

# Critical behaviour of the surface tension in the 3D Ising model

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September 22, 2018

# Summary

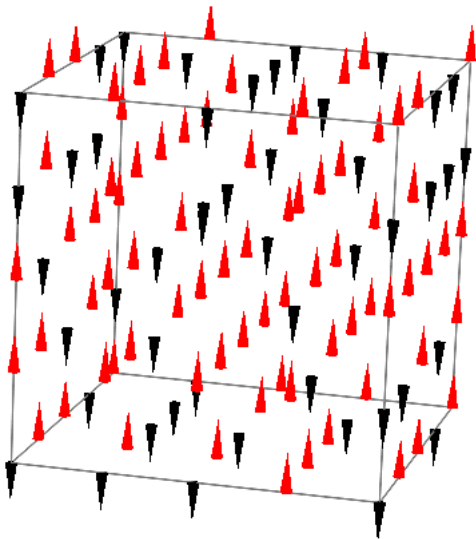
- 3D Ising models
- Definition of the surface tension
- Cluster algorithms and boundary flip
- Notes on the implementation
- Estimation of the errors and autocorrelation
- Fit of the free energy
- Fit of the critical behaviour
- Conclusions

## 3D Ising model

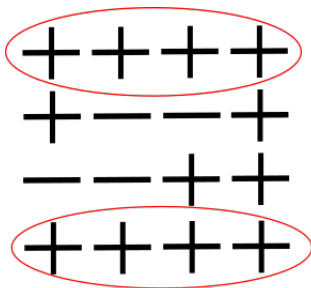
$$\mathcal{H} = - \sum_{\langle x,y \rangle} J_{\langle x,y \rangle} s_x s_y$$

$J_{\langle x,y \rangle} = 1$  ferromagnetic

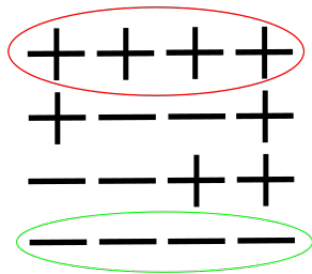
$J_{\langle x,y \rangle} = -1$  antiferromagnetic



## Definition of the surface tension

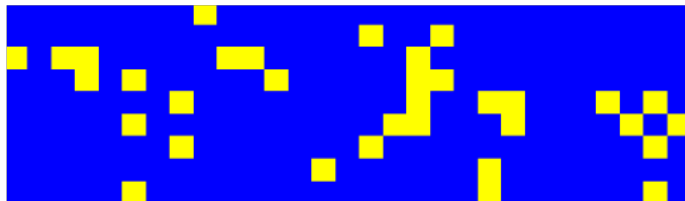


$Z_{++}$



$Z_{+-}$

$$\sigma = -\lim_{L \rightarrow \infty} \frac{1}{L^2} \log \frac{Z_{+-}}{Z_{++}} \quad L \times L \times T, \quad T = cL$$


 $Z_{+-}$ 

 $Z_{++}$ 

$$\sigma = - \lim_{L \rightarrow \infty} \frac{1}{L^2} \log \frac{Z_{+-}}{Z_{++}} = \lim_{L \rightarrow \infty} \frac{1}{L^2} (F_{+-} - F_{++}) = \lim_{L \rightarrow \infty} \frac{F_s}{L^2}$$

$\sigma$  = interface free energy per unit area

Redefinition of  $Z_{++}$  and  $Z_{+-}$ .

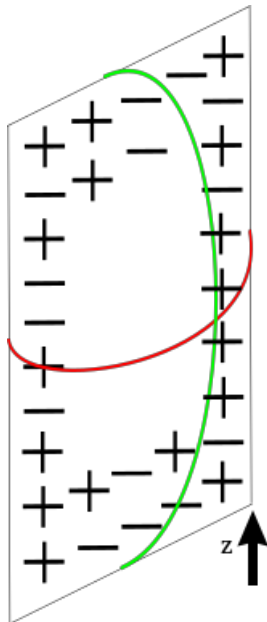
$Z_{++} \rightarrow$  ferromagnetic link  
between **top and bottom**.

$Z_{+-} \rightarrow$  **antiferromagnetic** link  
between **top and bottom**.

Always ferromagnetic link in  $x$   
and  $y$  directions.

Same definition for  $\sigma$ .

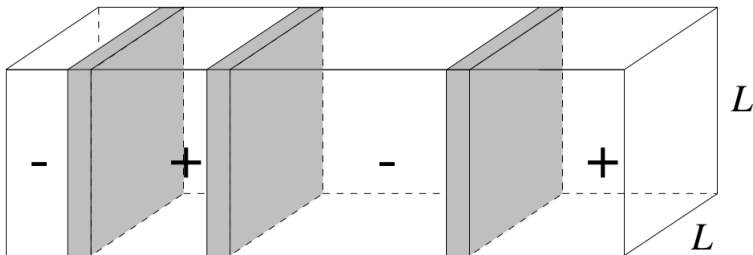
Periodic boundary conditions  
reduce the finite size effect.



We redefine the free energy of the interface in order to improve the convergence properties of  $\frac{F_s}{L^2}$  to  $\sigma$  when  $L \rightarrow \infty$ .

Thermodynamic limit  $\rightarrow$  only **one** interface

For finite  $L$  multiple interface can be present. An even number for  $Z_{++}$  and odd for  $Z_{+-}$ .



