Numerical study of the dimensionally reduced 3D Ising model

Stephan Durr, Tolga Kiel

University of Wuppertal

BERGISCHE UNIVERSITÄT WUPPERTAL

Introduction

- Study of the 3D Ising model [1] in the infinite volume limit $N_{x,y,z} \to \infty$, as well as the "dimensionally reduced" Ising model with fixed N_z in the limit of $N_{x,y} \to \infty$ by means of Monte-Carlo simulations.
- Determination of T_c as well as the critical exponents β, γ and ν, based on finite-size scaling and histogram reweighting techniques.

Ising model

- Simulation of the ferromagnetic Ising model with the well known Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle \in \Lambda} \sigma_i \sigma_j, \tag{1}$$

and the partition function

$$\mathcal{Z} = \sum_{\sigma_\mu \in \Omega} \exp(-\beta \mathcal{H}(\sigma_\mu)) = \sum_{\sigma_\mu \in \Omega} \exp(\tilde{J} \sum_{\langle ij \rangle} \sigma_i \sigma_j), \tag{2}$$

where $\beta = \frac{1}{k_B T}$ and we defined $\tilde{J} := \beta J$.

Observables

- We measure the following observables with $N = N_x N_y N_z$

$$e = \frac{1}{N} \sum_{\langle ij \rangle \in \Lambda} \sigma_i \sigma_j \tag{3}$$

$$m = \frac{1}{N} \sum_{i \in \Lambda} \sigma_i \tag{4}$$

$$C = \tilde{J}^2 N (\langle e^2 \rangle - \langle e \rangle^2) \tag{5}$$

$$\chi = \tilde{J} N (\langle |m|^2 \rangle - \langle |m| \rangle^2) \tag{6}$$

$$U_4 = 1 - \frac{\langle |m| \rangle^4}{3 \langle |m|^2 \rangle^2}, \tag{7}$$

where $\langle . \rangle$ denotes the ensemble average and U_4 is called the Binder cumulant.

Finite-size scaling and Binder cumulant crossing

- Make use of scaling relations to determine the infinite volume critical exponents.
- Define reduced temperature as

$$t := \frac{T - T_c}{T_c} \tag{8}$$

as $t \to 0$ and for large enough lattices, the following scaling relations hold:

$$\max C \propto L^{\alpha/\nu} \tag{9}$$

$$\max \chi \propto L^{\gamma/\nu} \tag{10}$$

$$\langle |m| \rangle|_{\tilde{J}=\tilde{J}_c} \propto L^{-\beta/\nu} \tag{11}$$

$$\left. \frac{\partial U_4}{\partial \tilde{J}} \right|_{\tilde{J}=\tilde{J}_c} \propto L^{1/\nu}, \tag{12}$$

where L denotes the size of the scaled dimension ($L = N_{x,y,z}$ for 3D and $L = N_{x,y}$ for "dimensionally reduced").
- Use crossing point of U_4 as a function of $\tilde{J}$ for different lattice sizes L to determine $\tilde{J}_c$.

Histogram reweighting

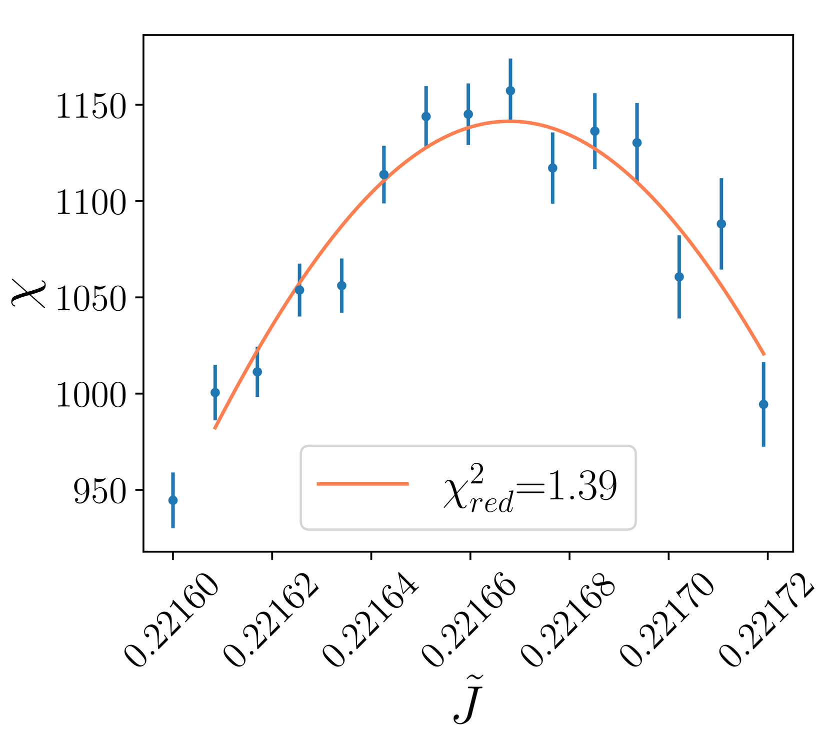
- Expectation value of observable $\mathcal{O}$ at $\tilde{J}$ can be determined from data measured at $\tilde{J}'$ via

