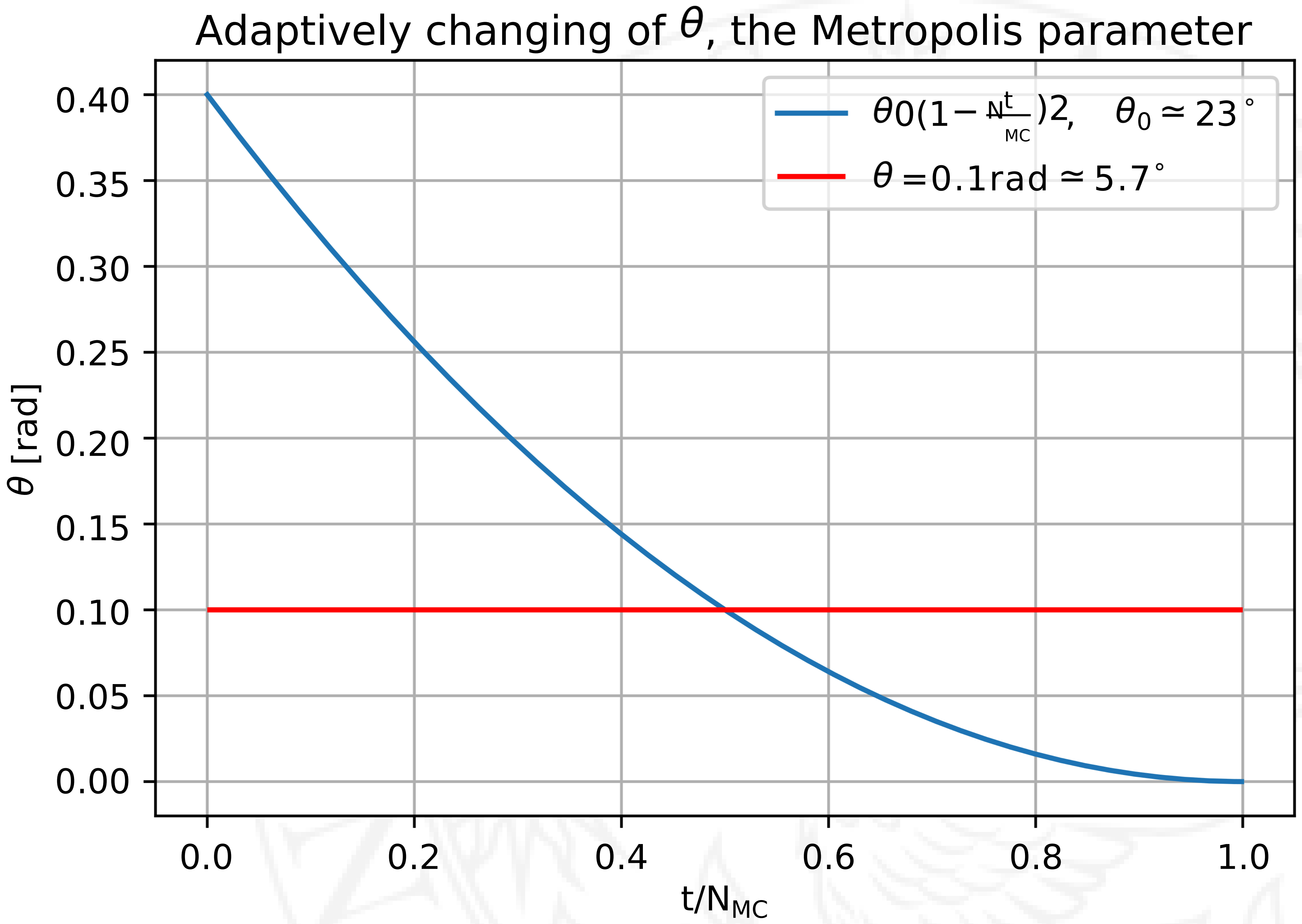


03 IMPLEMENTATION IN C++

METROPOLIS ALGORITHM

3 different strategies

- θ constant at θ=0.1rad
- θ changes adaptively during all the Monte Carlo cycles
- Mixed strategy: change θ adaptively for the first half and then leave it constant to thermalise



03

IMPLEMENTATION IN C++

OPTIMISATION TECHNIQUES

ARMADILLO

- Efficient **linear algebra** operations (like norm computing and matrix operations)
- Efficient **memory storage** for the interaction matrix (SpMat<double>)

OpenMP

- Parallel loop for temperature steps

challenge:

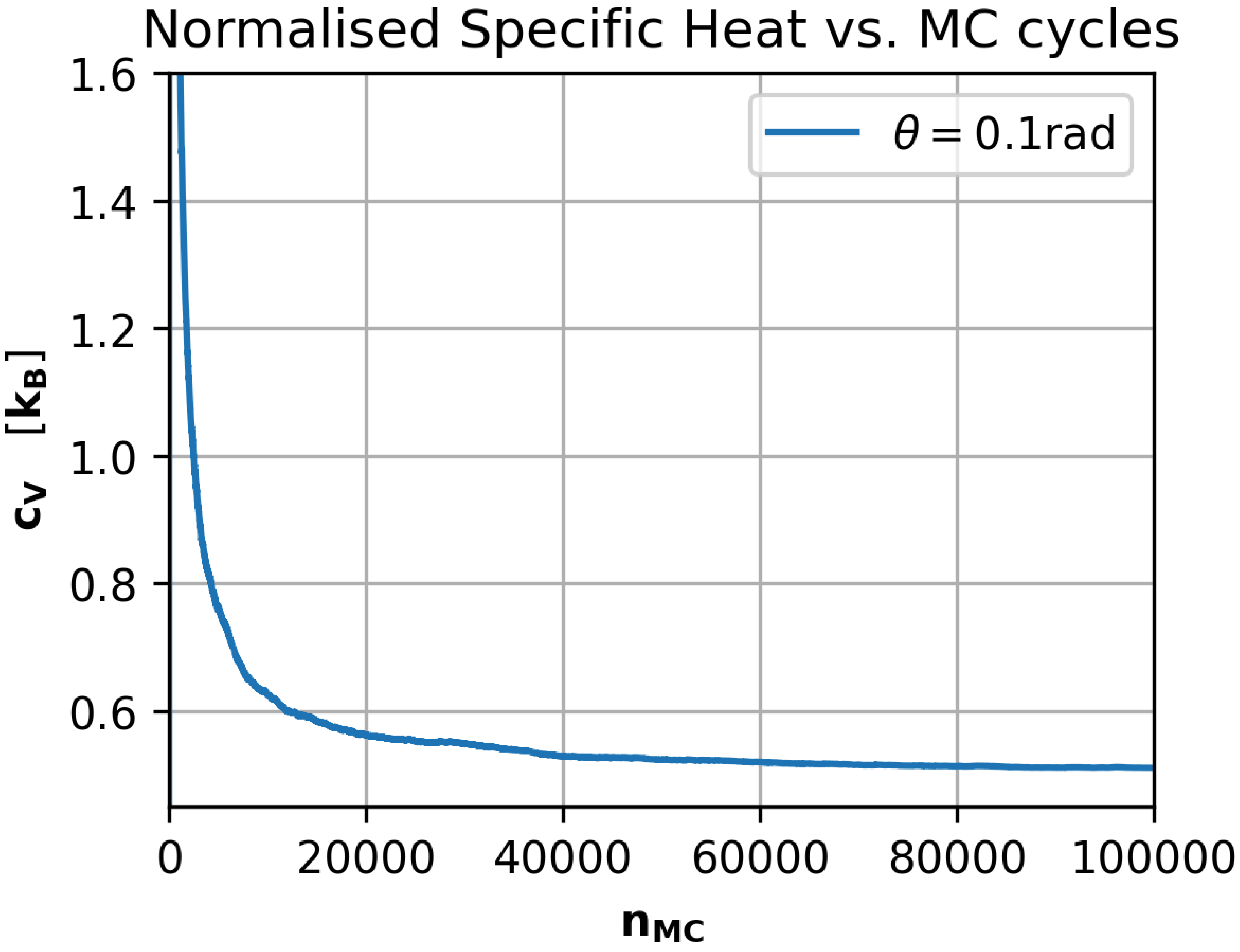
- Managing random seeds for reproducibility
- Risk of memory corruption

04

RESULTS

CONVERGENCE

- Fixed θ at a constant value of θ=0.1rad.