$F_s$  is the free energy of a single surface. There are  $\sim T$  different position for the interface.

$$Z_1 = T \exp(-F_s) = \exp(-F_s + \ln T)$$

$$\frac{Z_{+-}}{Z_{++}} = \frac{Z_1 + \frac{Z_1^3}{3!} + \frac{Z_1^5}{5!} + \dots}{1 + \frac{Z_1^2}{2!} + \frac{Z_1^4}{4!} + \dots} = \tanh(\exp(-F_s + \ln T))$$

$$F_s = \ln(T) - \ln\left(\frac{1}{2} \ln\left(\frac{1 + \frac{Z_{+-}}{Z_{++}}}{1 - \frac{Z_{+-}}{Z_{++}}}\right)\right) \quad \sigma = \lim_{L \rightarrow \infty} \frac{F_s}{L^2}$$



## General strategy

- Measure  $F_s$  on finite lattice size  $L$  at given  $\beta$  near  $\beta_c$ .
- Repeat for different  $L$ , same  $\beta$ .
- Find a theoretical formula to link  $F_s(L)$  and  $\sigma$ .
- Extrapolate  $\sigma$  at given  $\beta$ .
- Repeat the above procedure for different  $\beta$ , finding different  $\sigma(\beta)$ .
- Fit critical scaling law for  $\sigma(\beta)$ .

Montecarlo simulations can't measure  $Z$ !

Solution:  $J_{\langle x,y \rangle}$  between top and bottom becomes a **dinamical variable** that is summed over in  $Z$ .

$J_{\langle x,y \rangle} = 1$  (periodic b.c.)  $J_{\langle x,y \rangle} = -1$  (antiperiodic b.c.)  
Other  $J_{\langle x,y \rangle}$  remains ferromagnetic.

$$Z = \sum_{\{s\}, J} \exp \left( \beta \sum_{\langle x,y \rangle} J_{\langle x,y \rangle} s_x s_y \right)$$

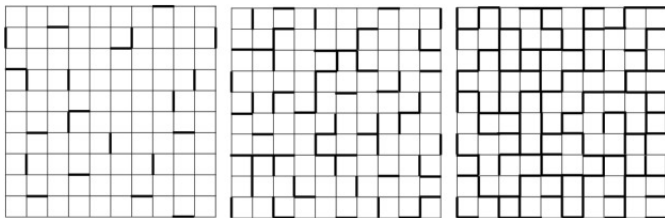
$$\frac{Z_{+-}}{Z_{++}} = \frac{\frac{Z_{+-}}{Z}}{\frac{Z_{++}}{Z}} = \frac{\langle \delta_{J=-1} \rangle}{\langle \delta_{J=+1} \rangle}$$

Ratio of measurable expectation values.

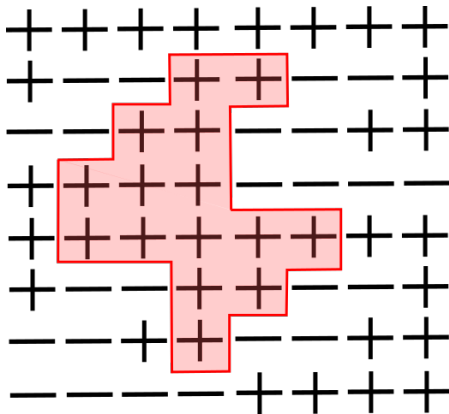
# Cluster algorithms and boundary flip

Cluster algorithms allow for simultaneous updates of large parts of the lattice. Thus reducing the autocorrelation time and the critical slowing down. Swendsen and Wang (1987).

Introduce link variables  $\sigma_{\langle x,y \rangle} = \{0, 1\}$  on the lattice and in the partition function:



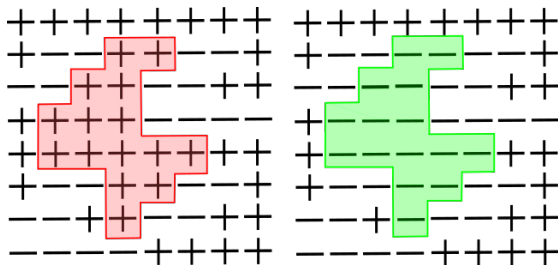
Definition: a **cluster** is a set of spins in the lattice path-connected by links with  $\sigma_{\langle x,y \rangle} = 1$ . If  $J_{\langle x,y \rangle} = 1$  all sites of a cluster are forced to have the same spin.



$\{\sigma\}$  uniquely **identifies** all the clusters. Vice versa given  $\{s\}$  we have some probability of generating a given link configuration.

## Single cluster update (Wolff):

In the Wolff algorithm we choose at random one site of the lattice and flip the cluster it belongs to. The probability of going from  $s_1$  to  $s_0$  and viceversa is obviously the same, being the probability of choosing the right cluster. Practically we build only **one cluster** starting from a seed.



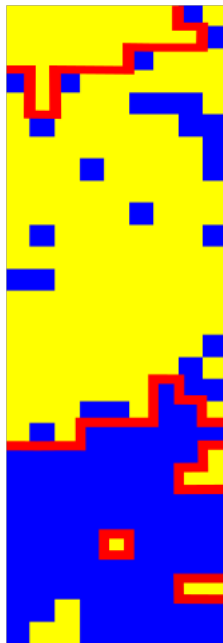
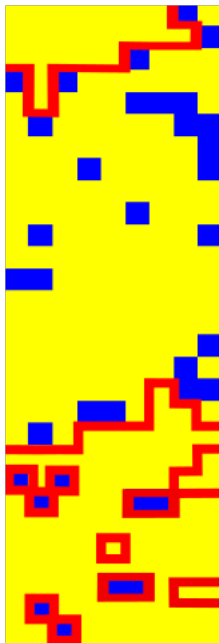
## Boundary flip algorithm:

$J = 1$  in the bulk, but the coupling between the top and the bottom is now a dynamical variable to simulate:

$\{s, \sigma, J_{0,T-1} = \pm 1\}$  is an element of the ensemble.

A link  $\sigma_{\langle 0, T-1 \rangle} = 1$  demands  $J_{0,T-1} s_0 s_{T-1} = 1$ . Thus we can flip  $J_{0,T-1}$ ,  $s_0$  and all the spins connected to  $s_0$  via some chain of links in the bulk obtaining a configuration compatible with  $\{\sigma_{\langle x,y \rangle}\}$ . This for all the spins on the bottom boundary.

