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

Federico Belliardo
Marco Costa

Dipartimento di Fisica
Università di Pisa

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Summary

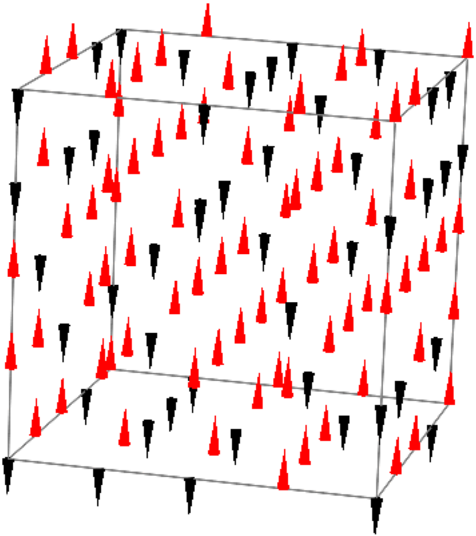
- 3D Ising models
- Definition of the surface tension
- Cluster algorithms and boundary flip
- Notes on the implementation
- Estimation of the errors and autocorrelation
- Fit of the free energy
- Fit of the critical behaviour
- Conclusions

3D Ising model

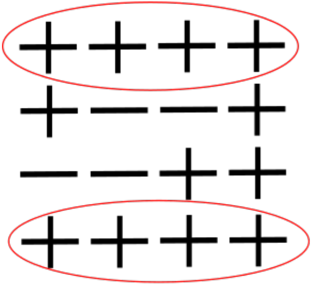
$$\mathcal{H} = -\sum_{\langle x,y\rangle} J_{\langle x,y\rangle} s_x s_y$$

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

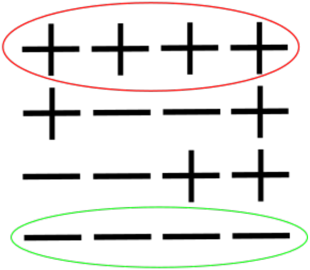
$J_{\langle x,y\rangle} = -1$ antiferromagnetic



Definition of the surface tension



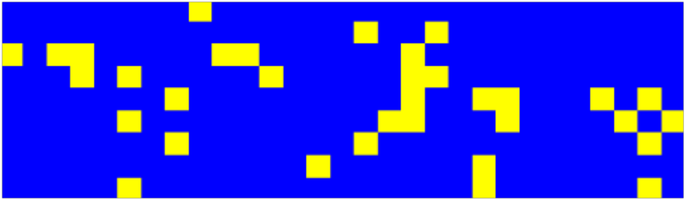
Z_{++}



Z_{+-}

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

Z_{+-}



Z_{++}

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

$\sigma =$ interface free energy per unit area

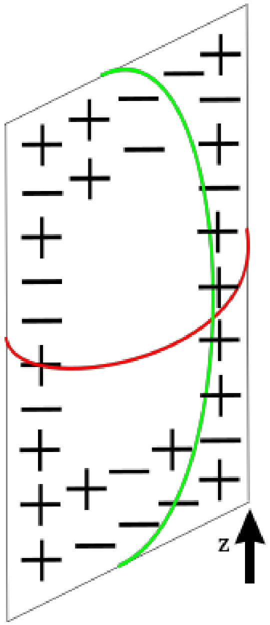
Redefinition of Z_{++} and Z_{+-}.

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

Always ferromagnetic link in x and y directions.

Same definition for σ.

Periodic boundary conditions reduce the finite size effect.



General strategy

- Measure F_s on finite lattice size L at given β near β_c.
- Repeat for different L, same β.
- Find a theoretical formula to link $F_s(L)$ and σ.
- Extrapolate σ at given β.
- Repeat the above procedure for different β, 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.

