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The 2-dimensional Ising model with minus boundary condition

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von

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1.1. The Ising model

The phenomenon of magnetism belongs to one of the oldest observations in nature which focused the academic interest of scientists as well as of philosophers and engineers while it remains a sophisticated subject of investigation till today. One remarkable effect in ferromagnets is the spontaneous magnetization on cooling down the substance below a critical temperture, the so called *Curie temperature*.

The Ising model represents one of the historical successes to qualitatively reproduce this critical behaviour. The crucial point is its simplicity of modelling the essential behaviours which lead to the observed phase transition. In general the system is modelled as a quadratic or cubic lattice of particles $i \in I = \{1, \ldots, N\}$ each carrying an elementary magnetization of only two distinct values $-\frac{1}{2}$ and $+\frac{1}{2}$ all oriented along the same axis. This concept finds its realistic counterparts in spin-$\frac{1}{2}$-particles like electrons in an embedding magnetic field. Each of those spins causes a magnetic field whose strength decreases with distance and influences the surrounding particles. For the sake of simplicity the Ising model assumes only the so called *nearest neighbours* to be coupled and neglects wider range interactions completely. Two particles are nearest neighbours if no other particle is located closer to one of them. In a one-dimensional Ising system an ordinary particle has two nearest neighbours, in two dimensions four, in a d-dimensional system $2d$. These magnetic interactions contribute to the energy of the whole system as well as to an interaction of an external field h which, again for simplicity, is parallel oriented to the axis of spin direction. Having a certain spin configuration $\sigma \in \mathcal{S} := \{I \to \{-1, +1\}, i \mapsto \sigma_i\}$ the Hamiltonian of the system is

$$H_h(\sigma) \;:=\; -\sum_{i,j \in I} J_{ij}\sigma_i\sigma_j - h\sum_{i \in I}\sigma_i$$

where $J_{ij} = 1$ if i and j are nearest neighbours and $J_{ij} = 0$ else. Formal simplification led

us to consider spins to be of values -1 or $+1$ and magnetic interaction constants equal 1.

Although the system has a quadratic or cubic topology there are freedoms to define the boundary of finite systems $N < \infty$. Common are *free* boundaries where corresponding edge particles have a reduced number of nearest neigbours or *periodic* boundaries where the matrix J_{ij} defines a nearest neighbourhood topology of a loop, a torus or a hyper-torus. Our case of interest is the *fixed* boundary of a system $I \cong \mathbb{Z}^2$ whose spins are all non-variable and negative except of a finite number forming a square of length L with $N = L^2$ particles. The set of all couplings with varying and fixed spins is called the *minus boundary*.

Determining the macroscopic behaviour leads in general to the more abstract problem of calculating the *partition function* (e.g. in Boltzmann statistics)

$$Z_{\beta,h} \;:=\; \sum_{\sigma\in\mathcal{S}} \exp\left(-\beta H_h\left(\sigma\right)\right), \quad \beta := 1/k_B T, \quad k_B := 1$$

or the *Gibbs measure* (the probability measure determining the Boltzmann statistics)

$$\mu\left(S \subset \mathcal{S}\right) \;:=\; Z_{\beta,h}^{-1} \cdot \sum_{\sigma\in S} \exp\left(-\beta H_h\left(\sigma\right)\right)$$

from which essential system information can be concluded, e.g.

$$\begin{aligned} E &= \langle H\rangle = \partial_\beta Z_{\beta,h} \\ m &= \langle M\rangle = \partial_h Z_{\beta,h}/\beta \\ &\ldots \end{aligned}$$

In practice difficulties arises from the fact that this partition sum has as many summands as the space of states $\mathcal{S}$ has elements, $\#\mathcal{S} = 2^N$. While properties of the thermodynamic limit get obvious for system sizes $N \sim 10^4 \ldots 10^6$ today's capability of single CPU cores enables calculation for lattices of sizes $N = 6^2$ or 7^2 at maximum. Approaches yielding concise formulas for $Z_{\beta h}$ (in thermodynamic limit $L \to \infty$) basing on *transfer matrix method* like the legendary Onsager solution for 2-dimensional Ising model with periodic boundary remain exceptions and solutions of 3-dimensional lattices or 2-dimensional with minus boundary are unknown – although this problem has a long tradition and is canonical content of lectures in statistical physics for decades. Despite that unsolved problem many partial aspects can be formulated explicitly which we will discuss next.

1.2. The matter of interest

One proud achievement made by statistical analysts is the explicit formulation of the *spontaneous magnetization* of the 2-dimensional Ising model with periodic boundary for $L \to \infty$: [13]

$$m^*_\beta \;=\; \begin{cases} \beta > \beta_c \;:\; \left(1 - \left(\sinh\left(2J\beta\right)\right)^{-4}\right)^{1/8} \\ \beta \leqslant \beta_c \;:\; 0 \end{cases} \quad , \quad \beta_c = \frac{\log\left(1+\sqrt{2}\right)}{2J}$$

Since magnetization has at least two different possible directions and the average magnetization is zero (without exterior field) theorists give a clear definition of m^*_β as a limit of ensembles prefering the plus phase. I met two conventions [11] [18]

$$\begin{aligned} \text{a)}\; m^*_\beta &:= \text{“}\lim_{L\to\infty} \langle m\rangle_{\beta,\text{fixed (+)-boundary}}\text{”} \\ \text{b)}\; m^*_\beta &:= \text{“}\lim_{h\to 0^+} m^*_{\beta,\text{periodic}}\left(h\right)\text{”} \end{aligned}$$

In detail: a) formulates a finite size scaling of the average magnetization $\langle m\rangle_L\left(\beta, h=0\right)$ of $(L\times L)$-lattice with temperature β, vanishing external field h and (+)-boundary condition, i.e. all out-of-boundary spins are positive. The positive boundary forces the (+)-phase to dominate the system while the limit $L\to\infty$ generally damps the influence of boundary condition until it vanishes. The limit represents the spontaneous magnetization as if the system has evolved into the positive branch. The formulation of b) is another avenue. Here we are considering the thermodynamic limits $m^*_\beta\left(h\right)$ of magnetizations with various fixed but *positive* exterior fields h. Here the one-side limit $h\to 0^+$ gives again the positive spontaneous magnetization. Both formulations result in equivalent definitions. But what happens if we combine both limits to competing influences

$$\text{c)}\; m \;=\; \text{“}\lim_{h\to 0^+}\lim_{L\to\infty} \langle m\rangle_{\text{fixed (−)-boundary}}\text{”}$$

having a (−)-boundary forcing the system in the minus phase while an external positive field h damps the boundary influence. **How large is h such that they compensate each other, i.e. $\langle m\rangle = 0$?** Or: **How are h and L related to each other such that “nobody wins” the magnetization “battle”?** This is the question this Diplom thesis was concerning with. A central role played the actual computational simulation which afterwards turned out to be a formidable and inherently difficult task. The most notable

result of my measurements is the critical field $h_c(\beta, L)$ and the magnetization $\langle m \rangle$ as well as the magnetical susceptibility $\langle \chi \rangle$ in dependence of β and $h = h_c(\beta)$. These obtained data shall provide an empirical counterpart to the theoretical paper [11].