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RESULTS

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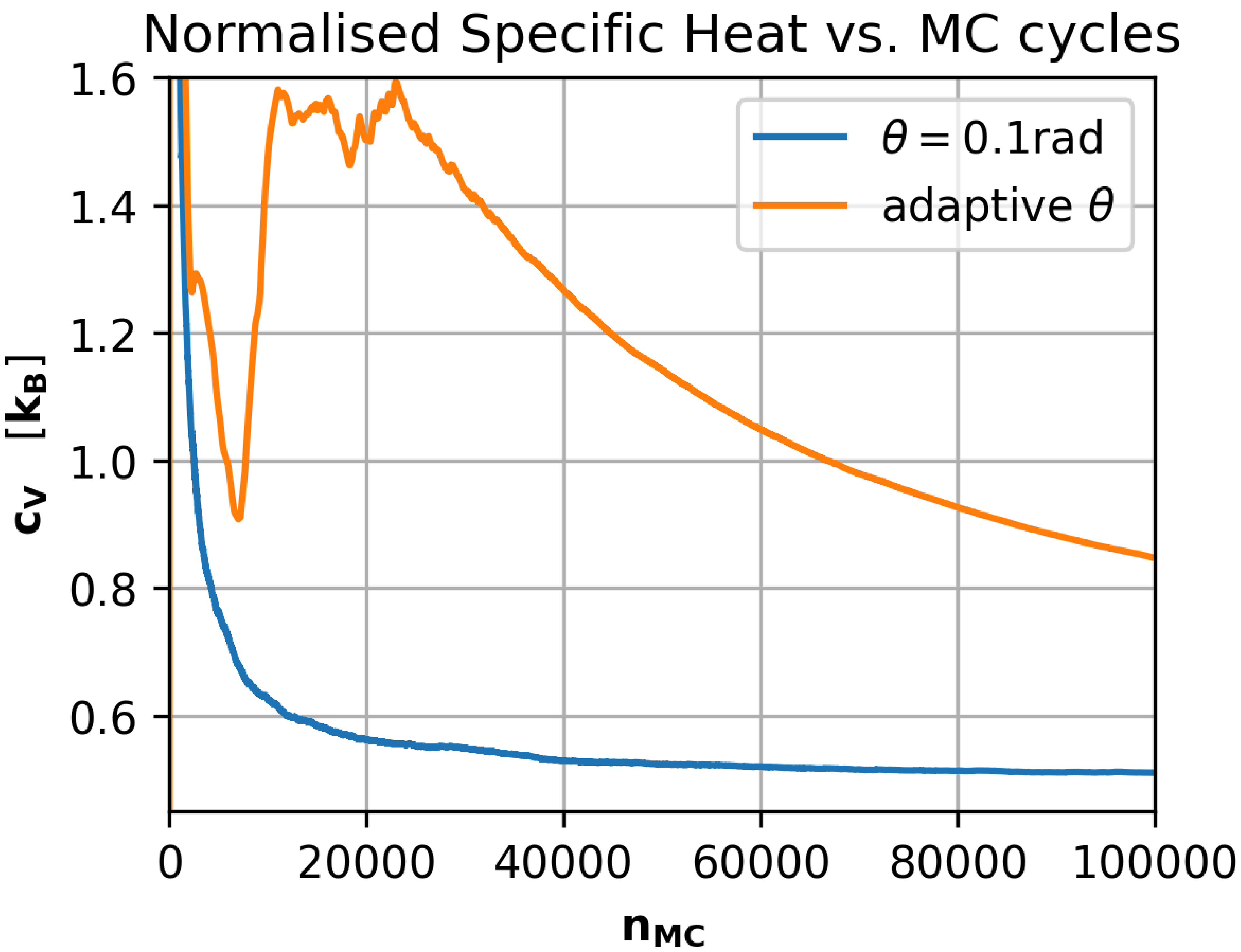
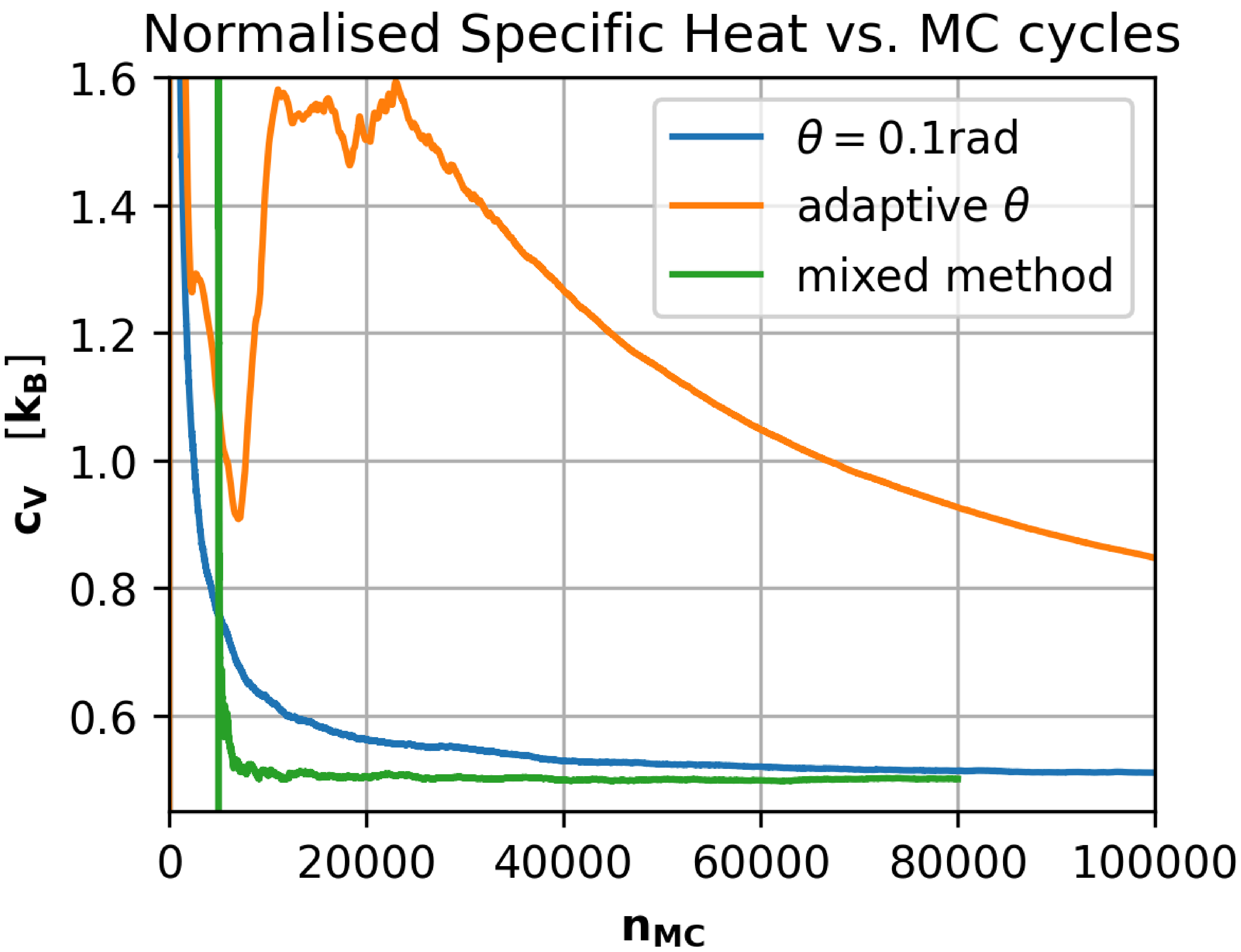


04

RESULTS

CONVERGENCE

- Fixed θ at a constant value of θ=0.1rad;
- θ changes adaptively during all the Monte Carlo cycles;
- θ changes adaptively during the first 5'000 cycles and then remains constant at θ=0.1rad.