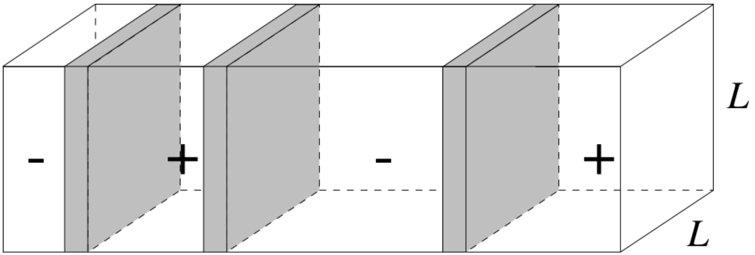
$$Z = \sum_{\{s\},J} \exp \left(\beta \sum_{\langle x,y \rangle} J_{\langle x,y \rangle} s_x s_y \right)$$

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

Ratio of measurable expectation values.

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

Thermodynamic limit $\longrightarrow$ 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.

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

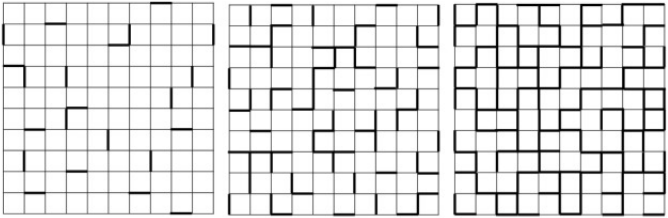
$$\frac{Z_{+-}}{Z_{++}} = \frac{Z_1 + \frac{Z_1^3}{3!} + \frac{Z_1^3}{5!} + \ldots}{1 + \frac{Z_1^2}{2!} + \frac{Z_1^4}{4!} + \ldots} = \tanh(\exp(-F_S + \ln T))$$

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

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 slowling down. Swendsen and Wang (1987).

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



$$Z = \sum_{\{s=\pm 1\}} \exp\left(\beta \sum_{\langle x,y\rangle} s_x s_y\right) = \sum_{\{s=\pm 1\}} \prod_{\langle x,y\rangle} e^{\beta s_x s_y} =$$

$$= e^{-dV\beta} \sum_{\{s=\pm 1\}} \prod_{\langle x,y\rangle} \left(1 + \delta_{s_x,s_y}\left(e^{2\beta} - 1\right)\right) =$$

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

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

$$Z = \sum_{\{s=\pm 1\}} \exp\left(\beta \sum_{\langle x,y\rangle} J_{\langle x,y\rangle} s_x s_y\right) = \sum_{\{s=\pm 1\}} \prod_{\langle x,y\rangle} e^{\beta J_{\langle x,y\rangle} s_x s_y} =$$

$$= e^{-dV\beta} \sum_{\{s=\pm 1\}} \prod_{\langle x,y\rangle} \left(1 + \delta_{J_{\langle x,y\rangle} s_x s_y,1} \left(e^{2\beta} - 1\right)\right) =$$

$$= e^{-dV\beta} \sum_{\{s\}} \prod_{\langle x,y\rangle} \sum_{\{\sigma_{\langle x,y\rangle}=0,1\}} \left(1 - \sigma_{\langle x,y\rangle}\right) +$$
$$+\sigma_{\langle x,y\rangle} \delta_{J_{\langle x,y\rangle} s_x s_y,1} \left(e^{2\beta} - 1\right)$$

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

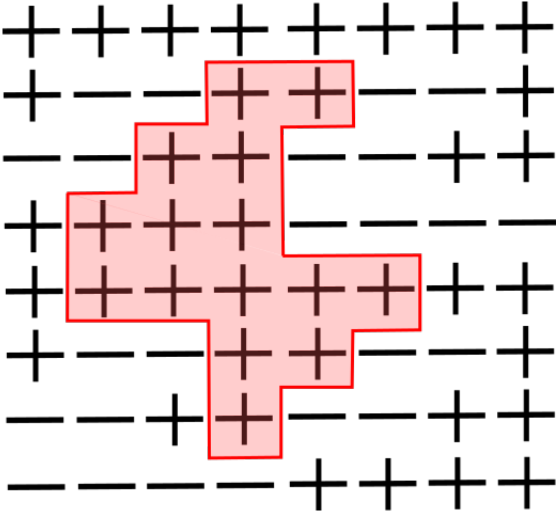
$$p_0 = p\left(\sigma_{\langle x,y\rangle} = 0\right) = \exp\left(-2\beta\delta_{J_{\langle x,y\rangle}s_x s_y,1}\right)$$