Let us assume the system is prepared with an exterior field such that $\langle m \rangle = 0$. As in the case of standard Ising model this does not imply configurations σ with $M(\sigma) \approx 0$ to be privileged. For subcritical temperatures $\beta > \beta_c$ we find the typical preference of magnetized phases again. In contrast to the standard Ising case there is an assymetry of how the system is magnetized depending on the phase, if it is positive or negative. While the minus phase takes the ordinary form of an omni-present cluster with few positive sprinkles due to thermal fluctuation the plus phase *must* have a surface between a positive region and the negative boundary. This surface consists of anti-binding couplings undermining the local energy minimum. To be close to the local minimum the system is forced to reduce the negative couplings, i.e. to reduce the length (or area) of the surface. The resulting *surface tension* turnes the plus phase to a droplet.

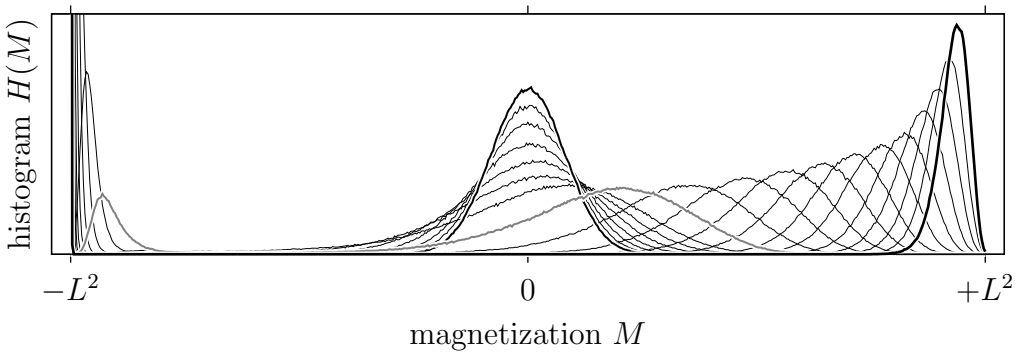

Fig. 1.1.: *Magnetization histograms for different β.*

The (in general direction-dependent) surface tension $\tau(\boldsymbol{n})$ is given by the ratio of the (free) energy of a plane surface perpendicular to $\boldsymbol{n}$ and the (free) energy of the phase without a surface. In the Ising structure we prepare plane surfaces of well-defined direction with boundary conditions again: A lattice of finite size is intersected by a half plane whose one half defines the fixed boundary spins to be positive and the other half the other fixed boundary spins to be negative. The case without surface is prepared as discussed above in a) receiving the spontaneous magnetization. Again with the limit $L \to \infty$ we yield the

thermodynamic limit.

$$\tau(\boldsymbol{n}) = \lim_{L\to\infty} -\frac{1}{\beta \cdot l_{\text{secant}}} \log \frac{Z_{\beta,h=0,\text{halfplane}(\boldsymbol{n})}(L)}{Z_{\beta,h=0,(+)\text{-boundary}}(L)}$$

[**Remark.** I could not figure out of how large l_{secant}, i.e. the length of our prepared minimal surface interesecting the boundary, is. An overview simulation yielding the different partition functions suggest that l_{secant} is *not* the Euclidean distance of the intersecting points, as proposed in [18].]

In [1] were presented successes to explicitely calculate the surface tension $\tau(\varphi)$ of a 2-dimensional Ising lattice in dependence of the direction given by an angle φ.

$$\begin{aligned}
x &:= \mathrm{e}^{-2\beta J}\ ,\ a := \left(1+x^2\right)^2\ ,\ p := 2x\left(1-x^2\right) \\
b &:= \left\{\left(\frac{a}{2}\sin 2\varphi\right)^2 + (p\cos 2\varphi)^2\right\}^{1/2} \\
\alpha_1 &:= \operatorname{ar\,cosh}\frac{\left(a^2\sin^2\varphi + p^2\cos 2\varphi\right)}{p\left(a\sin^2\varphi + b\right)} \\
\alpha_2 &:= \operatorname{ar\,cosh}\frac{\left(a^2\cos^2\varphi - p^2\cos 2\varphi\right)}{p\left(a\cos^2\varphi + b\right)} \\
\tau(\varphi) &= \beta^{-1}\left[\alpha_1\sin\varphi + \alpha_2\cos\varphi\right]
\end{aligned}$$

By applying studies of crystal growth originated in the chemical papers [19] of Wulff we are able to determine the average shape line of the surface tension minimizing droplet. This numerical concisely realizable method is known as *Wulff construction*: Let $L_{\lambda,\boldsymbol{n}}$ the half plane $\{\boldsymbol{x}\in\mathbb{R}^2 | \boldsymbol{x}\cdot\boldsymbol{n} \leqslant \lambda\}$ whose border $\partial L_{\lambda,\boldsymbol{n}}$ has the normal $\boldsymbol{n}$ and the distance λ from the origin, the origin lies within $L_{\lambda,\boldsymbol{n}}$. The construction

$$W_{\tau,\lambda} := \bigcap_{0\leqslant\varphi<2\pi} L_{\lambda\tau(\varphi),\boldsymbol{n}(\varphi)}$$

of intersecting non-concave sets gives the convex set of a *Wulff shape*. We define a parametrization of its border by

$$\gamma_\tau : \partial W_{\tau,\lambda} = \{\gamma_\tau(\varphi) \,|\, 0 \leqslant \varphi < 2\pi\}\,.$$

Behind the scenes this principle is a variational problem of crystal or droplet shapes minimizing the surface tension. The corresponding integral $\mathcal{W}_\tau(\gamma) := |W_{\tau,\lambda}|^{-1} \oint_\gamma \tau(\boldsymbol{n}_s)\,\mathrm{d}s$