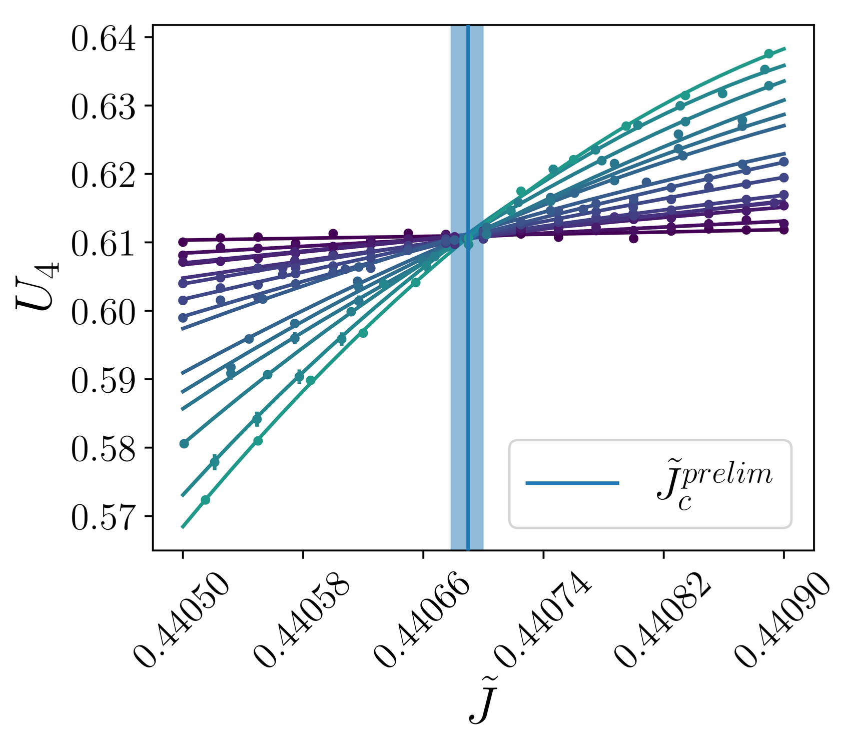
$$\langle \mathcal{O} \rangle_{\tilde{J}} = \frac{\left\langle \mathcal{O} e^{-(\tilde{J}-\tilde{J}')E} \right\rangle_{\tilde{J}'}}{\left\langle e^{-(\tilde{J}-\tilde{J}')E} \right\rangle_{\tilde{J}'}}. \tag{13}$$

- Estimate maxima of C and χ using Golden-Section search algorithm in $\tilde{J}$.
- Estimate crossings of U_4 using Newtons method on $\Delta U_4^{ij} = U_4^{L_i} - U_4^{L_j}$ for ascending pairs of lattice sizes $L_1 < L_2 < L_3 \dots$.
- Estimate $\left. \frac{\partial U_4}{\partial \tilde{J}} \right|_{\tilde{J}=\tilde{J}_c}$ using explicit form of observable by differentiating equation 13 symbolically.