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

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

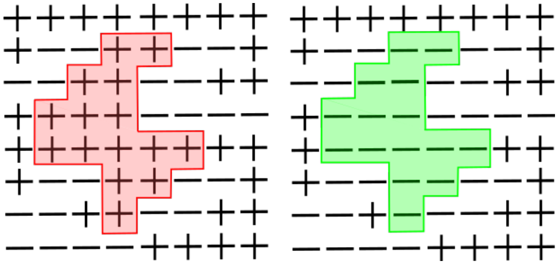
For simplicity let's put $J_{\langle x,y\rangle} = 1$. For fixed $\sigma_{\langle x,y\rangle}$ only configurations of spins that satisfy the constraint $s_x = s_y$ where $\sigma_{\langle x,y\rangle} = 1$ have a non zero probability. All configurations of spin that satisfy the constraint have the same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

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.



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 ad viceversa is obviously the same, beeing the probability of choosing the right cluster. Practically we build only **one cluster** starting from a seed.

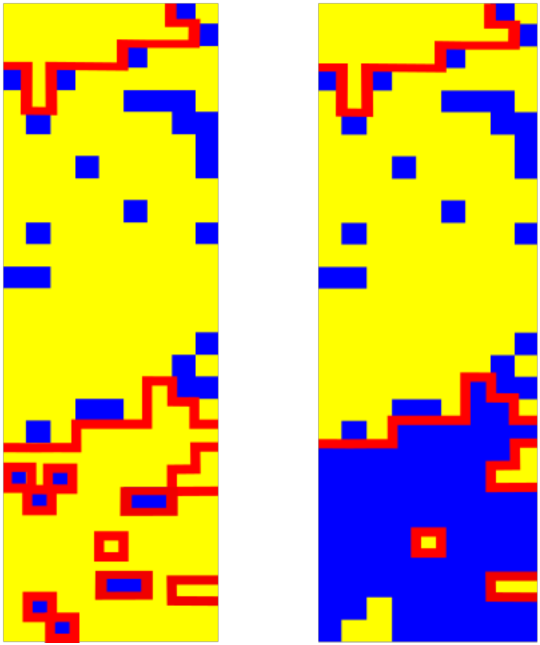


Boundary flip algorithm:

$J = 1$ 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 ensamble.

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 obtaing 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 $\beta = 0.250$

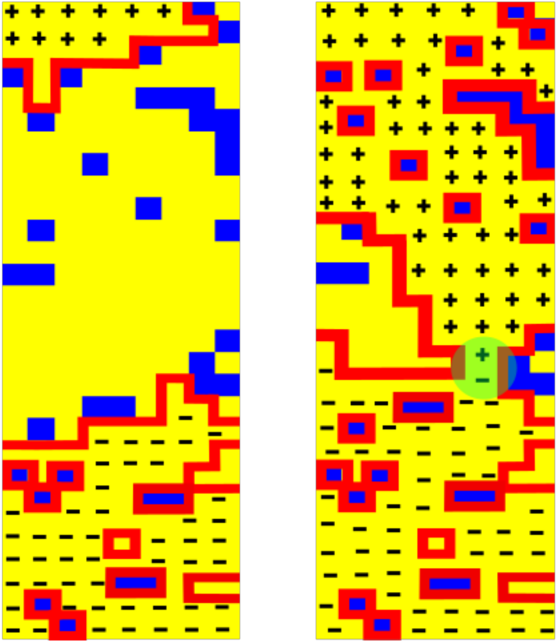


The boundary flip generates an interface between phases!

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.

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

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

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.

```
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
```

Algorithm properties: correlation

Estimate of integrated correlation time τ: 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

$\tau \simeq 1$: low correlation time even for $\beta = 0.2391, L = 10$

Algorithm properties: thermalization

Thermalization test: Kolmogorov-Smirnov If after thermalization time T the distribution of observbables is the same (2 sided KS test) system is in thermal equilibrium.