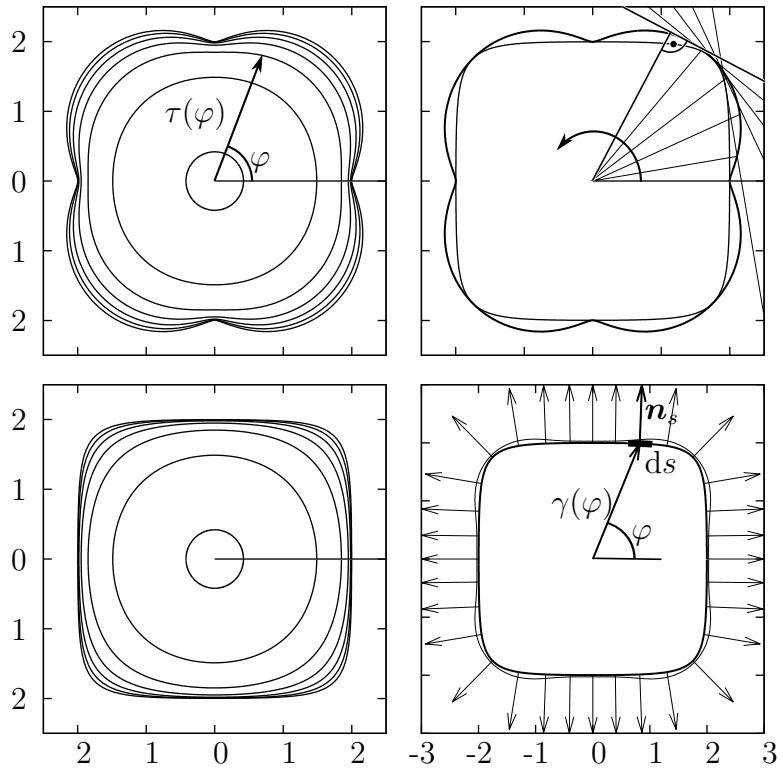

Fig. 1.2.: *Scheme of Wulff construction: the direction dependent surface tension, Wullf construction scheme, Wulff shapes and integration scheme for the Wulff functional. Different contures are of different temperature.*

of least action is called the *Wulff functional*. It is normed by the volume of the Wulff shape such that it is independent of the shape radius λ. All these numerical available data are combined by Schonman and Schlossmann [18] to determine the spontaneous magnetization of the droplet phase and the critical field for $L \to \infty$.

$$\begin{aligned} B_{0,\beta} &= \frac{4\bar{\tau}_\beta - w_\beta}{4m^*_\beta} \\ \kappa_\beta &= \frac{16\bar{\tau}^2_\beta - w^2_\beta}{2m^*_\beta} \end{aligned}$$

Where $\bar{\tau} := \tau(\varphi = 0)$ is the surface tension along a crystal main axis, $w := \mathcal{W}_\tau(\gamma_{\text{Wulff}})$ is the Wulff functional of the Wulff shape which is per construction the minimum of $\mathcal{W}_\tau$ and the solution of the variation problem.

R. Kotecký and I. Medved' claimed [11] to describe the spontaneous magnetization for the minus phase as well as the positive droplet phase not only for $L \to \infty$ but estimate

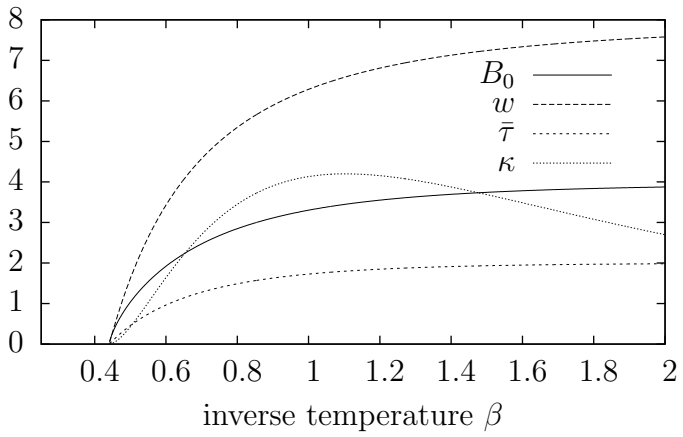

Fig. 1.3.: *Plot of the explicit computable surface tension along (0,1) and Wulff functional of minimizing Wulff shapes; from this derived quantities B_0 and κ.*

it for finite L with an error tending to zero for $L \to \infty$: The thermodynamic limit is

$$\lim_{L\to\infty} m_{L,\beta,h} = \begin{cases} -m^*_\beta & \text{for } Lh =: B < B_{0,\beta} \\ +m^*_\beta - \frac{\kappa_\beta}{(2B)^2} =: m(B) & \text{for } B > B_{0,\beta} \end{cases}$$

while the finite size scaling effords more abbreviating definitions. Let $h_\chi(L)$ the external field at which the susceptibility χ attains its maximum. It is not surprising that $h_\chi(L)$ should closely coincide with the critical field B_0/L. Let

$$\begin{aligned} B^* &:= \left(\frac{1}{2} + \frac{\kappa}{16 m^* B_0^2}\right) B_0 \\ m_+(B) &:= \begin{cases} m(B) & \text{for } B \geqslant B^* \\ m(B^*) & \text{for } B \leqslant B^* \end{cases} \\ \bar{m}(B) &:= (m_+(B) - m^*)/2 \\ \Delta m(B) &:= (m_+(B) + m^*)/2 \\ \Delta &:= \Delta m(B_0) \end{aligned}$$

The main result of Kotecký and Medved' reads as

$$\begin{aligned} h_\chi(L) \approx \tilde{h}_\chi(L) &:= B_0/L \\ m_L \approx \tilde{m}_L &:= \bar{m}(B) + \Delta m(B) \tanh\left(\beta\Delta\left(h - h_\chi(L)\right)L^2\right) \\ \chi_L \approx \tilde{\chi}_L &:= \left(\Delta m(B)\right)^2 \cosh^{-2}\left(\beta\Delta\left(h - h_\chi(L)\right)L^2\right) \end{aligned}$$

for $\beta > \beta_c$ and $h = B/L$. With error estimates

$$\begin{aligned} \left|\tilde{h}_\chi(L) - h_\chi(L) =: R_L^{(0)}\right| &\leqslant 3B_0^3 L^{-\delta}/\kappa \\ \sup_h \left|\tilde{m}_L - m_L =: R_L^{(1)}(h)\right| &\leqslant CL^{-\delta} \\ \sup_h \left|\tilde{\chi}_L - \chi_L =: R_L^{(2)}(h)\right| &\leqslant CL^{-\delta} \end{aligned}$$

The constants C and δ are not determined but it is claimed that for a fixed $0 < \delta < 1/4$ there is a fixed C and a L_0 such that these estimates are valid for all $L > L_0$.

