Spin correlations in the 3D Ising model on infinite cuboids

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- worm updates by N.V. Prokof'ev, B.V. Svistunov, PRL 87, 160601 (2001)
- sample graphs of the HTSE in the $3D$ Ising model
- calculate the two point functions $\Gamma(R)$ and χ
- H.G. Evertz and W. von der Linden in "Simulation on Infinite Lattices" PRL 86, 5164 (2001)

Simulations on Infinite-Size Lattices

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We introduce a Monte Carlo method, as a modification of existing cluster algorithms, which allows simulations directly on systems of infinite size, and for quantum models also at $\beta = \infty$. All two-point functions can be obtained, including dynamical information. When the number of iterations is increased, correlation functions at larger distances become available. Limits $q \to 0$ and $\omega \to 0$ can be approached directly. As examples we calculate spectra for the $d = 2$ Ising model and for Heisenberg quantum spin ladders with two and four legs.

- ”infinite hypercubic boxes” an example

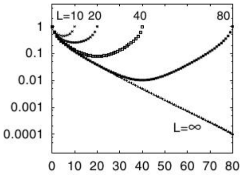


FIG. 1. Correlation functions $C(r)$ vs r of the $d = 2$ Ising model at $\beta = 0.42$.

- U. Wolff single cluster update, PRL 1989: a single bond-cluster is flipped, that contains a randomly chosen initial starting site x_0
- E+L:

$$\boxed{x_0 = \text{const}}$$

e.g. : x_0 origin of an Cartesian coordinate system

features of the infinite system method

- one never stores an infinite lattice Λ, only the flipped spins are kept in the computer
- after some "Computer Time" in local steps, $N_{\mathrm{Step}} = \mathcal{O}(10^{13-14})$ a region, domain of diameter $d(N_{\mathrm{Step}})$, including x_0 in the center, is equilibrated
- and in $D = 3$ d can be of size $d^3 = \mathcal{O}(2048^3)$ (multispin-coding)
- detailed balance and ergodicity is granted
- measurements of improved estimators of observables for $R << d$
- $\Gamma(R)$, ξ_{exp}, ξ_{secnd} and χ
- the theory has no boundary and therefore is of infinite size

$\boxed{\text{can be efficient as only the "needed" dof's are kept and updated}}$

Ising Model

- partition function at β with two spin insertions

$$Z(u,v) = \sum_{Conf.} e^{\beta \sum_{Bonds} s(i)s(j)} s(u)s(v)$$

- two point function

$$G(u-v) = \frac{Z(u,v)}{Z(u,u)}$$

- zero momentum correlator

$$\Gamma(R) = \frac{1}{N_y N_z} \sum_{u,v} G(u-v)\delta^1(R - u_x + v_x)$$

$$\boxed{\Gamma(R) \propto e^{-R/\xi_{\text{exp}}} \quad R >> \xi_{\text{exp}}}$$

- magnetic susceptibility: $\chi := \mathcal{N}^{-1} \sum_R \Gamma(R)$

Loop Representation for Partition Function

$$Z(u, v)$$

- dimers $k_{i,\eta} = 0, 1$, $\eta = 1, 3$
- local dimer sum

$$\Sigma(i) = \sum_{\eta=1,2,3} (k_{i,\eta} + k_{i-\eta,\eta})$$

- odd at u and v

$$\mathrm{mod}(\Sigma(u), 2) = \mathrm{mod}(\Sigma(v), 2) = 1$$

- even at $i \neq u, v$

$$\mathrm{mod}(\Sigma(i), 2) = 0$$

Loops of Dimers and one Worm

- dimer chemical potential

$$\tanh(\beta) = e^{-\mu}$$

$$\mu = -\ln[\tanh(\beta)]$$

- dimer representation

$$Z(u,v) = \sum_{Dimers} e^{-\mu \sum_{i,\eta} k_{i,\eta}} \times \delta^1(1 - \mathrm{mod}(\Sigma(u),2))$$
$$\times\, \delta^1(1 - \mathrm{mod}(\Sigma(v),2))$$
$$\times \prod_{i\neq u,v} \delta^1(0 - \mathrm{mod}(\Sigma(i),2))$$