Boundary  
condition  
update.  
Section of a  
 $7 \times 7 \times 21$   
lattice at  
temperature  
 $\beta = 0.250$



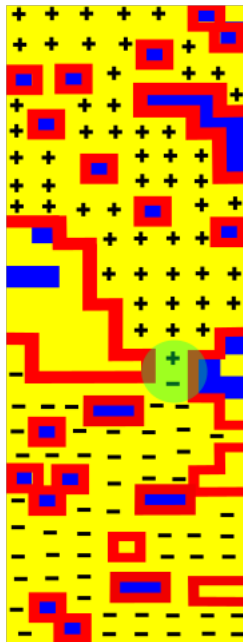
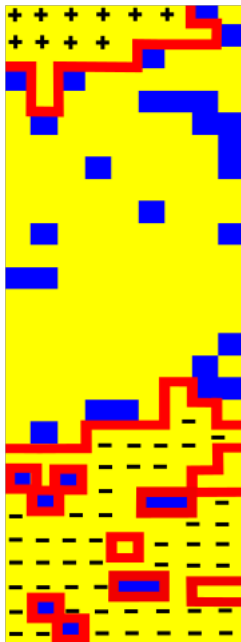
The boundary flip generates an interface between phases!

We must check this update can be done without violating the constraints imposed by the bulk links ( $\sigma_{\langle x,y \rangle} = 1$  implies  $s_x = s_y$ ).

Check all the clusters that contain sites of the lower surface and flip the boundary condition only if it can be done consistently in all the lattice.



Introduce extra  
variables  $c_x = \pm 1$   
that get  
propagated in the  
bulk during the  
costruction of the  
cluster but change  
sign when crossing  
the boundary.



We do  $N$  total steps alternating the Wolff algorithm with the boundary flip.

After each update we count if the current configuration has ferromagnetic or antiferromagnetic coupling between top and bottom.

$$\langle \delta_{J=-1} \rangle = \frac{\# \text{Antiferromagnetic}}{N}$$

$$\langle \delta_{J=+1} \rangle = \frac{\# \text{Ferromagnetic}}{N}$$

## Recap on the algorithm

- ① Hot/cold start
- ② Single cluster update
- ③ For all sites on the lower boundary we generate the correspondig clusters.
- ④ All cluster propagate a variable  $c_x$  which changes sign if there is a boundary cross.
- ⑤  $J_{0,T-1}$  is switched if  $c_x$  is consistent on all the lattice.
- ⑥ We repeat from point 2  $N$  times.
- ⑦ We count the number of configurations with ferromagnetic and antiferromagnetic boundary coupling.
- ⑧ The ratio of this values is the estimator of  $\frac{Z_{+-}}{Z_{++}}$  to be substited in  $F_s$ .

## Notes on the implementation

C++ for the Montecarlo and Jackknife algorithms, Python for data analysis, fits and plots.

The hot function of the simulation generates a cluster starting in a given position and exploring the neighbouring links. If a link is chosen to be  $\sigma_{\langle x,y \rangle} = 1$  then the adjacent site is included in the cluster and the procedure is repeated. The extra variable  $c_x$  is also propagated.

## Algorithm properties: correlation

Estimate of integrated correlation time  $\tau$ : data blocking

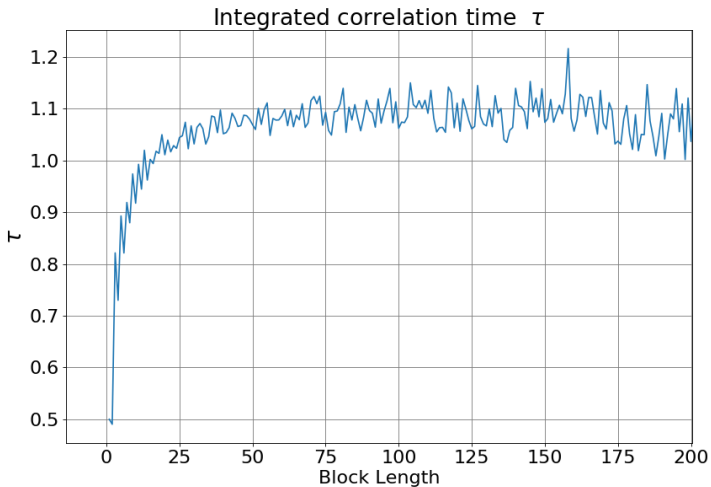
$$\sigma_{\bar{x}}^2 = 2\tau\sigma_x^2/N$$

Idea: study the fluctuation around average of block averages.

$$\sigma_B^2 = \frac{1}{N_B - 1} \sum_{i=1}^{N_B} (x_{B_i} - \bar{x})^2$$

If  $k \gg \tau$ , blocks are uncorrelated and we get  $\sigma_B^2/N_B = \sigma_{\bar{x}}^2$ .  
Asymptotically in  $k$  we have:

$$2\tau = k\sigma_B^2/\sigma_x^2$$



**Figure:** Integrated correlation time for boundary condition value ( $\beta = 0.2391, L = 10$ )

$\tau \simeq 1$ : low correlation time even for low  $T$ , big  $L$ .

## Algorithm properties: thermalization

Thermalization test: 2-sample Kolmogorov-Smirnov on magnetization distribution (almost continuous distribution).

Sample A :  $x_{T+l}, x_{T+2l}, \dots, x_{T+NI}$

Sample B :  $x_{T+(N+1)l}, x_{T+(N+2)l}, \dots, x_{T+2NI}$

T thermalization time,  $N \simeq 1000$ ,  $l \geq \tau$ .

Thermal equilibrium  $\rightarrow$  A,B same distribution (pass KS test).

T  $\simeq 5 - 10\%$  of total events passes the test for  $l \geq 3$

## Data analysis strategy

- Measure  $F_s$  at given  $\beta$ ,  $L$  through estimator
- Study statistical uncertainty on  $F_s$  estimate.

$$F_s = \ln(T) - \ln\left(\frac{1}{2} \ln\left(\frac{1 + \frac{Z_{+-}}{Z_{++}}}{1 - \frac{Z_{+-}}{Z_{++}}}\right)\right)$$

- Get  $\sigma(\beta)$  in thermodynamic limit  $L \rightarrow \infty$  from finite size lattice at different  $L$ .