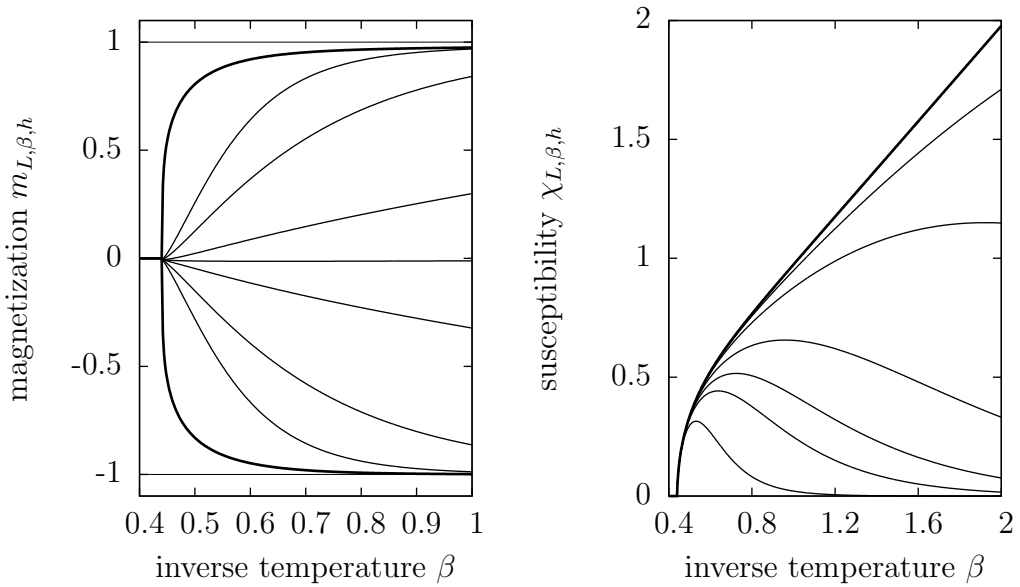

Fig. 1.4.: *Plots of the explicit results of Kotecký and Medved' over β.*

[**Remark.** In the paper [18] the authors took $B_0 := (4\bar{\tau} - w)/(2m^*)$ which results in a wrong factor of 1/2. For the above calculations I did not use their definition, rather the result of [11]. Further, I took the definition $\chi = \beta \operatorname{var}(M)$ instead of $\chi = \operatorname{var}(M)$.]

Discussion. These results are remarkable in a certain sense: Contrary to my expectation, the estimates $\tilde{h}_\chi(L)$, $\tilde{m}_L$ and $\tilde{\chi}_L$ still show a singular point at $\beta = \beta_c$ rather than a continuous smeared finite size version which actually occur. While the residues $R_L^{(1)}$ and $R_L^{(2)}$ have an undetermined scaling behaviour their still finite (i.e. non-zero) at the critical temperature. But in fact the estimate $\left|R_L^{(i)}\right| < C \cdot L^{-\delta}$ for unknown C and $\delta > 0$ only states that the scaling over L is better than logarithmic. It is getting worser for $R_L^{(0)}$: Although $\tilde{h}_\chi(\beta = \beta_c, L < \infty) = 0$ and $h_\chi(\beta = \beta_c, L < \infty) > 0$ the residue $R_L^{(0)}$ is also zero at $\beta = \beta_c$. Since the finite size scalings are given only for $\beta > \beta_c$ the statements remain mathematically true – we only need to choose a δ which is small enough that for some L_0 all $L > L_0$ underlie the scaling. That means if we get closer to β_c we will find an **arbitrary bad** constraint $R_L^{(0)}$ of the actual finite size scaling.

Conclusion. *The results of Kotecký and Medved' might be of theoretical relevance but are impractical for computational purposes, especially the estimate of the critical field which we need prior the simulation.*

1.3. Algorithms

1.3.1. Monte Carlo Methods

Despite the practical difficulties to enumerate the partition function exactly many states $\sigma \in \mathcal{S}$ fortunately have similar or same Boltzmann factors $\exp\left(-\beta H_h\left(\sigma\right)\right)$ which allows us to choose a *representable* tiny fraction of $\mathcal{S}' \subset \mathcal{S}$ without striking the Law of Large Numbers. To this end, we decompose the Hamiltonian in *spin sum* $M\left(\sigma\right) := \sum_i \sigma_i \in \mathbb{Z}$ and *coupling sum* $K\left(\sigma\right) := \sum_{i<j} \sigma_i \sigma_j + \sum_i F_i \in \mathbb{Z}$ and thus we yield

$$H\left(\sigma\right) \quad = \quad -JK\left(\sigma\right) - hM\left(\sigma\right).$$

Correspondingly, we decompose the set of states in disjoint subsets

$$S_{m,k} \quad := \quad \left\{\sigma \in S | M\left(\sigma\right) = m, K\left(\sigma\right) = k\right\}$$

and call the characteristic couple $(m,k) \in \mathbb{Z} \times \mathbb{Z}$ a *bin*. For each bin all states have the same energy

$$H_{m,k} \quad := \quad H\left(\sigma \in S_{m,k}\right) \equiv \text{const}\,.$$

The essence of *binning* the set S is a simplification of the partition function

$$\begin{aligned} Z\left(\beta, h\right) \quad &= \quad \sum_{m,k \in \mathbb{Z}} \sum_{\sigma \in S_{m,k}} \exp\left(-\beta H\left(\sigma\right)\left(h\right)\right) \\ &= \quad \sum_{m,k \in \mathbb{Z}} \left|S_{m,k}\right| \cdot \exp\left(\beta Jk + \beta hm\right) \end{aligned}$$

which is now a sum over few bins $\#\left\{(m,k)\right\} \sim L^4$ instead over the whole state space $\#S = 2^L$. The very question now is how to choose the states σ representable.