- the worm update of PS performs single dimer moves only at v uniform in the directions η and $-\eta$, while in accord with Evertz et. al. $u = \mathrm{const}$ is kept constant
- with a Metropolis accept reject decision
- yields a 'Random Walk' of the worm, which always returns to the origin of the coordinate system
- after the worm returns , a new worm is created always emanating form the origin

Biased Sampling [Multicanonical]

- biased

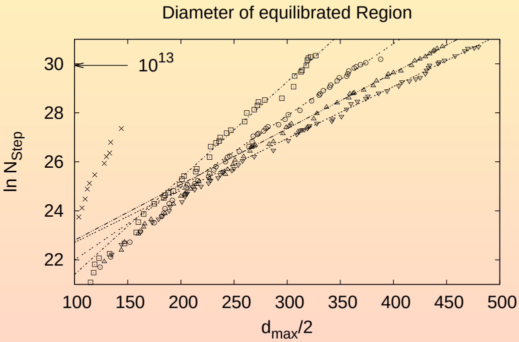
$$Z(u,v,s) = \sum_{Dimers} e^{-\mu \sum_{i,\eta} k_{i,\eta}} \times \delta^1(1 - \mathrm{mod}(\Sigma(u),2))$$
$$\times \delta^1(1 - \mathrm{mod}(\Sigma(v),2))$$
$$\times \prod_{i \neq u,v} \delta^1(0 - \mathrm{mod}(\Sigma(i),2))$$
$$\times e^{+(1-\frac{1}{s})(u_x - v_x)/\xi_{\mathrm{exp}}}$$

$$Z \propto \exp[-\frac{u_x - v_x}{\xi_{\mathrm{exp}}} + (1 - \frac{1}{s})\frac{u_x - v_x}{\xi_{\mathrm{exp}}}] \propto \exp[-\frac{u_x - v_x}{s\xi_{\mathrm{exp}}}]$$

- domain size boost : $s = 1.4$

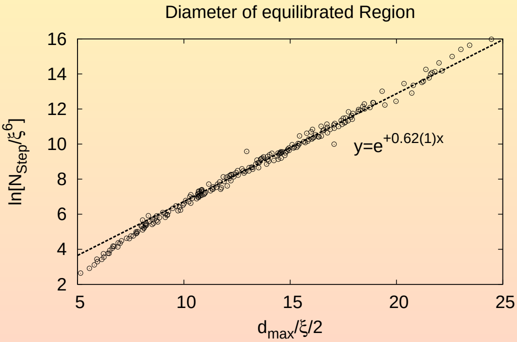
the effort to expand a domain of diameter d is exponential large

- D=3 Ising $\beta < \beta_c$



and scales in units of ξ

- D=3 Ising $\beta < \beta_c$



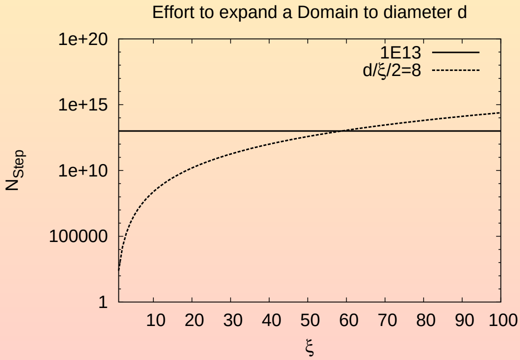
- scaling variables d/ξ and N_{Step}/ξ^6

however

the effort to evolve a domain to fixed diameter $d/\xi = \mathrm{const}$

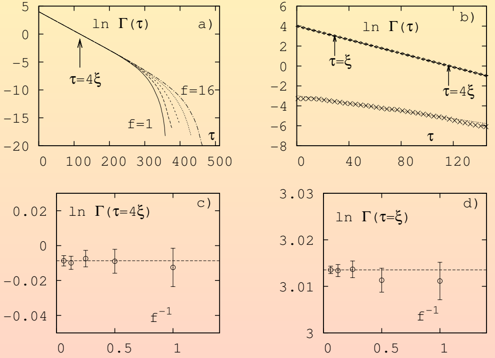
scales polynomial in ξ

- D=3 Ising $\beta < \beta_c$



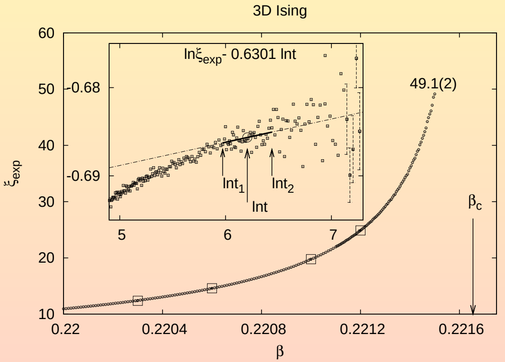
within the domain $\Gamma(R)$ is measured