Estimation of peak parameters

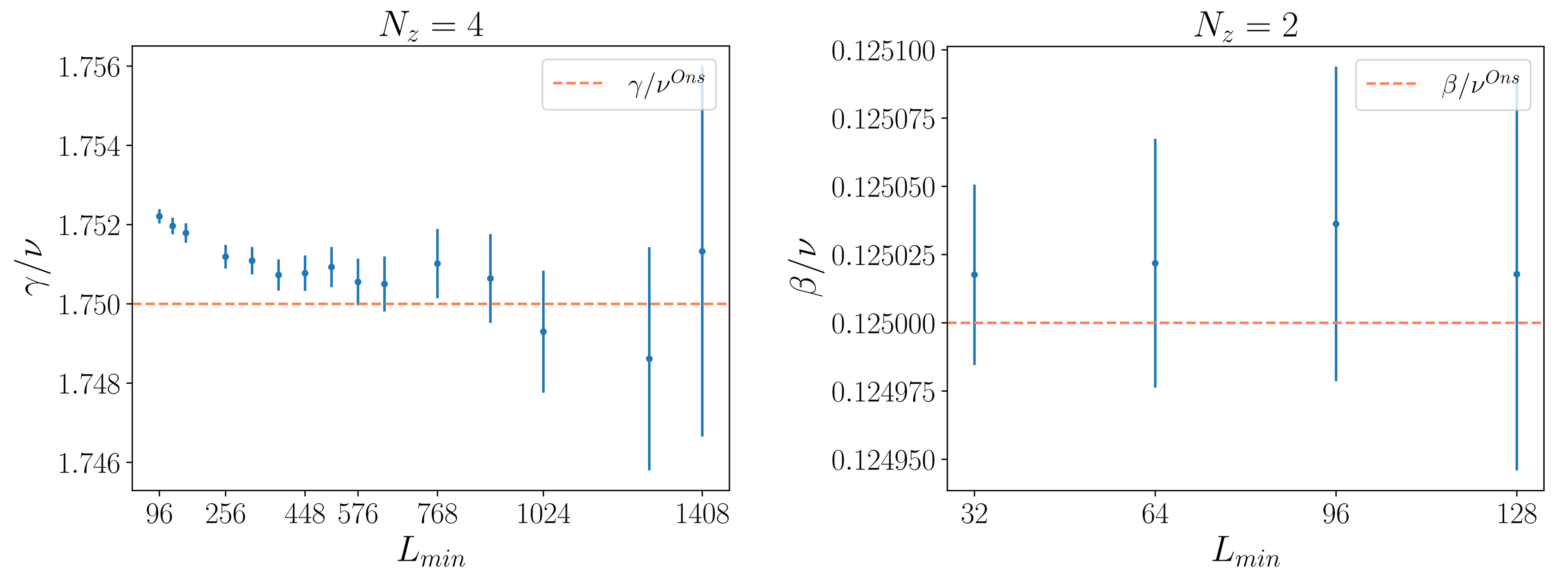
- Histogram reweighting only feasible in close proximity to simulated coupling.
- Estimation of simulation temperatures using fits to bunches of simulations in neighborhood of estimated peak/critical coupling.





Error estimation

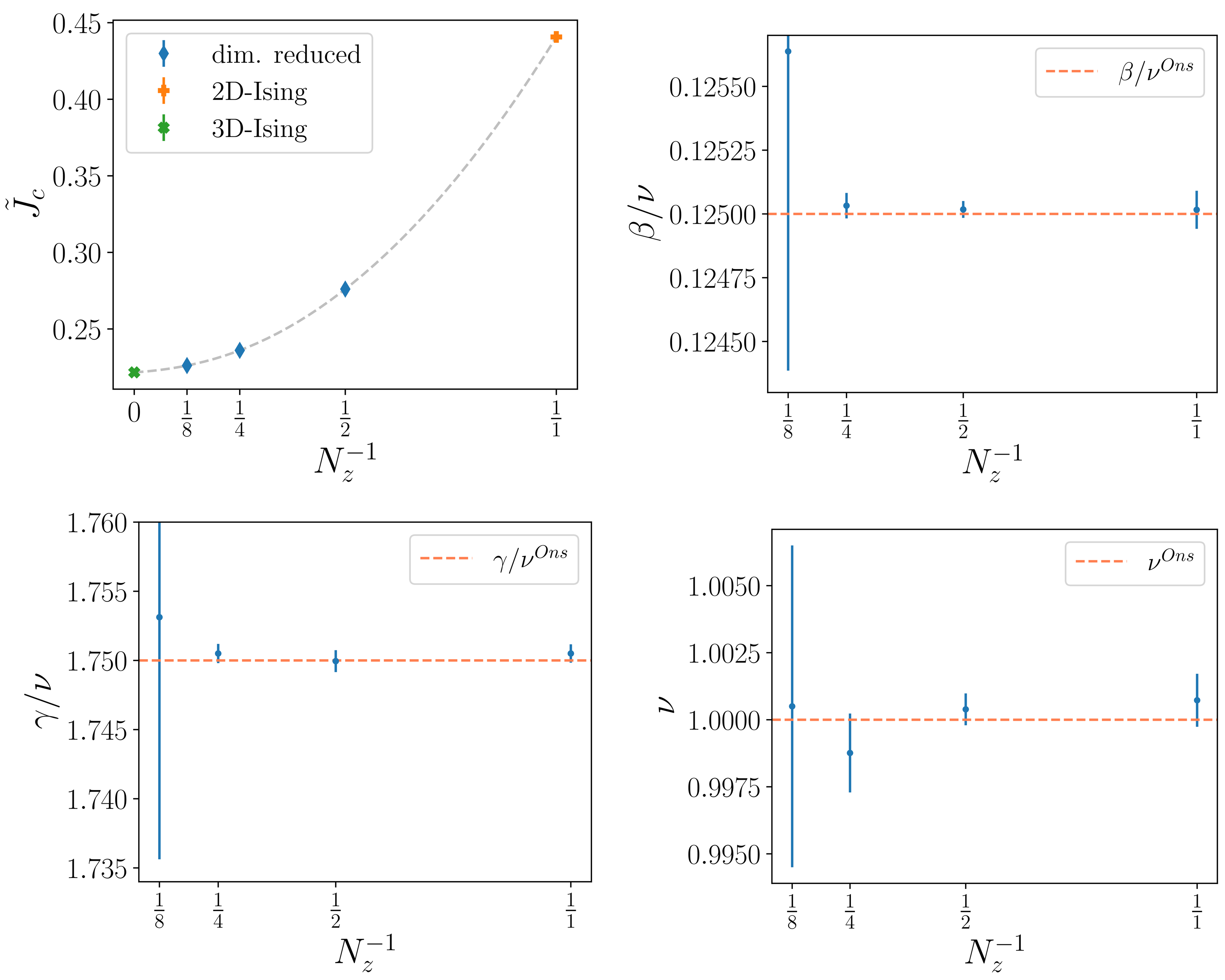
- Use of delete-d-jackknife to estimate statistical errors.
- d is chosen such that the data is divided into 10000 jackknife-blocks.
- Ensemble sizes between 10^6-10^8 and autocorrelation times between 1-15 $\Rightarrow d \gg 2\tau_{int} + 1$.
- Scaling relations only asymptotically valid $\Rightarrow$ systematic deviation from true exponent if smallest $L = L_{min}$ included in fit is not large enough.
- Exclude smallest L from fit one by one until estimator of exponent does not change significantly (see below for estimators of γ/ν and β/ν obtained from fits as a function of minimal lattice size L_{min} included).