Estimation of the errors

We want to estimate reduced free energies F at given β, L.

$$\hat{F}_N = \frac{\#\text{Antiferromagnetic}}{\#\text{Ferromagnetic}}$$

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.

$$\hat{F}_{N-k,i} = \frac{\sum_{\text{no block i}} \#\text{Antiferromagnetic}}{\sum_{\text{no block i}} \#\text{Ferromagnetic}}$$

Statistical error: fluctuation around $\hat{F}_N$ evaluated on resamples.

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

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

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

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-termalized 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 β near β_c.

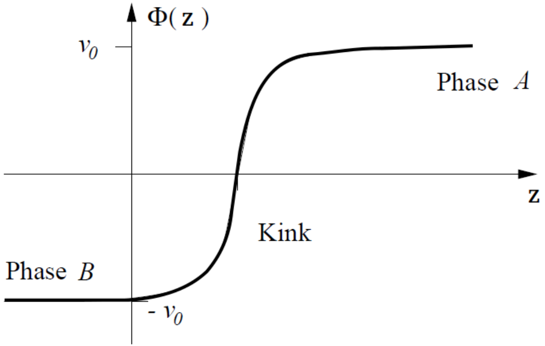


Figure: Semiclassical "kink" solution for average magnetization φ between 2 phases

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 φ^4, focus on the kink interface between the two phases.

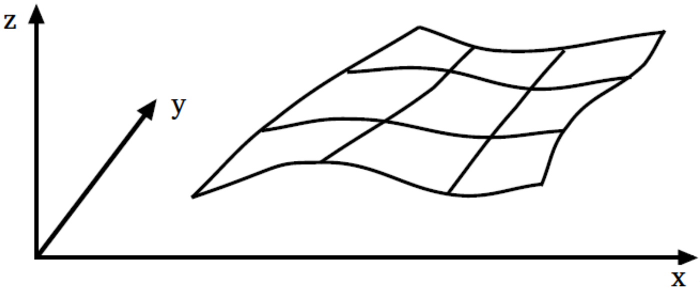


Figure: Effective 2D description of the interface.

Energy proportional to surface area:

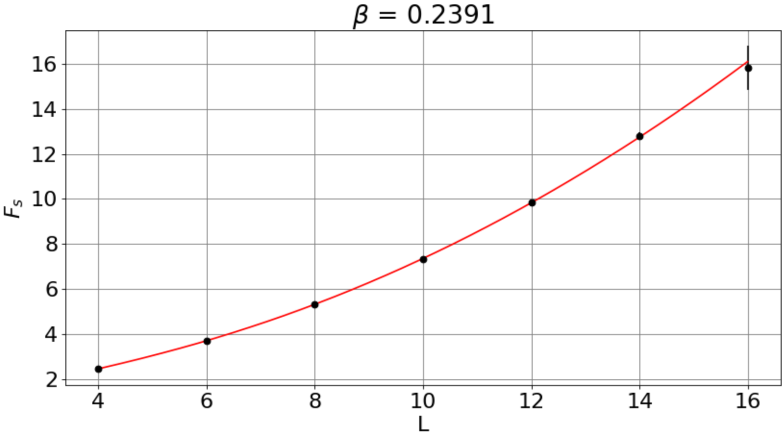
$$\mathcal{H} = \sigma(\beta) \int_0^L dx \int_0^L dy \sqrt{1 + \left(\frac{\partial h}{\partial x}\right)^2 + \left(\frac{\partial h}{\partial y}\right)^2}$$