The first idea may be selecting each state with same probability. This is easy to implement by choosing each spin with a 50-50 chance (simple sampling Monte Carlo). Formally, this method corresponds to selecting each state with its Boltzmann factor $1/Z_{\beta h}$ at temperature $\beta = 0$. But this method fails since *nearly all* states in $\mathcal{S}$ become highly unlikely, i.e. their Boltzmann factors tend to zero, as the inverse temperature β increases. Relevant states with significant factors occure rarely, irrelevant states with unsignificantly small factors will dominate the simulation time. The best would be if we had an algorithm

preparing states $S_{m,k}$ with probabilities

$$P_{\beta,h}(m,k) := \frac{\#S_{m,k} \cdot \exp(\beta Jk + \beta hm)}{\#S}$$

A direct method to construct states with probability of their Boltzmann factors with a *general*, *determining* and *sufficiently fast* algorithm seems to be impossible since the algorithm must use an inner larger symmetry of the system to have the states of arbitrary complexity calculated with an algorithm of low complexity. If there would be such a symmetry a concise formula implementing this algorithm would exist. But as already mentioned no formula is known yet except for some special cases and as far as I know no such algorithm has been published yet.

Today's successfull approaches use *non-determining* algorithms which relie on time evolving, energy minimizing techniques which transform each state to a close, similar state. One possibility orients on the *equation of motion*, i.e. following the natural laws of certain dynamics. But this method is not optimal since stationary points or cycles (which widely occure in nature) would trap the simulation for a small selection of states and this selection can not be representable. *Importance Sampling Monte Carlo* methods give a more powerful tool. The basic and very intuitive picture is to propose a small set of states at each time step which are close to the current state and to choose one of them with the probability given by their Boltzmann factors. Stationary points or cycles may occure in finite time intervals but with increasing time the system becomes more likely to change its orbit and cover the full range of $\mathcal{S}$. (And the Monte Carlo principle is closer to quantum dynamics whose common interpretation suggest random driven events). But even those temporal orbits can get a long life time when $\beta \gtrsim \beta_c$ (*critical slowing down*) and these are further problems that need to be taken into account.

Regarding our problem we will focus our consideration on the *Heat Bath* algorithm which belongs to the single spin update algorithms. For the Ising model the Metropolis algorithm, also a single spin update algorithm, is slightly more efficient. Nevertheless we will use Heat Bath for two reasons: first it is formally a bit more comfortable and second the aim of this thesis is to provide a starting point to generalize the elaborated methods to those for the Potts model where Heat Bath is slightly more efficient than Metropolis. We improve critical slowing down by applying the *Parallel Tempering* method.

In certain cases it is possible to improve the slowing down with Cluster algorithms. But while the famous Wolff algorithm does not work for systems with exterior fields,

Swendsen-Wang does but has no clear advantage.

1.3.2. Independent Monte Carlo steps and autocorrelation

The aim of a Monte Carlo simulation is a set of independently generated states $\sigma \in S$ following the distribution $P_{\beta,h}\left(M\left(\sigma\right), K\left(\sigma\right)\right)$. But since such importance sampling methods rely on a Markov chain producing states each with a memory to its preceding state, we can not eliminate remanent effects. We expect an exponentially decreasing correlation of states which we discuss quantitatively with the autocorrelation function $A\left(\Delta t\right)$ for an observable $X\left(t\right)$ of interest:

$$A\left(\Delta t\right) \;:=\; \frac{\frac{1}{\mathrm{MCS}-\Delta t}\sum_{t=1}^{\mathrm{MCS}-\Delta t} X\left(t\right) X\left(t+\Delta t\right) - \left\langle X\right\rangle^2}{\mathrm{var}\left(X\right)} \quad\sim\quad \exp\left(-t/\tau\right).$$

The factor $\tau > 0$ determines the time scaling of autocorrelations, it has the unit of time so it is called *correlation time*. The smaller the correlation time the larger the number of states which are allowed to be considered as nearly independent. Actually, measurements reveal an "overlap" of multiple exponentials

$$A\left(\Delta t\right) \;\sim\; C_1 \mathrm{e}^{-t/\tau_1} + C_2 \mathrm{e}^{-t/\tau_2} + C_3 \mathrm{e}^{-t/\tau_3} + \ldots$$

and suggest a multitude of influences which autocorrelate the simulation. The largest impact is caused by significant local minima in $P_{\beta,h}$ over magnetization m. Since single spin flip algorithms turn only one spin at once the system undergoes a *random walk* $m_t \to m_{t+1} \pm 2$ within the binned state space $\{S_{m,k}\}$ or the histogram $P_{\beta,h}$. Two distant states $\sigma_1, \sigma_2 \in S$ with similar energies $H_h\left(\sigma_1\right) \approx H_h\left(\sigma_2\right)$ are highly unlikely to be transformed into each other when a significant energy "barrier" makes a walk from σ_1 to σ_2 to a rare "tunneling" event although statistics demand a $\approx$ 50-50 transition probability. This simulational problem has its physical counter part in spontaneous symmetry breaking, i.e. *spontaneous magnetization* in our case.

While this effect causes a *critical slowing down* around $\beta = \beta_c$ the simulation will be "subcritically trapped" in one magnetization phase for $\beta \gg \beta_c$. Computational physics provide a wide arsenal of methods to reduce this trapping effect, e.g. Cluster flip algorithms and umbrella techniques like Multicanonical sampling or Wang-Landau algorithm. We decided for *Parallel Tempering* [4] method which will be discussed soon.

A second correlation effect inherently comes from the simulation principle itself: as we

will discuss in the next section, the Heat Bath sinlge-spin flip systematically "rejects" spin flip proposals if they would turn the system into a less probable state, i.e. the Boltzmann weight factor $\mathrm{e}^{-\beta H_h(\sigma)}$ would decreases. The lower the temperature T the larger is β and the larger it amplifies the differences in the weight factors. In turn this increases the probability of rejection in the case the system is in equilibrium, i.e. if it is already forced into a local optimum. This effect slows down the simulation but not in such a large scale like the above mentioned random walk trap. Rejects can be avoided completely with a reformulation of the original algorithm, as we will show in the next section.

The result will be a time line of states each holding the additional information of its average lifetime and avoiding subsequent repetitions. Before calculating τ we unfold the compressed time line to the actual $A(\Delta t)$. Since analytical methods would be non-trivial we calculate τ from the integral or sum of $A(\Delta t)$. After that, we normalize τ with the acceptance rate.