- D=3 Ising $\beta < \beta_c$



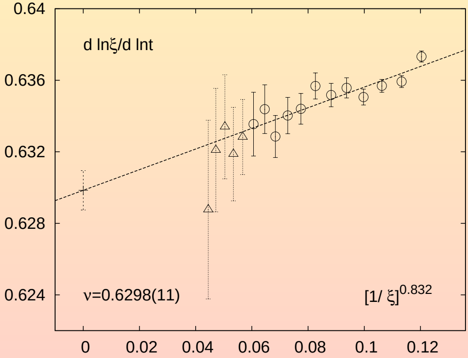
and the correlation length $\xi_{\exp}$ is fitted on the interval $1 \leq R/\xi_{\exp} \leq 4$

- squares by Kim, Souza, Landau, PRE 1996



- reduced temperature $t = 1 - \frac{\beta}{\beta_c}$ with $\beta_c = 0.22165463$ Hasenbusch PRB 2010.

- determines $\nu = 0.6298(11)$ **without the use of finite size scaling theory**



Conclusion

- encouraging demonstration of Monte Carlo simulations and scaling behavior on infinite Cuboids with quantitative result for ν and γ
- competitive method for the ξ determination
- it is not simple to determine a correlation length of $\xi = 50$ in the 3D Ising model
- ongoing project: dedicated workstation in Leipzig to determine large correlation length values in the nearest neighbor 3*D* Ising theory

Appendix 1 comparison to Hasenbusch

β	$\xi_{\exp}$	$\xi_{\exp}$	$\frac{\xi_{\exp}}{\xi_{\exp}} - 1$	BIT
0.204210	2.36429(22)	2.363(1)	0.00054(43)	1
0.211890	3.47865(42)	3.477(2)	0.00047(58)	0
0.215810	4.86348(77)	4.864(3)	-0.00010(63)	0
0.217310	5.8954(17)	5.892(3)	0.00057(58)	0
0.219310	8.7636(34)	8.766(5)	-0.00027(69)	0
0.220200	11.8844(39)	11.884(9)	0.00004(82)	0
β	χ	χ	$\frac{\chi}{\chi} - 1$	BIT
0.204210	25.2552(34)	25.254(16)	0.00001(64)	0
0.211890	52.1502(92)	52.090(40)	0.00115(78)	1
0.215810	98.840(20)	98.90(10)	-0.0006(10)	0
0.217310	143.033(53)	143.03(12)	-0.00004(91)	0
0.219310	308.17(16)	308.57(31)	-0.0013(11)	1
0.220200	557.60(31)	557.57(61)	0.0000(12)	0

Table: Comparison of χ and correlation length values to Hasenbusch 1997.

Appendix 2 comparison to Landau

β	ξ_{2nd}	ξ_{2nd}	$\frac{\xi_{2nd}}{\xi_{2nd}} - 1$	BIT
0.217000	5.63039(71)	5.62 (1)	0.0018(17)	1
0.219000	8.0865(23)	8.03 (4)	0.0070(50)	1
0.220300	12.4302(37)	12.38(15)	0.004(12)	0
0.220600	14.5823(58)	14.61(6)	-0.0018(41)	0
0.221000	19.744(11)	19.77(12)	-0.0012(60)	0
0.221200	24.861(18)	24.87(12)	-0.0007(48)	0
β	χ	χ	$\frac{\chi}{\chi} - 1$	BIT
0.217000	131.285(25)	130.89(40)	0.0029(30)	0
0.219000	264.14(12)	261.6(21)	0.0097(81)	1
0.220300	609.11(30)	605.5(88)	0.005(14)	0
0.220600	831.46(48)	837.0(57)	-0.0066(67)	0
0.221000	1502.63(93)	1518(15)	-0.0101(98)	1
0.221200	2360.3(26)	2382(14)	-0.0090(59)	1

Table: Comparison of ξ and χ values to Landau 1996.