## Estimation of statistical errors

We want to estimate reduced free energies  $F$  at given  $\beta, L$ .

$$\hat{F}_N = \ln(T) - \ln \left( \frac{1}{2} \ln \left( \frac{1 + \frac{\#J=-1}{\#J=1}}{1 - \frac{\#J=-1}{\#J=1}} \right) \right)$$

$N_B$  resamples created via blocked Jackknife.

We divide initial sample in  $N_B$  block with fixed length  $k \gg \tau$ .

$i$ -th resample: all blocks except block  $i$

We calculate the free energy on the resamples.

$$\hat{F}_{N-k,i} = \ln(T) - \ln \left( \frac{1}{2} \ln \left( \frac{1 + \frac{\#J=-1 \notin i}{\#J=1 \notin i}}{1 - \frac{\#J=-1 \notin i}{\#J=1 \notin i}} \right) \right)$$

Statistical error: fluctuation around average  $\bar{F}_{N-k}$  evaluated on resamples.

$$\sigma_{\bar{F}, N-k}^2 = \frac{1}{N_B - 1} \sum_i^{N_B} \left( \hat{F}_{N-k,i} - \bar{F}_{N-k} \right)^2$$

To relate fluctuation of  $N - k$ -long samples to  $N$ -long original sample multiply to get correct sum of errors.

$$\sigma_{F_N}^2 = \frac{N_B - 1}{N_B} \sum_i^{N_B} \left( \hat{F}_{N-k,i} - \bar{F}_{N-k} \right)^2$$

## Bias

By Great Numbers' Law  $\hat{F}_N$  is consistent. Is it biased?

$$\mathbb{E} \left[ \hat{F}_N \right] = F + \frac{\alpha_1}{N} + \frac{\alpha_2}{N^2} \dots$$

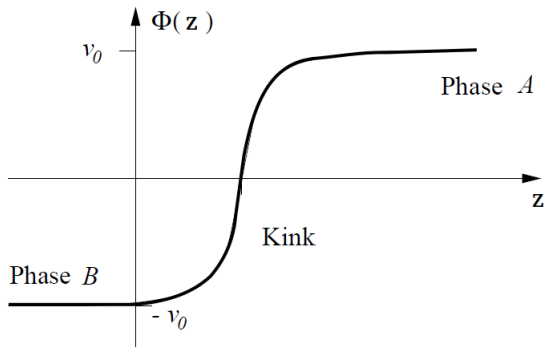
Jackknife resamples help to construct a less biased estimator

$$\hat{F}_N^{(u)} = N_B \hat{F}_N - \frac{N-k}{N} \sum_{i=1}^{N_B} \hat{F}_{N-k,i}$$

From data: bias  $\ll$  statistical uncertainty

- The simulations were executed with  $N = 10^6$  steps of the Markov chain.
- The first 10% of the Markov chain is ignored to avoid non-thermalized configurations.
- The Jackknife is executed for blocks of sizes that are divisors of 900000 going from 300 to 10000. No strong dependence of results on block length is observed.

We need model to relate  $F$  and  $L$  at given  $\beta$  near  $\beta_c$ .



**Figure:** Semiclassical "kink" solution for average magnetization  $\varphi$  between 2 phases

Near critical point, 3D Ising  $\simeq \varphi^4$ .  $F$  is related to fluctuations around kink solution.

# Capillary Wave Model

**Idea:** instead of doing calculation in  $\varphi^4$ , focus on the kink interface between the two phases.

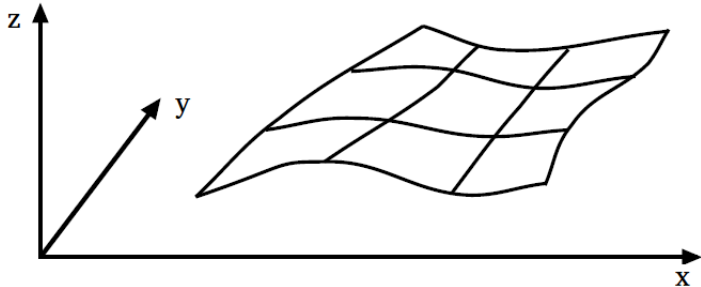


Figure: Effective 2D description of the interface.

Energy proportional to surface area:

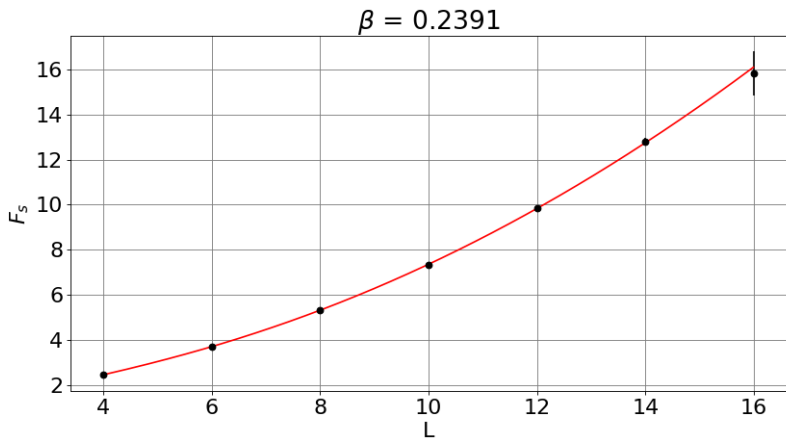
$$\mathcal{H} = \sigma(\beta) \int_0^L dx \int_0^L dy \sqrt{1 + \left(\frac{\partial h}{\partial x}\right)^2 + \left(\frac{\partial h}{\partial y}\right)^2}$$

$$\mathcal{H} = \sigma(\beta) \int_0^L dx \int_0^L dy \left(1 + \frac{1}{2}(\nabla h)^2 - \frac{1}{8}\left((\nabla h)^2\right)^2\right)$$