A further influence should be kept in mind: the type of (pseudo!) random number generator determines the quality of random distribution. Standard generators produces numbers which are not sufficiently uncorrelated for scientific demands. To avoid unpredictable artefacts I used a Mersenne twister generator. [17]

1.3.3. Heat Bath Update and a slight improvement

The classical Heat Bath algorithm performs repeated single-spin-flip transitions of given spin configuration $\sigma^0 \to \sigma^1$ to produce a Markov chain obeying the Boltzmann statistics. This is done by taking a particle i at uniform randomness, calculating the transition energy ΔE_i and deriving the transition probability

$$w\left(\sigma^0 \to \sigma^1(i)\right) \;=\; \mathrm{e}^{-\beta\Delta E_i} / \left(1 + \mathrm{e}^{-\beta\Delta E_i}\right)$$

which determines the probability to accept the flip request. But the main disadvantage of an increasing reject rate of the flip request when temperature decreases (,,critical slowing down") is that this method slows down. However it is possible to reformulate the algorithm in such a way that effectively the same simulation takes place with the rejects *rejected*. We use simplifications which result from the simplicity of the model: The individual flip energy of each particle i depends only on its spin $\sigma_i^0 \in \{-1, +1\}$ and on the local field, i.e. the sum ν_i of the spins of its nearest neighbour particles. These sums ν_i are one of $\{-4, -2, 0, +2, +4\}$. Later on, we can tabularize further derived quantities with low

costs. The flip energy is

$$\Delta E_{\sigma,\nu} \;=\; 2\sigma \cdot (J\nu + h) \;,\; \Delta E_i = \Delta E_{\sigma_i,\nu_i}$$

We sort all particles in sets $I_{\nu,s} := \{i \in I | \nu_i^0 = \nu, \sigma_i^0 = s\}$ in dependence of their nearest neighbour configuration and the spin. The probability to visit particle i is

$$\begin{aligned} p_{\text{visit}}(i) &= N^{-1} \\ &= \frac{N_{\nu,s}}{N} \cdot \frac{1}{N_{\nu,s}} \end{aligned}$$

where $N_{\nu,\sigma} := \#I_{\nu,\sigma}$. In classical Heat Bath it means we may equivalently choose a subset $I_{\nu,\sigma} \subset I$ with probability $N_{\nu,\sigma}/N$ and subsequently we choose a particle $i \in I_{\nu,\sigma}$ with probability $1/N_{\nu,\sigma}$ to get the same effect. In classical Heat Bath, the probability of acceptance, i.e. to flip any arbitrary particle's spin is

$$\begin{aligned} p_{\text{flip}} &= \sum_{i \in I} p_{\text{visit}}(i) \cdot w\left(\sigma^0 \to \sigma^1(i)\right) \\ &= \sum_{\nu,\sigma} \frac{N_{\nu,\sigma}}{N} \cdot \sum_{i \in I_{\nu,\sigma}} \frac{1}{N_{\nu,\sigma}} \cdot \frac{\mathrm{e}^{-\beta \Delta E_{\nu,\sigma}}}{1 + \mathrm{e}^{-\beta \Delta E_{\nu,\sigma}}} \\ &= \sum_{\nu,\sigma} \frac{N_{\nu,\sigma}}{N} \cdot \frac{N_{\nu,\sigma}}{N_{\nu,\sigma}} \cdot \frac{1}{\mathrm{e}^{\beta \Delta E_{\nu,\sigma}} + 1} \\ &=: \sum_{\nu,\sigma} n_{\nu,\sigma} \cdot w_{\nu,\sigma} \end{aligned}$$

This means a state σ^0 needs $1/p_{\text{flip}}$ requests on average until a flip is accepted.

Algorithm. In our faster variant of Heat Bath the current state's expected lifetime $1/p_{\text{Flip}}$ is added to the histogram (instead of counting the "matches") and the flip will definitely be carried out (this means an effective 100% acceptance rate). The probability to choose a specific subset $I_{\nu,\sigma}$ is $n_{\nu,\sigma} \cdot w_{\nu,\sigma}/p_{\text{flip}}$, the probability to choose a particle in $I_{\nu,\sigma}$ is uniformly $1/N_{\nu,\sigma}$. Implementational drawback of this method may be the complicated list data structures for the $I_{\nu,s}$.

The deeper meaning of $p_{\text{flip}}(\sigma)$. Let be $(t \mapsto \sigma_t) : T \to S$ a Markov chain of states $\sigma_t \in S$ over a discrete time $t \in T = \{1, \ldots, \text{MCS}\}$ as a product of our faster Heat Bath

sweeps. Consider the selection of states with specific energy

$$T_{m,k} \quad = \quad \{t \in T | \sigma \in S_{m,k}\}.$$

By the above discussion we have

$$P_{\beta,h}(m,k) \quad \sim \quad \sum_{t \in T_{m,k}} p_{\text{flip}}(\sigma_t)^{-1}$$

If we forget the binning over (m,k) for a short time and consider a certain $\sigma \in S$ we will have

$$Z_{\beta,h}^{-1} \cdot \mathrm{e}^{-\beta H_h(\sigma)} = P_{\beta,h}(\sigma) \quad = \quad c(\sigma) \cdot p_{\text{flip}}(\sigma)^{-1}$$

and we will see that

$$c(\sigma) \quad \sim \quad \mathrm{e}^{-\beta H_h(\sigma)} \cdot p_{\text{flip}}(\sigma)$$

counts the frequency of the state σ in the fast Heat Bath variant – it is the probability measure in the statistics of our algorithm. If we are interested in transition probabilities for arbitrary states (and we are for parallel tempering method) we should take this circumstance into account. Long living states which are the significant in Boltzmann statistics will be under-representated by the factor $p_{\text{flip}}(\sigma)^{-1}$ in the fast Heat Bath statistics where $c(\cdot)$ is the probability measure.

$$\langle \chi_{m,k} \rangle_{\text{Gibbs}} = P_{\beta,h}(m,k) \quad = \quad \left\langle p_{\text{flip}}^{-1} \chi_{m,k} \right\rangle_c$$

where $\chi_{m,k}(\sigma) := \begin{cases} \sigma \in S_{m,k} & : \ 1 \\ \text{else} & : \ 0 \end{cases}$. A transition probability like $w_{\sigma_1,\sigma_2} := \frac{c(\sigma_2)}{c(\sigma_1)+c(\sigma_2)}$ preserves detailed balance in fast Heat Bath statistics.