04

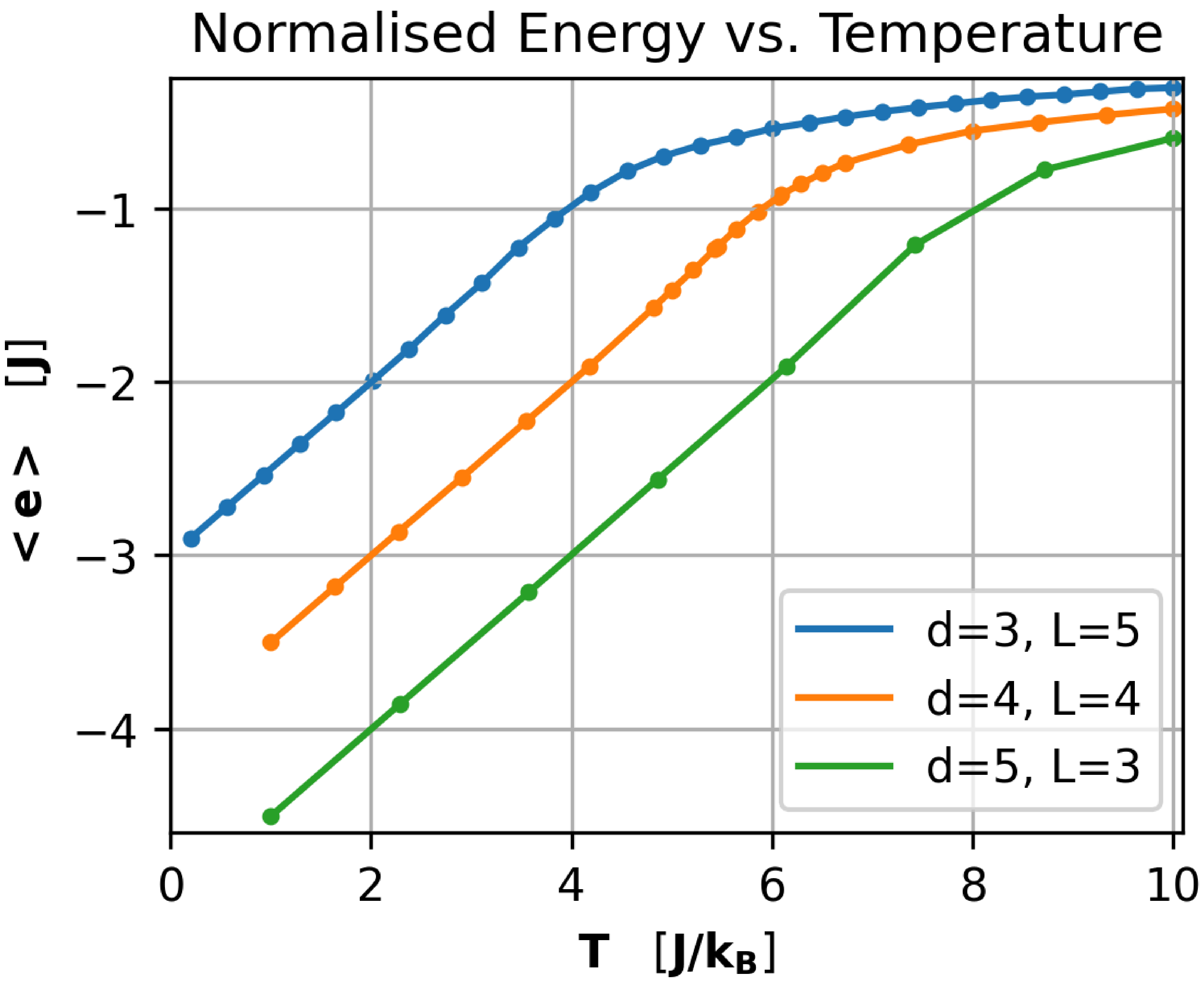
RESULTS

ENERGY

Three simulations at 3 different dimensions:

- **3D:** L=5
- **4D:** L=4
- **5D:** L=3

Zero field (H=0) and J=1



04

RESULTS

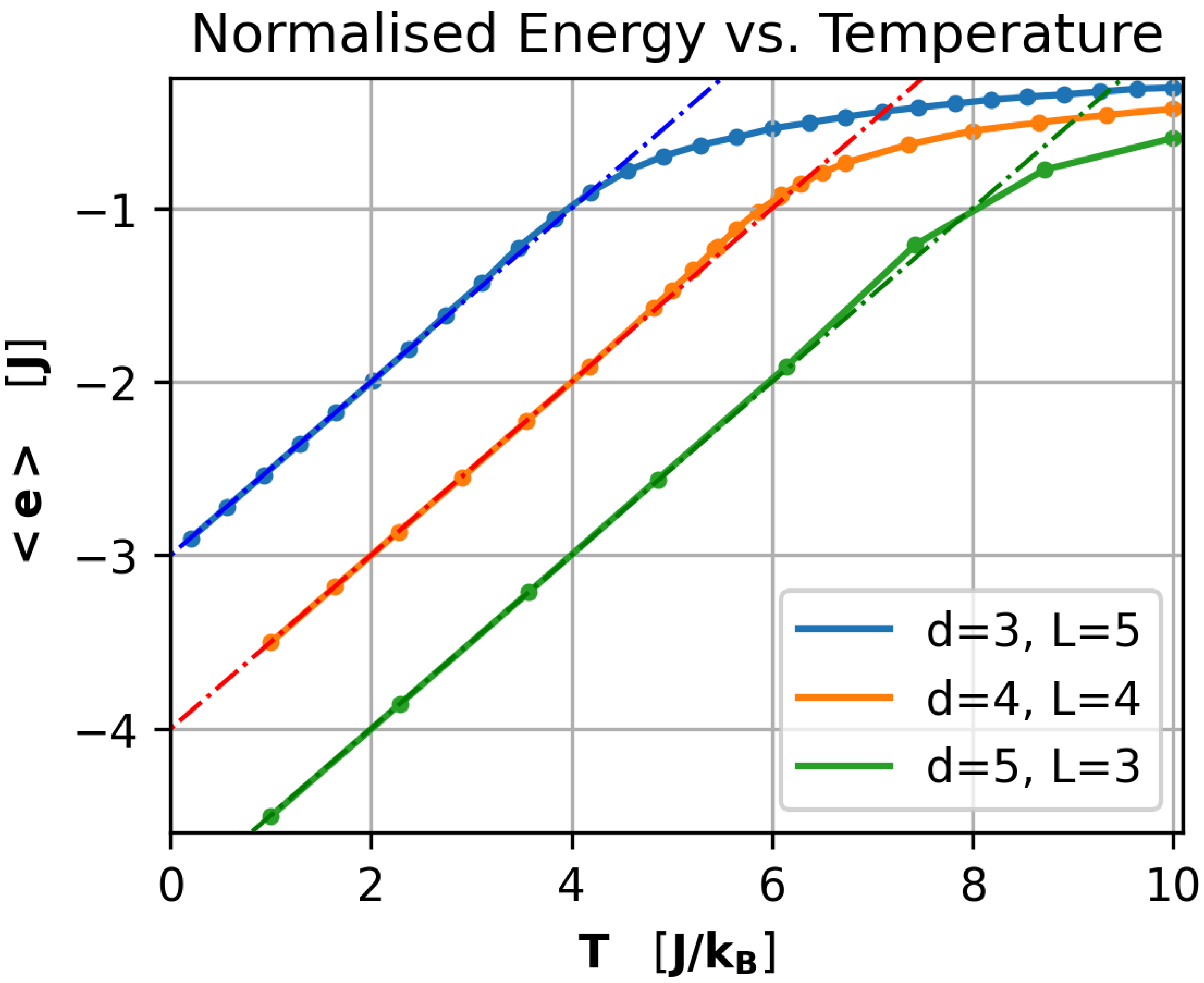
ENERGY

Reminding the analytical solution for the internal energy:

$$u_- = \frac{1}{2}k_B T - Jd \quad \text{for } T < T_c$$

It means that:

$$\begin{aligned}\langle e \rangle = u^{(3)} &= \frac{1}{2}T - 3 \\ = u^{(4)} &= \frac{1}{2}T - 4 \\ = u^{(5)} &= \frac{1}{2}T - 5\end{aligned}$$