Quartic expansion + 2-Loop calculations:

$$F = C + \sigma L^2 - \log\left(1 + \frac{1}{4\sigma L^2}\right)$$

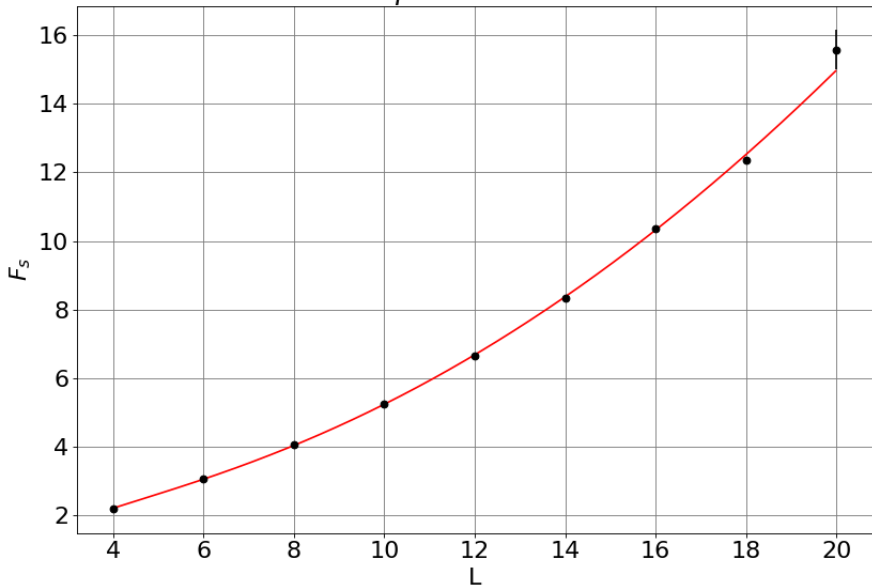
## Fit of the free energy - results



Low T, Big L: MCMC too short to flip boundary.  $F_s = \sigma L^2$  is a good fit.

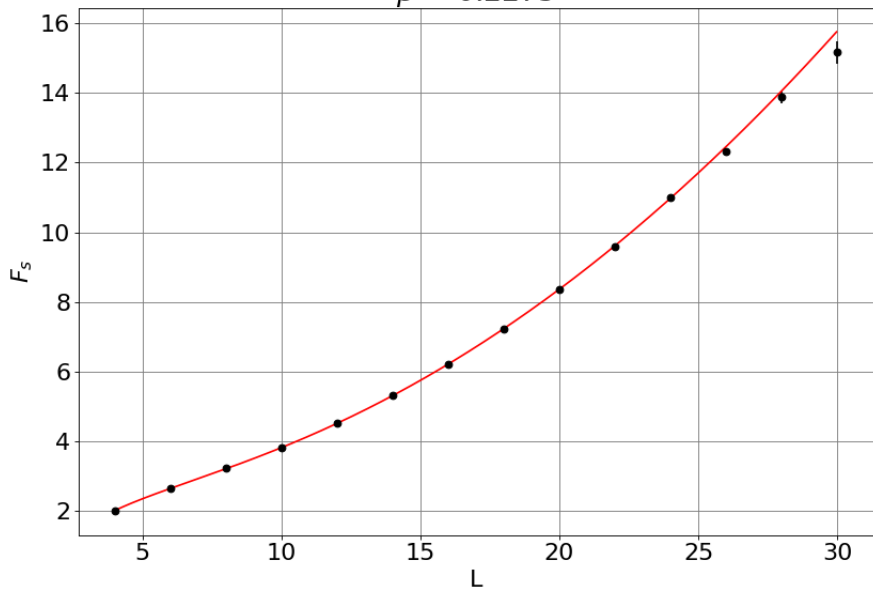


$$\beta = 0.2327$$

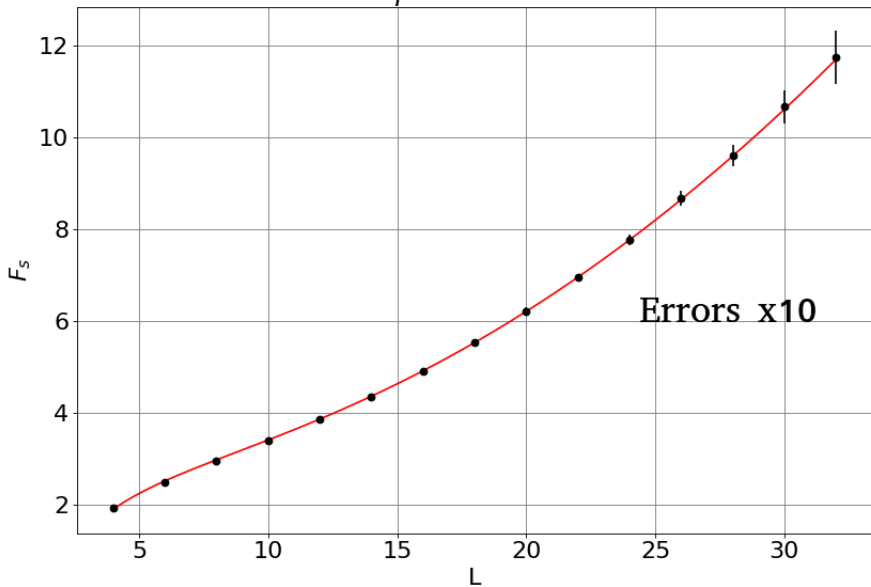


$F_s = \sigma L^2$  is a good fit.