- Smallest L_{min}, for which the asymptotic scaling relation can be used, varies strongly between exponents ($\mathcal{O}(30)$-$\mathcal{O}(500)$). Generally L_{min} becomes larger for large N_z.

Results

- The critical temperature and the critical exponents for $N_z = 1, 2, 4, 8$ are shown below.



- With the help of the hyperscaling relation and the Rushbrook equation, it is possible to determine the effective dimension of the system using

$$d_{\text{eff}} = \frac{2\beta + \gamma}{\nu}. \tag{14}$$

- Critical temperatures, critical exponents and effective dimensions for different N_z:

N_z	$\tilde{J}_c$	β/ν	γ/ν	ν	d_{eff}
1	0.440 687 0(19)	0.125 041(85)	1.750 50(66)	1.0003(15)	2.000 58(69)
2	0.276 032 19(13)	0.125 018(33)	1.749 95(79)	1.000 39(59)	1.999 98(79)
4	0.236 027 75(14)	0.125 032(50)	1.750 50(70)	0.9988(15)	2.000 57(70)
8	0.226 102 78(51)	0.1256(13)	1.753(17)	1.0005(60)	2.004(18)
3D	0.221 654 94(49)	0.5193(13)	1.9632(50)	0.628 75(82)	3.0019(61)

Conclusions

- For $\tilde{J}_c$ we find a smooth transition curve which connects the well known critical temperatures of the 2D and the 3D Ising model.
- In contrast to previous work on this topic [2][3][4], our data suggests that the "dimensionally reduced" Ising model is in the same universality class as the 2D Ising model, regardless of N_z.

References

[1] E. Ising, *Beitrag zur Theorie des Ferromagnetismus*, Z. Physik 31, 253-258 (1925).

[2] D. Sabogal-Suárez, J.D. Alzate-Cardona, E. Restrepo-Parra, *Static and dynamic critical behavior of thin magnetic Ising films*, Physica A: Statistical Mechanics and its Applications 434, 60-67 (2015).

[3] X.T. Pham Phu, V. Thanh Ngo, H.T. Diep, *Critical behavior of magnetic thin films*, Surface Science 603, 109-116 (2009).

[4] M. I. Marqués, J. A. Gonzalo, *Thickness Dependence of Effective Critical Exponents in Three-Dimensional Ising Plates*, Acta Physica Polonica A 97(6), 1033–1037 (2000).