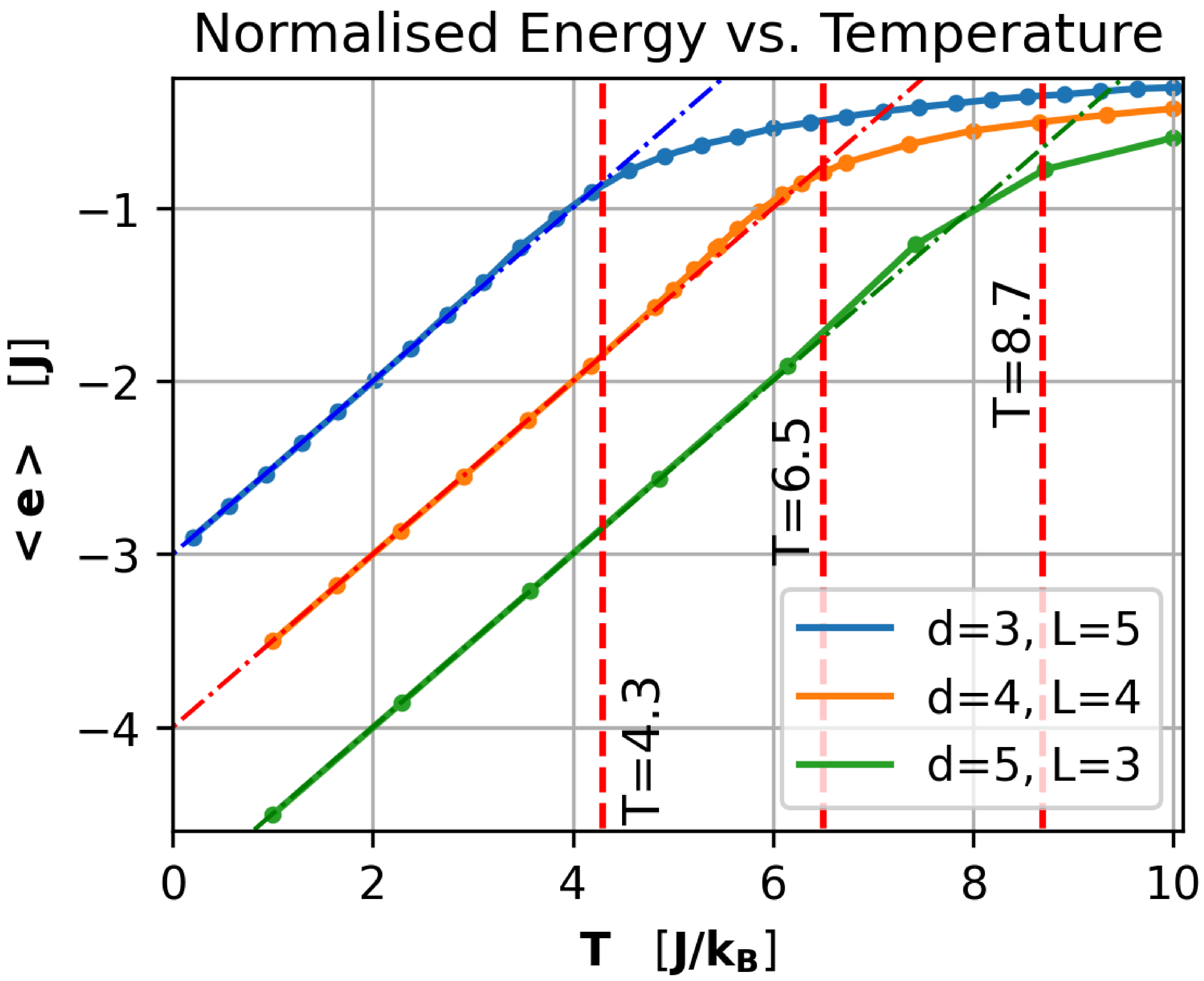
04

RESULTS

ENERGY

Numerically solving the analytical solution, one can find that:

$$T_C^{(3)} \simeq 4.3 J/k_B$$
$$T_C^{(4)} \simeq 6.5 J/k_B$$
$$T_C^{(5)} \simeq 8.7 J/k_B$$



04

RESULTS

MAGNETISATION

Three simulations at 3 different dimensions:

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- **4D:** L=4
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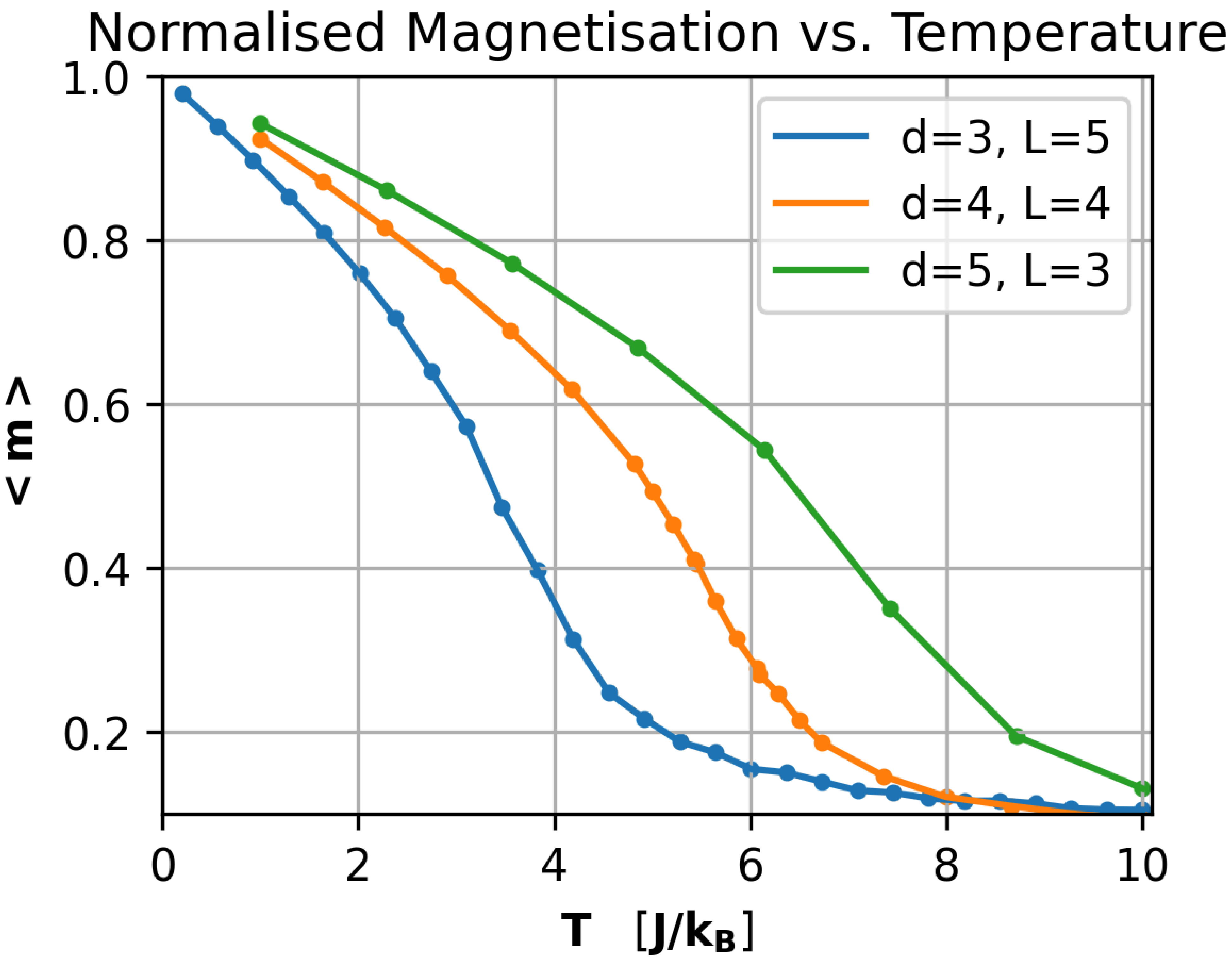
Zero field (H=0) and J=1