$$\beta = 0.2275$$

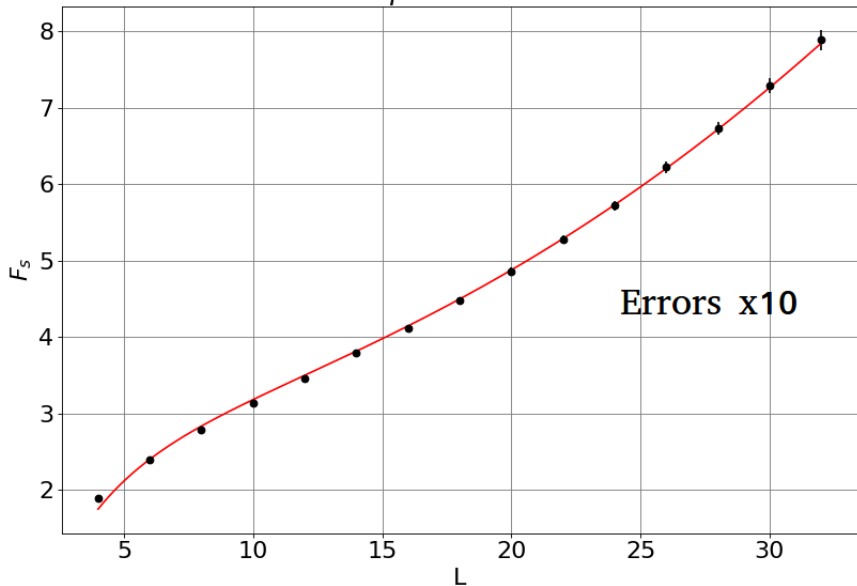


$$\beta = 0.2255$$



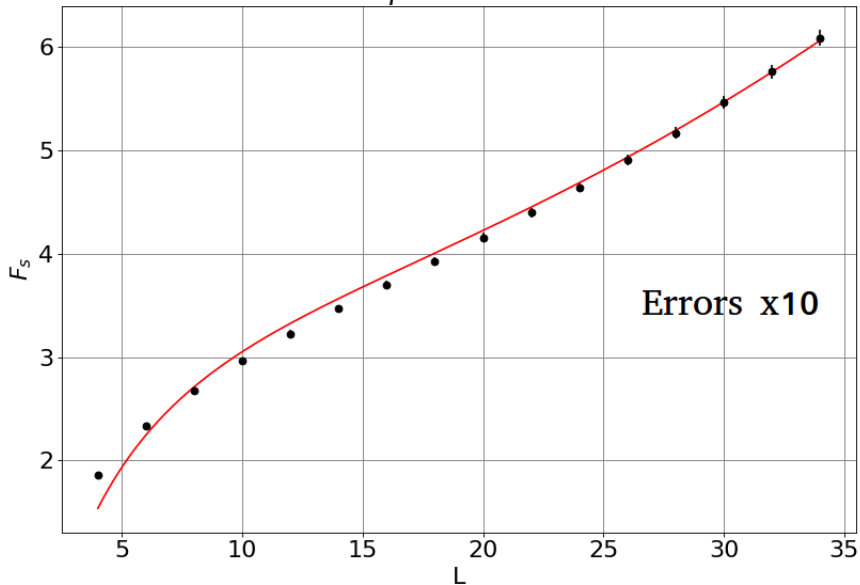
Fluctuations contribution  $-\log\left(1 + \frac{1}{4\sigma L^2}\right)$  becomes evident.

$$\beta = 0.224$$



Fluctuations contributions  $-\log\left(1 + \frac{1}{4\sigma L^2}\right)$  becomes evident.

$$\beta = 0.223$$



Systematics becomes important.

## Results

$\beta$	$\sigma$	$\chi^2/n$
0.223	$2.226(5) \cdot 10^{-3}$	1154.8
0.224	$4.637(6) \cdot 10^{-3}$	236.5
0.2255	$8.73(1) \cdot 10^{-3}$	19.9
0.2275	$1.476(2) \cdot 10^{-2}$	4.9
0.2327	$3.225(4) \cdot 10^{-2}$	22.4
0.2391	$5.60(1) \cdot 10^{-2}$	5.4

Table: Fit results for  $\sigma$ .

- Low statistical error.
- High systematics: finite  $L$  and  $T$  + truncated action + 2-loops only.
- High  $\chi^2/\text{ndof}$ .

## Fit of the critical behaviour

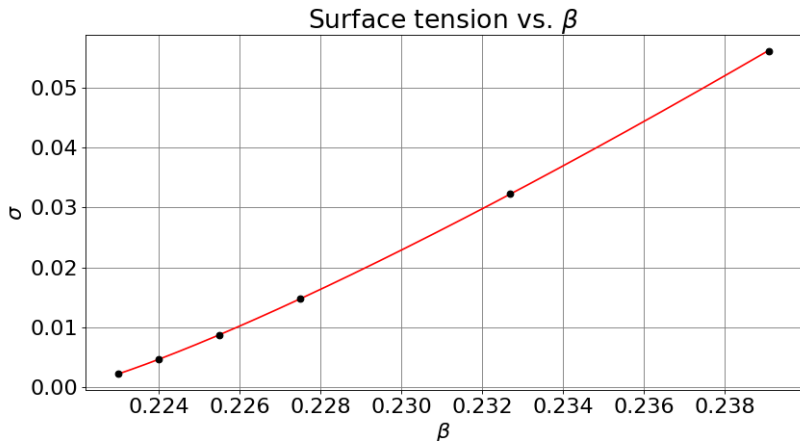


Figure: Critical scaling law fit.

Scaling law at critical point:

$$\sigma(\beta) = \sigma_0 \left| \frac{\beta - \beta_c}{\beta_c} \right|^\mu$$

$\sigma_0$	$\mu$	$\beta_c$	$\chi^2/n$
1.209(6)	1.202(2)	0.22182(1)	5.4

Table: Fit results ( $n = 3$ )

- $\mu$  correct to first digit. ( $\mu_{th} = 2\nu_{th} \simeq 1.25 - 1.26$ ).
- High  $\chi^2$ : points outside scaling region!
- High systematics! Need of corrected scaling law.