1.3.4. Parallel tempering

An efficient method [4] to reduce critical slowing down is the trick of swapping replicas of the system simulated with different parameters (β, h). The idea is that configurations in a deep temperature environment with large slowing down profits from the uncorrelating effect of high temperature environment when they randomly diffuse through the field

of parallel simulated environments. While the local simulation within a replica may be arbitrary, e.g. Heat Bath or Wang-Landau, the replica swapping must obey detailed balance. But as proposed in the previous section, swapping states between two simulations does not only mean changing spin configurations within the probability of the underlying statistics but of *two* statistics which are different in general caused by different simulation parameters β and h.

Assume two parallel, isolated simulations. The first with parameters β, h and the resulting probability measure $c(\cdot)$ and the second one with β', h' and $c'(\cdot)$. Let $\sigma_1, \sigma_2 \in S$ and let us, with the notation $(\sigma, \sigma') \in S \times S$, abbreviate the fact "first system has state σ, second σ'." Since both simulations are independent from each other the probability of a configuration (σ_1, σ_2) of the total system is $c(\sigma_1) \cdot c'(\sigma_2)$. The function $w(X \to Y)$ stands for transition probability from a circumstance X to a circumstance Y. *Detailed balance* for swapping demands us

$$\begin{aligned}
\frac{w((\sigma_1,\sigma_2)\to(\sigma_2,\sigma_1))}{w((\sigma_2,\sigma_1)\to(\sigma_1,\sigma_2))} &= \frac{c(\sigma_2)\cdot c'(\sigma_1)}{c(\sigma_1)\cdot c'(\sigma_2)} \\
&= \frac{\mathrm{e}^{-\beta H_h(\sigma_2)}\cdot p_{\text{flip}}(\sigma_2)\cdot \mathrm{e}^{-\beta' H_{h'}(\sigma_1)}\cdot p'_{\text{flip}}(\sigma_1)}{\mathrm{e}^{-\beta H_h(\sigma_1)}\cdot p_{\text{flip}}(\sigma_1)\cdot \mathrm{e}^{-\beta' H_{h'}(\sigma_2)}\cdot p'_{\text{flip}}(\sigma_2)} \\
&= \mathrm{e}^{J(\beta-\beta')(K_2-K_1)+(\beta h-\beta' h')(M_2-M_1)}\cdot\frac{p_{\text{flip}}(\sigma_2)\,p'_{\text{flip}}(\sigma_1)}{p_{\text{flip}}(\sigma_1)\,p'_{\text{flip}}(\sigma_2)} \\
&=: W_{\sigma_1,\sigma_2}(\beta,h;\beta',h')
\end{aligned}$$

which is fulfilled e.g. for

$$w((\sigma_1,\sigma_2)\to(\sigma_2,\sigma_1)) = \min\left\{1, W_{\sigma_1,\sigma_2}(\beta,h;\beta',h')\right\}.$$

In general, the selection of the simulation parameters (β_i, h_i) is a non-trivial task: The parallel tempering method works optimal if the different overlapping histogram regions of adjacent simulation are 'balanced'. There are methods "*making life simple*" [3]. But for reasons of comparability I chose an apriori distribution of β_i such that $\beta_i/\beta_{i+1} = \text{const}$.

The distribution of N measure points $\beta_1 < \ldots < \beta_N$ for given β_1, β_N is

$$\begin{aligned} C &:= \beta_2/\beta_1 \\ \beta_{i+1} &= C\beta_i \\ \Longrightarrow \beta_i &\stackrel{!}{=} C^i\beta_1 \\ \Longrightarrow C &= \sqrt[N]{\beta_N/\beta_1} \\ \Longrightarrow \beta_i &= (\beta_N/\beta_1)^{(i-1)/N}\,\beta_1 \end{aligned}$$

1.4. Evaluation techniques and error estimation

1.4.1. Reweighting techniques.

Reweighting techniques. Once we are in knowledge of $P_{\beta_0,h_0}(m,k)$ for a certain temperature β_0 and a certain external field h_0 we are able transform it with an easy-to-calculate factor in order to generalise it for arbitrary temperatures β and fields h

$$P_{\beta,h}(m,k) \quad = \quad P_{\beta_0,h_0}(m,k) \cdot \exp\left(\left(\beta_0 - \beta\right) Jk + \left(\beta_0 h_0 - \beta h\right) m\right).$$

This factor is called *reweighting factor* $R_{m,k}(\beta, h; \beta_0, h_0)$ since it formally replaces the Boltzmann weights $\mathrm{e}^{-\beta_0 H_{h_0}(m,k)}$ by $\mathrm{e}^{-\beta H_h(m,k)}$ which are implicitely contained in $P_{\beta_0,h_0}(m,k)$. Transforming one histogram P_{β_0,h_0} into another histogram $P_{\beta,h}$ suggests this method to name *(single) Histogram Reweighting*. It has the advantage to carry out a single simulate only once and have data for an infinite ensemble of different parameters. But one needs to bear in mind that statistical errors scale exponentially with $R_{m,k}(\beta, h; \beta_0, h_0)$, which are huge for larger $\Delta\beta$ and Δh and constrain the reliability of reweighting to the neighbourhood of (β_0, h_0).

To get data for a wider range of simulation parameters – as we need for $\beta = \beta_c \cdots 2.0$ – we have to measure at few distant parameters $(\beta_0, h_0), \ldots, (\beta_k, h_k)$. The question is how to combine the multiple histograms to a single one. The difficulty is, that

$$P_{\beta_p,h_p}(m,k) \cong C_p \cdot \varrho(m,k) \cdot \mathrm{e}^{-\beta_p H_{h_p}(m,k)}$$

for which the factors $C_p \in \mathbb{R}^+$ are unknown. An idea that naturally comes into mind is to get the correct *ratios* between adjacent histograms P_{β_p,h_p} and $P_{\beta_{p+1},h_{p+1}}$ by reweighting the histogram $p+1$ as $(\beta_{p+1}, h_{p+1}) \longrightarrow (\beta_p, h_p)$ so that comparison is allowed from which we conclude all normalizations

$$\tilde{C}_p \quad = \quad C \cdot C_p$$

in correct ratios, with the remaining unknown C to be of no problem. And if we have, e.g. $\beta_0 = 0$, we are able to conclude the absolute C_p and get the density of states without biases from cut off effects. But the problem of statistical errors remains problematical since our chain of conclusion is $C_0 \Rightarrow C_1 \Rightarrow C_2 \Rightarrow \ldots \Rightarrow C_k$ so C_k is less correct. Luckily there is a fixed point iteration suggested by Swendsen and Ferrenberg [5] which solves

these difficulties: Let us reweight all histograms to the same parameter, e.g. $(\beta_0, h_0) = 0$ and sum them

$$\begin{aligned} P'(m,k) &= \sum_{p=0}^{k} P_{\beta_p,h_p}(m,k) \cdot \mathrm{e}^{-\beta_p H_{h_p}(m,k)} \\ t_p &= \sum_{m,k} P_{\beta_p,h_p}(m,k) \end{aligned}$$

and iterate the two formulas

$$\begin{aligned} P^{\mathrm{new}}(m,k) &= P'(m,k) \cdot \left(\sum_{p=0}^{k} t_p \cdot \mathrm{e}^{-\beta_p H_{h_p}(m,k)} \cdot C_p^{-1} \right)^{-1} \\ C_p &= \sum_{m,k} P^{\mathrm{new}}(m,k) \cdot \exp\left(-\beta_p H_{h_p}(m,k)\right) \end{aligned}$$