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

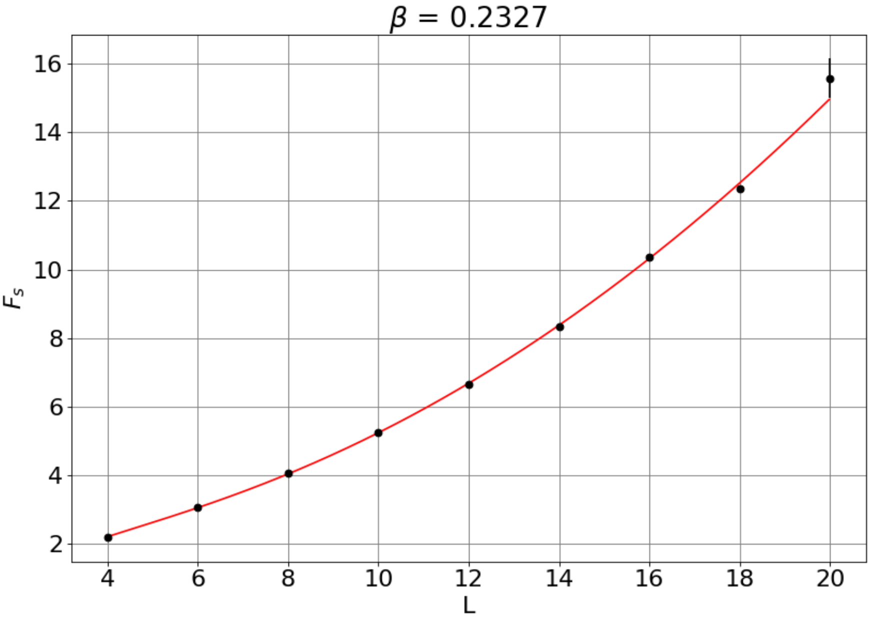
Quartic expansion + 2-Loop calculations:

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

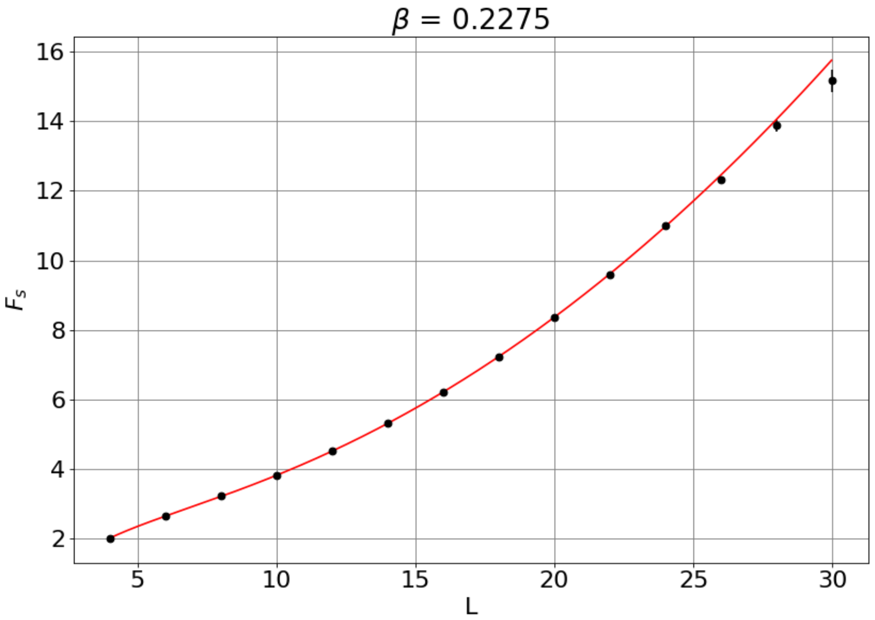
Fit of the free energy - results



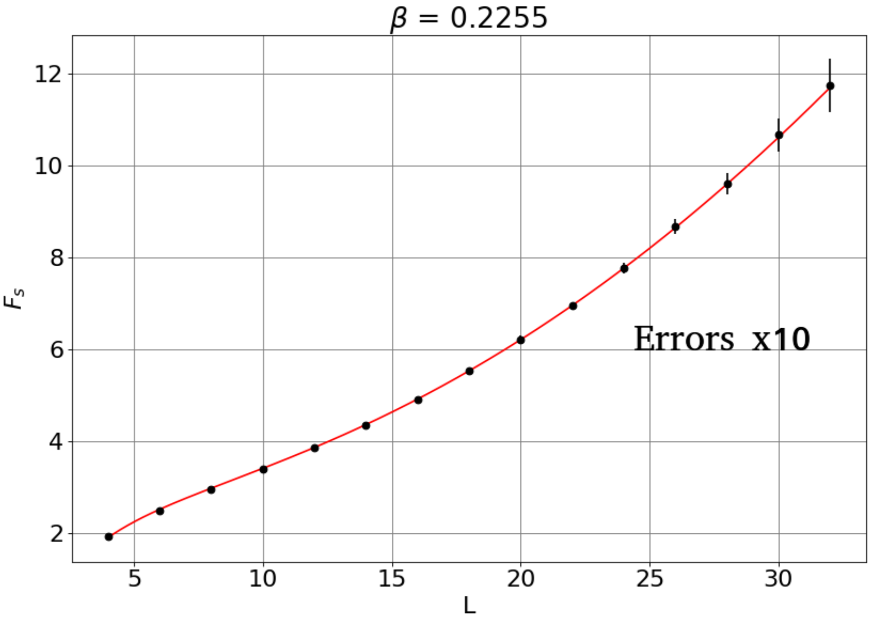
Low T, Big L: MCMC too short to flip boundary. $F_s = \sigma L^2$ is a good fit.



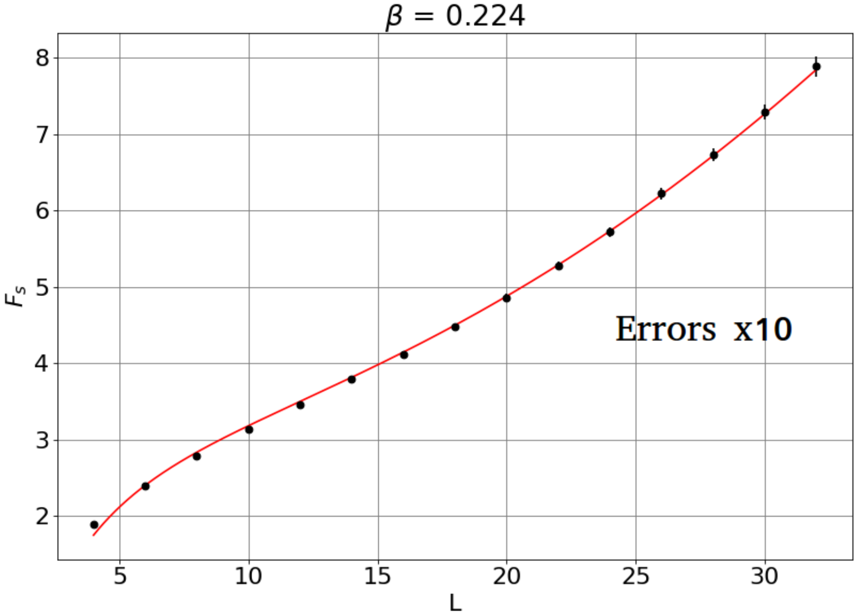
$F_s = \sigma L^2$ is a good fit.



β = 0.2275
F_s
L
2
4
6
8
10
12
14
16
5
10
15
20
25
30



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



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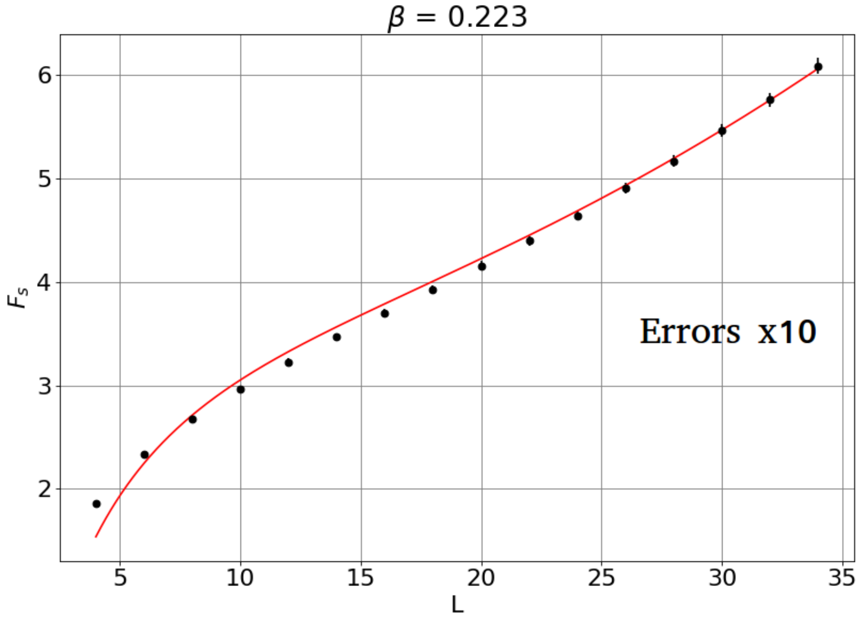