## Wegner's scaling correction

From linearized RG flow near critical point:

$$\sigma(\beta) = \sigma_0 t^\mu (1 + a_\theta t^\theta + at) \text{ with } \theta = 0.5$$

Fit input:  $\mu$  (variable),  $\theta = 0.51$ ,  $\beta_c = 0.2218$ . Fit result:

$\mu$	$\sigma_0$	$a_\theta$	$a$	$\chi^2/n$
1.209	1.198(6)	0.33(7)	0.4(2)	0.8
1.220	1.294(7)	0.01(7)	0.8(2)	1.2
1.230	1.387(7)	-0.26(6)	1.2(1)	1.8
1.240	1.486(7)	-0.53(6)	1.6(2)	2.8
1.250	1.592(8)	-0.79(6)	2.0(1)	4.1
1.256	1.658(8)	-0.93(5)	2.2(2)	5.0
1.260	1.704(8)	-1.03(6)	2.3(2)	5.8

Table: Improved fit results ( $n = 3$ )

$\sigma_0$  VERY dependent on  $\mu$  value.

# Conclusions

Year	Author(s)	Ref.	$\sigma_0$
1982	Binder	218	1.05(5)
1984	Mon and Jasnow	222	1.2(1)
1988	Mon	220	1.58(5)
1992	Klessinger and Münster	215	1.29–1.64
1993	Berg <i>et al.</i>	219	1.52(5)
1993	Ito	221	1.42(4)
1993	Hasenbusch and Pinn	60	1.22–1.49
1993	Hasenbusch	58	1.5(1)
1993	Gausterer <i>et al.</i>	223	1.92(15)
1994	Caselle <i>et al.</i>	61	1.32–1.55
1996	Zinn and Fisher	224	1.50(1)
1997	Hasenbusch and Pinn	62	1.55(5)

Figure: Previous results for  $\sigma_0$  in 3D Ising

- Our result for  $\sigma_0$  agree with other results.
- Need for better theoretical understanding of parameters of the theory ( $\mu$ ).

Thanks for your attention!

## Backup slides

$$\begin{aligned} Z &= \sum_{\{s=\pm 1\}} \exp \left( \beta \sum_{\langle x,y \rangle} s_x s_y \right) = \sum_{\{s=\pm 1\}} \prod_{\langle x,y \rangle} e^{\beta s_x s_y} = \\ &= e^{-dV\beta} \sum_{\{s=\pm 1\}} \prod_{\langle x,y \rangle} (1 + \delta_{s_x, s_y} (e^{2\beta} - 1)) = \\ &= e^{-dV\beta} \sum_{\{s\}} \prod_{\langle x,y \rangle} \sum_{\{\sigma_{\langle x,y \rangle}=0,1\}} [(1 - \sigma_{\langle x,y \rangle}) + \sigma_{\langle x,y \rangle} \delta_{s_x, s_y} (e^{2\beta} - 1)] \end{aligned}$$

Also valid for generic coupling  $J_{\langle x,y \rangle}$ :

$$\begin{aligned}
 Z &= \sum_{\{s=\pm 1\}} \exp \left( \beta \sum_{\langle x,y \rangle} J_{\langle x,y \rangle} s_x s_y \right) = \sum_{\{s=\pm 1\}} \prod_{\langle x,y \rangle} e^{\beta J_{\langle x,y \rangle} s_x s_y} = \\
 &= e^{-dV\beta} \sum_{\{s=\pm 1\}} \prod_{\langle x,y \rangle} \left( 1 + \delta_{J_{\langle x,y \rangle} s_x s_y, 1} (e^{2\beta} - 1) \right) = \\
 &= e^{-dV\beta} \sum_{\{s\}} \prod_{\langle x,y \rangle} \sum_{\{\sigma_{\langle x,y \rangle}=0,1\}} (1 - \sigma_{\langle x,y \rangle}) + \\
 &\quad + \sigma_{\langle x,y \rangle} \delta_{J_{\langle x,y \rangle} s_x s_y, 1} (e^{2\beta} - 1)
 \end{aligned}$$

For a fixed spin configuration  $\{s\}$  the links are independent.

$$p_0 = p(\sigma_{\langle x,y \rangle} = 0) = \exp\left(-2\beta\delta_{J_{\langle x,y \rangle} s_x s_y, 1}\right)$$

$$p_1 = p(\sigma_{\langle x,y \rangle} = 1) = 1 - p(\sigma_{\langle x,y \rangle} = 0)$$

(if  $J_{\langle x,y \rangle} s_x s_y = 1$  the weights in  $Z$  are normalized to  $e^{2\beta}$ )

For simplicity let's put  $J_{\langle x,y \rangle} = 1$ . For fixed  $\sigma_{\langle x,y \rangle}$  only configurations of spins that satisfy the constraint  $s_x = s_y$  where  $\sigma_{\langle x,y \rangle} = 1$  have a non zero probability. All configurations of spin that satisfy the constraint have the same weight.

## Swendsen and Wang algorithm:

- Generate a link configuration  $\sigma_{\langle x,y \rangle}$  based on the current spin configuration by using probabilities  $p_0$  and  $p_1$ .
- For each cluster choose a spin ( $s = \pm 1$ ) with probability  $\frac{1}{2}$ . In general the update step must be compatible with the constraint  $J_{\langle x,y \rangle} s_x s_y = 1$ .
- The newly generated spin configuration is the next element of the Markov chain.

The SW is **ergodic**. It can be proved it satisfies the **detailed balance**.

We now prove all our cluster algorithms satisfy the detailed balance condition.

In the cluster algorithm we update both the spins  $\{s\}$  and the links  $\{\sigma_{x,y}\}$ . The ensemble contains both spins and links configurations:  $\{s, \sigma\}$ .

$$\frac{P(\{s_0, \sigma_0\} \rightarrow \{s_1, \sigma\})}{P(\{s_1, \sigma_0\} \rightarrow \{s_0, \sigma\})} = \frac{P(\{s_1\}|\{\sigma, s_0\}) P(\{\sigma\}|\{s_0\})}{P(\{s_0\}|\{\sigma, s_1\}) P(\{\sigma\}|\{s_1\})}$$

(this is not the detailed balance in the ensemble of  $\{s, \sigma\}$  as the link configurations don't get exchanged!)