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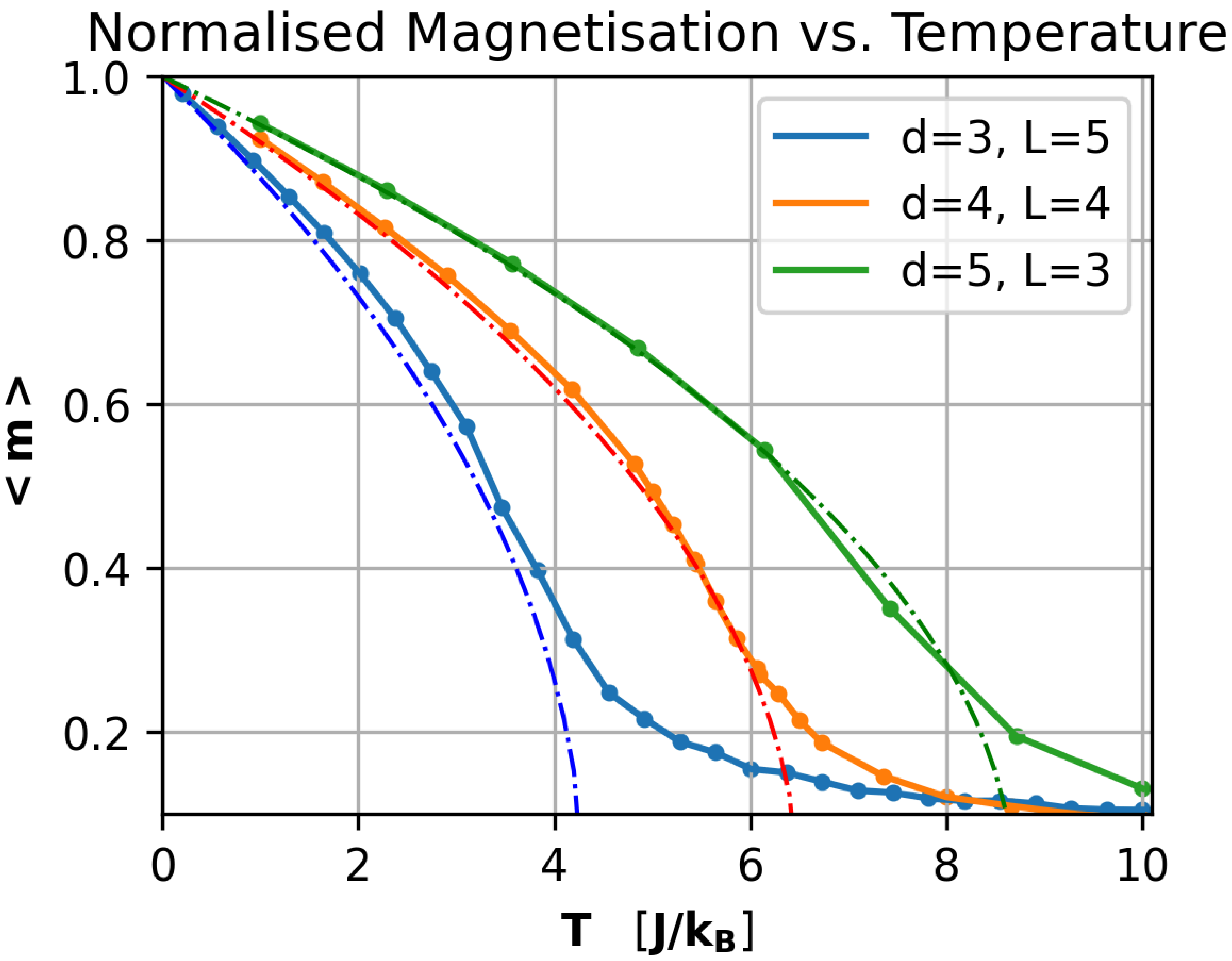
RESULTS

MAGNETISATION



Reminding the analytical solution for the magnetisation:

$$M = \mathrm{sgn}(H)\left(1 - \frac{T}{T_c}\right)^{1/2}, \qquad T < T_c$$
$$M = 0, \qquad T > T_c$$

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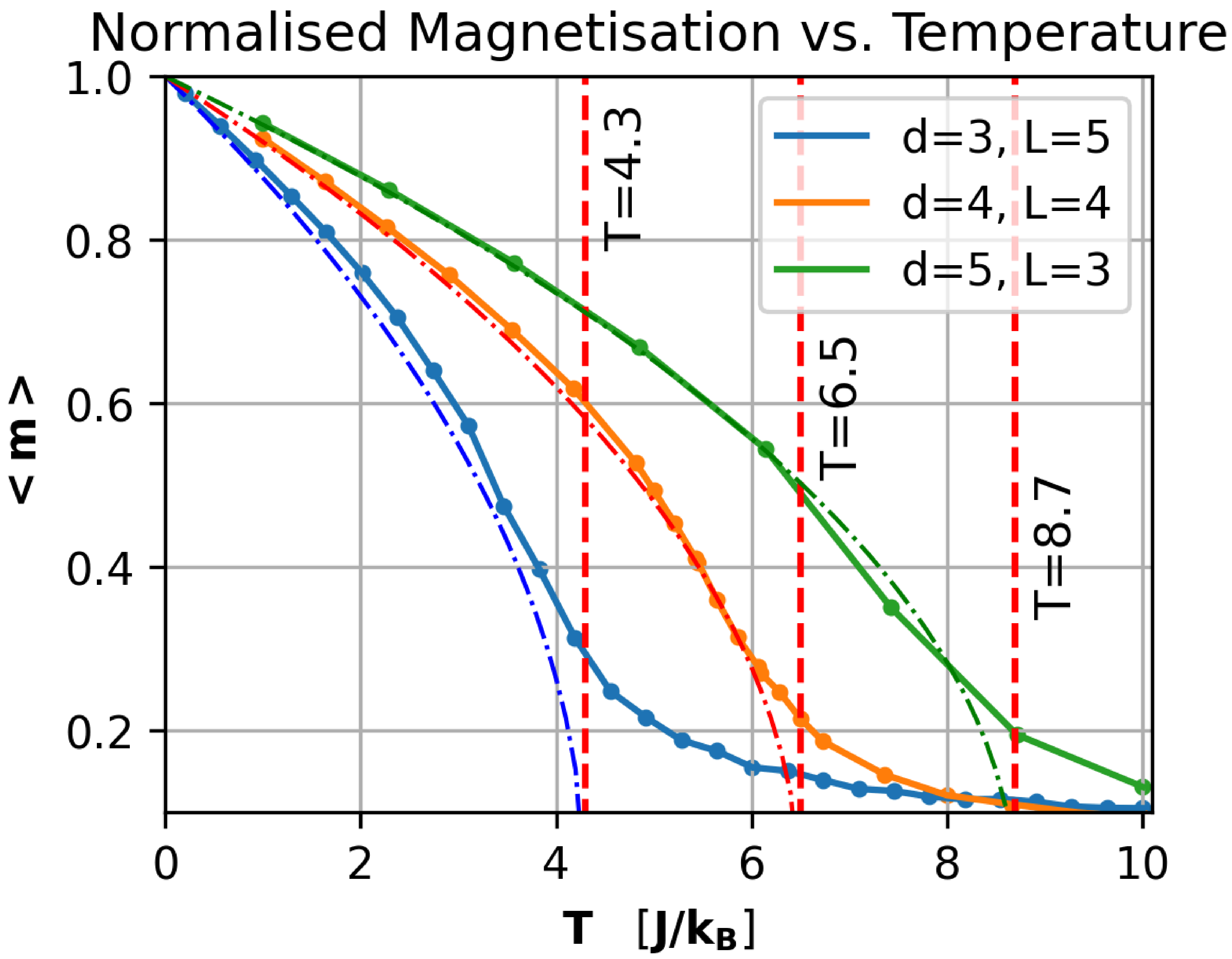