Systematics becomes important.

Results

β	σ	χ^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 σ.

- Low statistical error.
- High systematics: finite L and T + truncated action + 2-loops only.
- High χ^2/ndof.

Fit of the critical behaviour

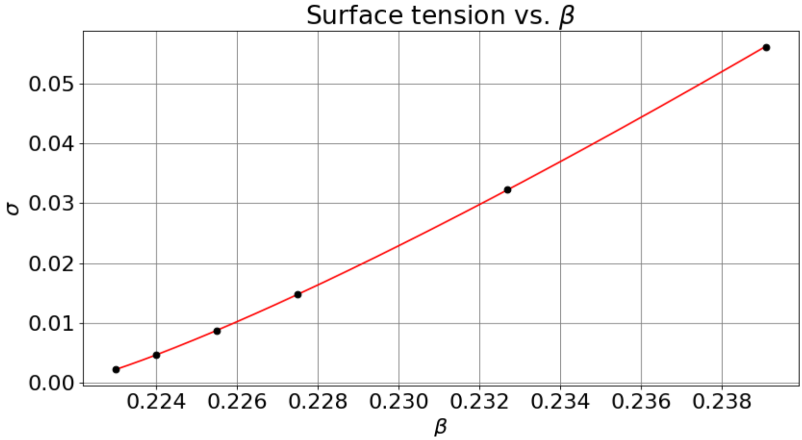

Figure: Critical scaling law fit.

Scaling law at critical point:

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

σ_0	μ	β_c	χ^2/n
1.209(6)	1.202(2)	0.22182(1)	5.4

Table: Fit results ($n = 3$)

- Correct critical exponent from Widom law.
- High χ^2: points outside scaling region!
- High systematics! Need of corrected scaling law.

Wegner's scaling correction

From linearized RG flow near critical point:
$\sigma(\beta) = \sigma_0 t^{\mu}\left(1 + a_\theta t^\theta + at\right)$ with $\theta = 0.5$

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

μ	σ_0	a_θ	a	χ^2/n
1.200	1.124(6)	0.61(8)	0.0(2)	0.6
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
1.256	1.658(8)	-0.93(5)	2.2(2)	5.0

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

σ_0 VERY dependent on μ value.

Conclusions

Year	Author(s)	Ref.	σ_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 *et al.*	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 *et al.*	223	1.92(15)
1994	Caselle *et al.*	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 σ_0 in 3D Ising

- Our result for σ_0 agree with other results.
- Need for better theoretical understanding of parameters of the theory (μ).

Swendsen and Wang algorithm:

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

The SW is **ergodic**. It can be prooved it satisfy 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 ensamble contains both spin and link configurations: $\{s, \sigma\}$.

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

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

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

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

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

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

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 neglettend in the sequent.

We obtain:

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

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

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

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

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:

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

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

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

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

We arrived at:

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

$$P\left(\{s_0\} \to \{s_1\}\right) = \sum_{\{\sigma\},\{\sigma_0\}} P\left(\{s_0, \sigma_0\} \to \{s_1, \sigma\}\right)$$

We thus obtain the detailed balance:

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

- The only requirement on the update step is that $P\left(\{s_1\}|\{\sigma, s_0\}\right) = P\left(\{s_0\}|\{\sigma, s_1\}\right)$.
- 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.