$P(\{s\}|\{\sigma, s_0\}) = \frac{1}{2^{\#cluster}}$  if  $\{s\}$  is compatible with  $\{\sigma\}$ , null otherwise. Notice that in the SW algorithm  $\{s\}$  is actually independent on  $\{s_0\}$ .

$$\text{Thus } P(\{s_1\}|\{\sigma, s_0\}) = P(\{s_0\}|\{\sigma, s_1\}).$$

In general this is the condition we ask to cluster algorithms.

$$P(\{\sigma\}|\{s\}) = \prod_{\substack{\sigma_{\langle x,y \rangle}=0 \\ J_{\langle x,y \rangle} s_x s_y=1}} e^{-2\beta} \prod_{\sigma_{\langle x,y \rangle}=1} (1 - e^{-2\beta})$$

for  $\{s\}$  compatible with  $\{\sigma\}$ .

The first factor arise from the unconnected links for which  $J_{\langle x,y \rangle} s_x s_y = 1$  each being in this state with probability  $e^{-2\beta}$ .

The second one is from the connected links (for which  $J_{\langle x,y \rangle} s_x s_y = 1$  necessarily).

The second factor is **independent of  $\{s\}$**  and will be neglected in the sequent.

We obtain:

$$P(\{\sigma\}|\{s\}) = \prod_{\substack{\sigma_{\langle x,y \rangle}=0 \\ J_{\langle x,y \rangle} s_x s_y=1}} e^{-2\beta}$$

Now we compute (reminding  $\{s_0\}$  and  $\{s_1\}$  share the same  $\{\sigma\}$ ):

$$\frac{e^{-\beta \mathcal{H}(\{s_1\})}}{e^{-\beta \mathcal{H}(\{s_0\})}} = \frac{\prod_{\langle x,y \rangle} e^{J_{\langle x,y \rangle} s_x^1 s_y^1}}{\prod_{\langle x,y \rangle} e^{J_{\langle x,y \rangle} s_x^0 s_y^0}} =$$

$$\frac{\prod_{J_{s_x^1 s_y^1}=+1}^{\sigma=0} e^{\beta} \prod_{J_{s_x^1 s_y^1}=-1}^{\sigma=0} e^{-\beta} \prod_{J_{s_x^1 s_y^1}=+1}^{\sigma=1} e^{\beta}}{\prod_{J_{s_x^0 s_y^0}=+1}^{\sigma=0} e^{\beta} \prod_{J_{s_x^0 s_y^0}=-1}^{\sigma=0} e^{-\beta} \prod_{J_{s_x^0 s_y^0}=+1}^{\sigma=1} e^{\beta}}$$

The last part having  $\sigma = 1$  obviously depends only on  $\{\sigma\}$  for all  $J_{\langle x,y \rangle} s_x s_y$  beeing forced to 1 if  $\sigma = 1$ .

We observe that:

$$\prod_{\substack{\sigma=0 \\ J s_x^1 s_y^1 = -1}} e^{-\beta} \times \prod_{\substack{\sigma=0 \\ J s_x^1 s_y^1 = 1}} e^{-\beta} = \prod_{\sigma=0} e^{-\beta} = k$$

$k$  depends only on the link configuration  $\{\sigma\}$

$$\prod_{\substack{\sigma=0 \\ J s_x^1 s_y^1 = -1}} e^{-\beta} = k \prod_{\substack{\sigma=0 \\ J s_x^1 s_y^1 = 1}} e^{\beta}$$

$$\frac{e^{-\beta \mathcal{H}(\{s_1\})}}{e^{-\beta \mathcal{H}(\{s_0\})}} = \frac{\prod_{J s_x^1 s_y^1 = +1}^{\sigma=0} e^{2\beta}}{\prod_{J s_x^0 s_y^0 = +1}^{\sigma=0} e^{2\beta}} = \frac{\prod_{J s_x^0 s_y^0 = +1}^{\sigma=0} e^{-2\beta}}{\prod_{J s_x^1 s_y^1 = +1}^{\sigma=0} e^{-2\beta}}$$

We arrived at:

$$\frac{P(\{s_0, \sigma_0\} \rightarrow \{s_1, \sigma\})}{P(\{s_1, \sigma_0\} \rightarrow \{s_0, \sigma\})} = \frac{e^{-\beta \mathcal{H}(\{s_1\})}}{e^{-\beta \mathcal{H}(\{s_0\})}}$$

$$P(\{s_0\} \rightarrow \{s_1\}) = \sum_{\{\sigma\}, \{\sigma_0\}} P(\{s_0, \sigma_0\} \rightarrow \{s_1, \sigma\})$$

We thus obtain the detailed balance:

$$\frac{P(\{s_0\} \rightarrow \{s_1\})}{P(\{s_1\} \rightarrow \{s_0\})} = \frac{e^{-\beta \mathcal{H}(\{s_1\})}}{e^{-\beta \mathcal{H}(\{s_0\})}}$$

- The only requirement on the update step is that  $P(\{s_1\}|\{\sigma, s_0\}) = P(\{s_0\}|\{\sigma, s_1\})$ .
- We can also update the coupling constants  $J_{\langle x,y \rangle}$  as long as  $J_{\langle x,y \rangle} s_x s_y = 1$  where  $\sigma = 1$ .

This two observations give rise to two key modification of the SW algorithm: the Wolff algorithm and the boundary flip.

```
stack<site> stack
stack.push(seed)
while(!stack.empty())
    site current = stack.top()
    if(cluster[current] is incostintent) flag = 1;
    else if(cluster[current] == 0)
        cluster[current] = cluster[old];
        for(d = 0; d < 3; d++)
            for(a = -1; a < 2; a = a + 2)
                next = current + a
                check if we are on the boundary
                if(cluster[next] == 0)
                    if(p > 0 and random < p) stack.push(next)
return flag
```