04

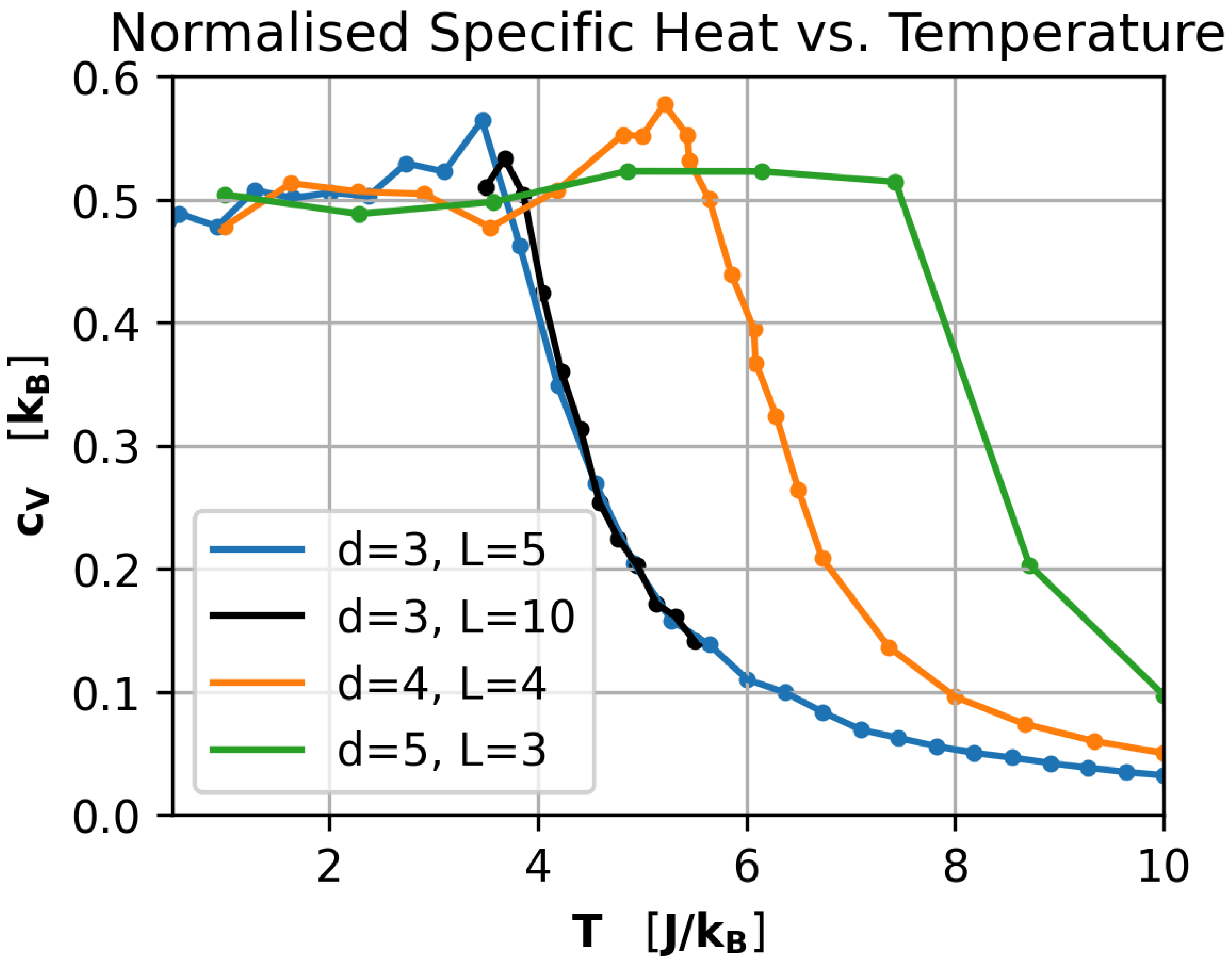
RESULTS

SPECIFIC HEAT

Three simulations at 3 different dimensions:

- **3D:** L=5
- **3D:** L=10
- **4D:** L=4
- **5D:** L=3

Zero field (H=0) and J=1

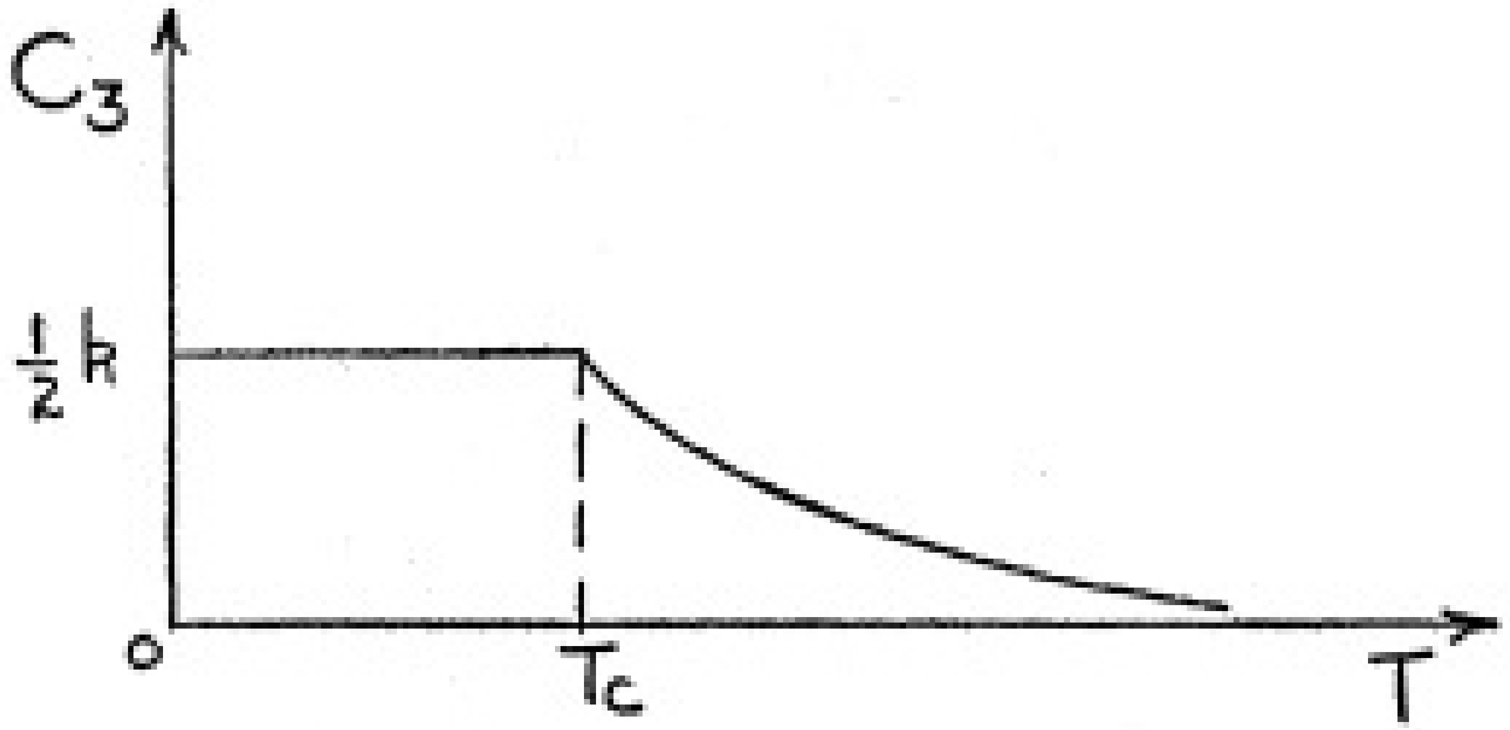


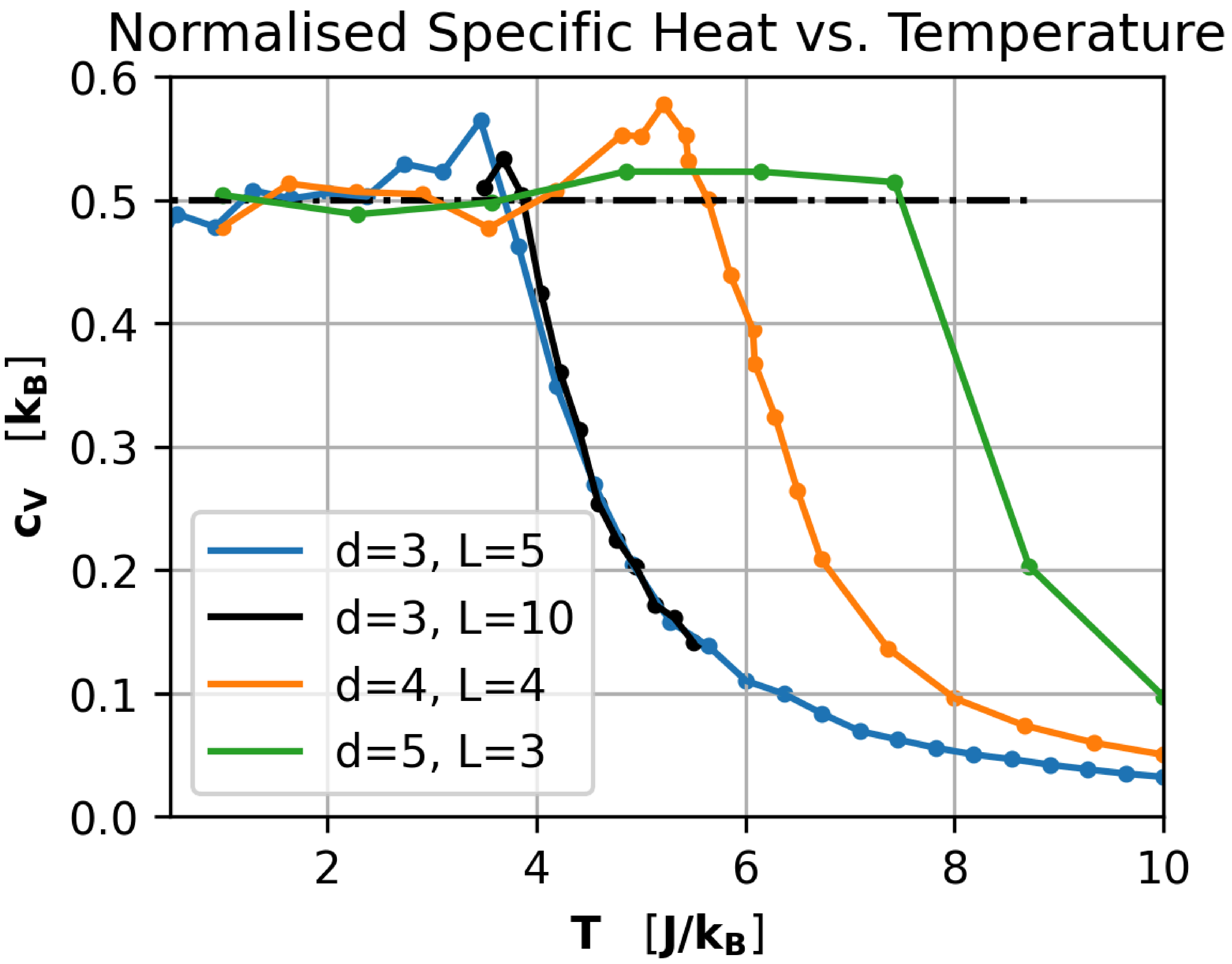
04

RESULTS

SPECIFIC HEAT

Reminding the analytical solution for the specific heat:





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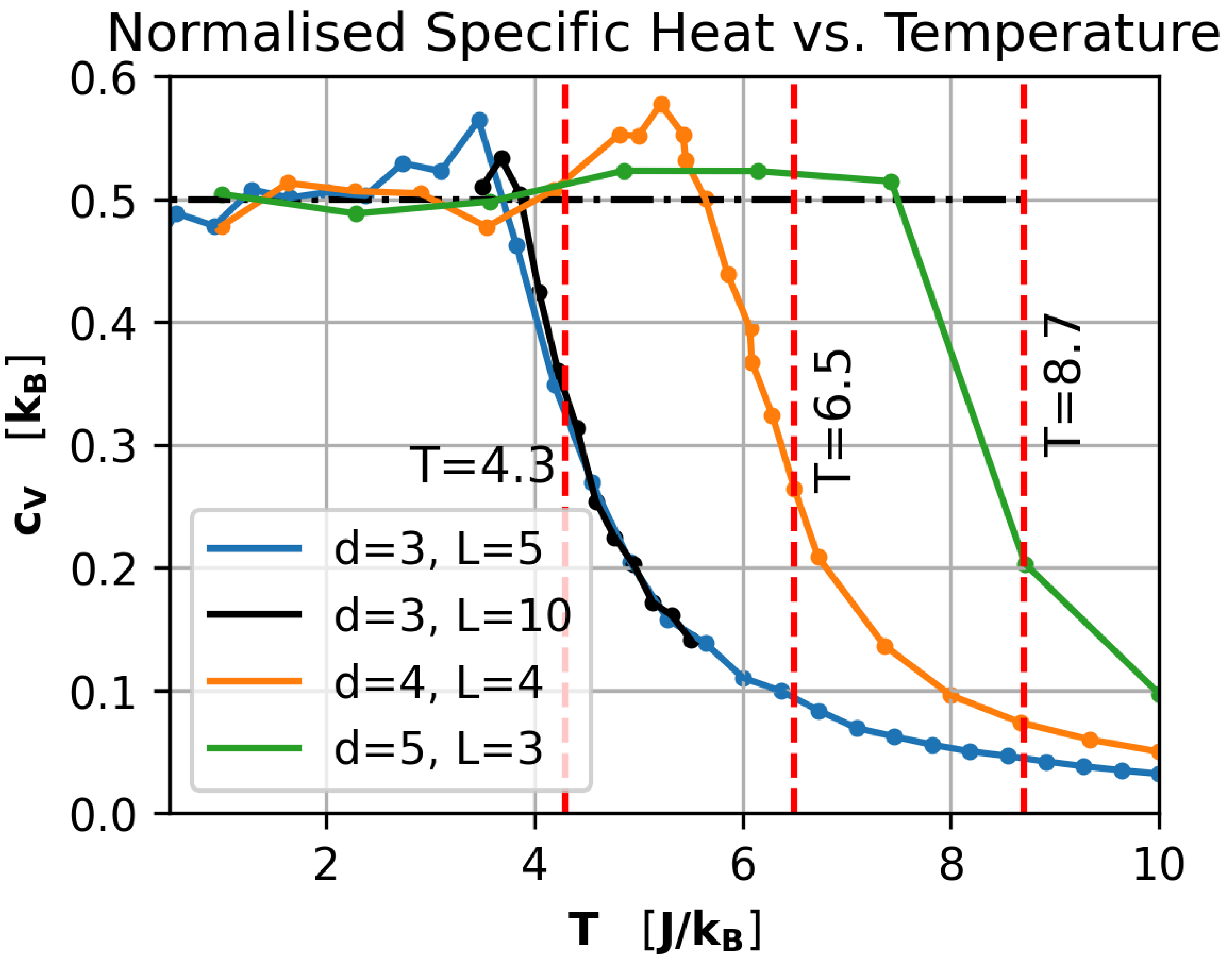
RESULTS

SPECIFIC HEAT

- For each system, the critical temperature is smaller than the theoretical one
- For the dimension d=3, the bigger system has a better estimation



04

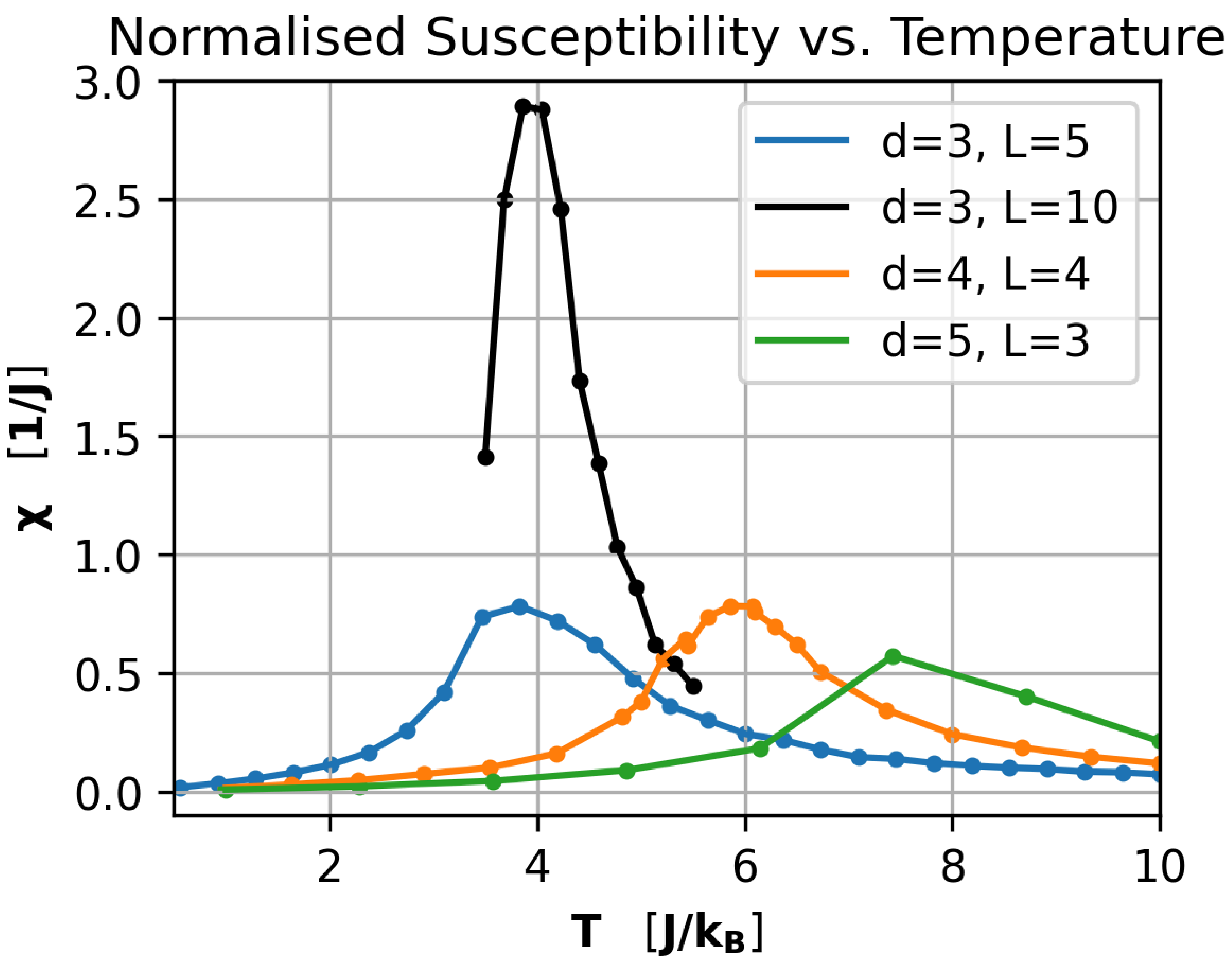
RESULTS

SUSCEPTIBILITY

Four simulations at 3 different dimensions:

- **3D:** L=5
- **3D:** L=10
- **4D:** L=4
- **5D:** L=3

Zero field (H=0) and J=1



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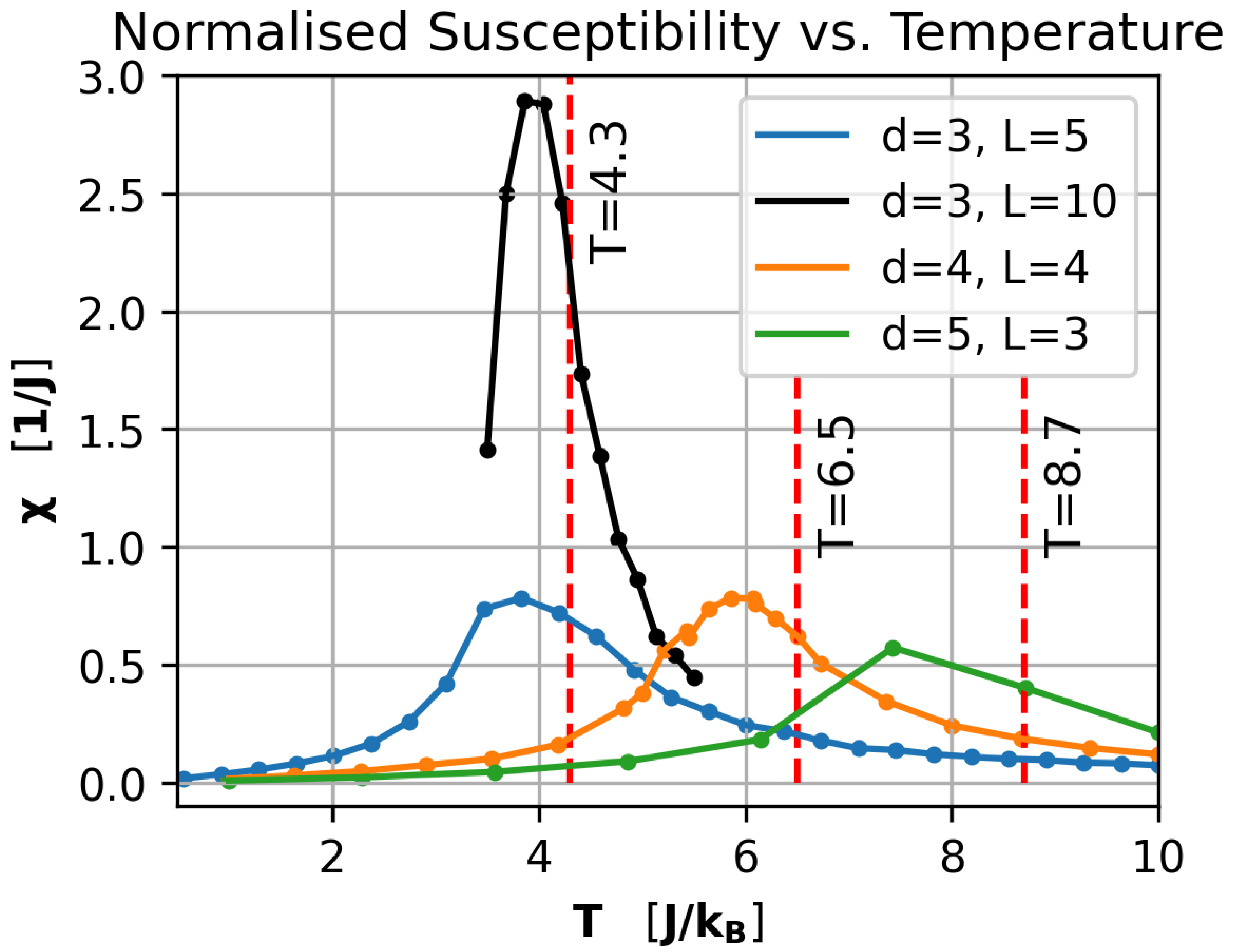
RESULTS

SUSCEPTIBILITY

Reminding that, near the critical temperature, the susceptibility diverges, for dimension d=3:

- The bigger system has a bigger peak
- The bigger system has a closer peak to the theoretical value



05

Conclusion

The Mixed Metropolis Algorithm converges faster than the Standard Algorithm.

The simulations follow the results expected from the theory, with finite size dependence.

Reference

01 Berlin and Kac, “The spherical model of a ferromagnet”. 1952.

02 R. J. Baxter. Exactly solved models in statistical mechanics. 1982.

03 R.K. Pathria and Paul D. Beale. Statistical mechanics. 2011.

04 H. E. Stanley. “Spherical Model as the Limit of Infinite Spin Dimensionality”. 1968.

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Thank You

01

BACKGROUND

ISING MODEL

Simple and useful but
Exactly solvable only for 1D
and 2D with zero field

GAUSSIAN MODEL

More general but fails
under the critical
temperature

03

IMPLEMENTATION IN C++

CODE ORGANISATION

CLASS:

The class represents the system as a **d** dimensional hyper-lattice and has functions to:

- Create the system
- Evolve the system
- Export the state of the system

MAIN:

The main file runs the simulation:

- Reads all the input parameters
- Parallelise the code
- Observes the temperature evolution of the system

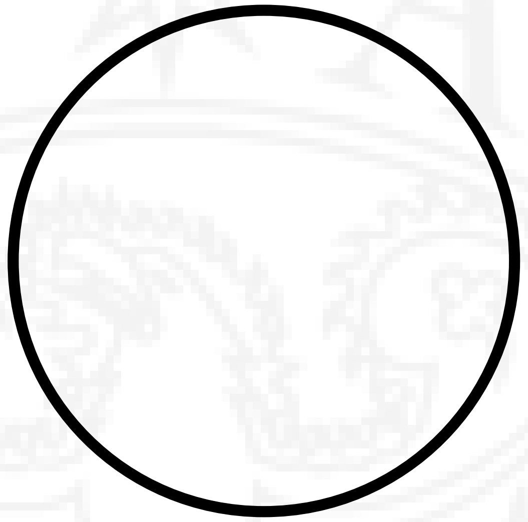
03

IMPLEMENTATION IN C++

SYSTEM VISUALISATION

We represent the system, a hyper-dimensional lattice, as a vector containing all the spins: $\bar{\sigma}$

1D



2D