1.4.2. Range of Magnitudes

The tremendous magnitudes of the reweighting factors do not only lead to a limiting effect of the applicable ranges of β and h but also to a pragmatical difficulty when we want to unite multiple histograms of very different parameters β and h to a single one: Since the $R_{m,k}(\beta, h; \beta_0, h_0)$ is an exponential, we need to face the serious question of magnitudes it spans in machine numbers. For our specific problem of a 2-dimensional spin lattice of linear length L the coupling sum ranges within $-2L(L+1) \ldots +2L(L+1)$, the spin sum within $-L^2 \ldots + L^2$ but which is multiplied by the external field h which never exceeds $4J/L$. Thus, the Hamiltonian never exceeds

$$H \leqslant 2L(L+3)$$

The partition function can generously be estimated via

$$Z = \sum \mathrm{e}^{-\beta H(\sigma)} < |S| \cdot \mathrm{e}^{-0 \ldots 2H} = 2^{L^2} \cdot \mathrm{e}^{4L(L+3)} < \mathrm{e}^{L^2 + L(4L+12)} = \mathrm{e}^{L(5L+12)}$$

The comparison with realistic system sizes shows us the significance of magnitudes

L	16	32	64	128	256
$\ln(Z)$	1472	5504	21248	83456	330752

So even a 16×16-Lattice is to large to be handled with machine numbers of double precision standard IEEE 754, whose values range within $-2^{-1023} \ldots + 2^{+1024}$. The pro-

grammer needs to handle these issues by using multi precision libraries or by implementing necessary functionality on his own – as it has been done in this work – when a logarithmic storage of the large numbers seems to be an inattractive alternative.

1.4.3. Calculation of magnetization $\langle M \rangle (\beta, h)$ and $\chi (\beta, h)$

The average magnetization and its i-th powers are the expectation values of $M^i(\sigma)$ in Boltzmann statistics and calculates from histogram as

$$\begin{aligned} \left\langle M^i \right\rangle (\beta, h) &= \sum_{\sigma \in S} M(\sigma)^i \cdot \exp\left(-\beta H_h(\sigma)\right) / \sum_{\sigma \in S} \exp\left(-\beta H_h(\sigma)\right) \\ &= \sum_{m,k} m^i \cdot P_{\beta,h}(m,k) \end{aligned}$$

when $P_{\beta,h}(m,k)$ is normalized. The magnetic susceptibility $\chi(\beta, h)$ is defined as

$$\chi(\beta, h) := \left. \frac{\partial \langle M \rangle}{\partial h} \right|_\beta$$

and can be reformulated using the above formula for $\langle M \rangle$. Consider

$$\begin{aligned} Z'_{\beta,h} := \left(\left. \frac{\partial}{\partial h} \right|_\beta \right) Z_{\beta,h} &= \left(\left. \frac{\partial}{\partial h} \right|_\beta \right) \sum_{\sigma \in S} \exp\left(\beta J K(\sigma) + \beta h M(\sigma)\right) \\ &= \sum_{\sigma \in S} \beta M(\sigma) \cdot \exp\left(-\beta H_h(\sigma)\right) / Z_{\beta,h} \cdot Z_{\beta,h} \\ &= \beta \langle M \rangle \cdot Z_{\beta,h} \\ \text{analogously } Z''_{\beta,h} &= \beta^2 \left\langle M^2 \right\rangle \cdot Z_{\beta,h} \end{aligned}$$

and thus

$$\begin{aligned} \chi(\beta, h) &= \left(\frac{Z'_{\beta,h}}{\beta Z_{\beta,h}} \right)' = \frac{1}{\beta} \cdot \frac{Z''_{\beta,h} \cdot Z_{\beta,h} - \left(Z'_{\beta,h}\right)^2}{Z^2_{\beta,h}} \\ &= \frac{1}{\beta} \cdot \left(\frac{Z''_{\beta,h}}{Z_{\beta,h}} - \left(\frac{Z'_{\beta,h}}{Z_{\beta,h}} \right)^2 \right) = \beta^{-1} \left(\beta^2 \left\langle M^2 \right\rangle - \left(\beta \langle M \rangle\right)^2 \right) \\ &= \beta \left(\left\langle M^2 \right\rangle - \langle M \rangle^2 \right). \end{aligned}$$

Since $\mathrm{var}(M) = \beta^{-1}\chi(\beta, h)$ we also calculated the error of the magnetization estimator $\varepsilon_M := \sqrt{\frac{\mathrm{var}(M)}{\mathrm{MCS}}} = \sqrt{\frac{\chi(\beta,h)}{\beta \cdot \mathrm{MCS}}}$ where MCS is the number of (independent!) *M*onte *C*arlo *s*teps of the simulation. The errors of $\chi(\beta, h)$ are of interest, too. As the susceptibility is not an observable derived from the normally distributed histogram bins $P_{\beta,h}(m, k)$ directly, we need a different method to get error estimates. A common method – the *blocking* – divides the whole block $\{X_1, \ldots, X_{\mathrm{MCS}}\}$ of Monte Carlo steps into a set of B disjoint sub blocks $\{X\}_1, \ldots, \{X\}_B$ of width b and consider each as a single simulation. From all these sub blocks the susceptibility will be calculated as mentioned above so in turn $\chi(\beta, h)$ is made to a random variable on which we apply statistics. The *Jackknife* method is an improved version of that concept and reduces uncomfortable bias effects from the given distribution. The fundamental difference of simple blocking is that the Jackknife uses the set-theoretical complements $\{X\}'_j := \{X_1, \ldots, X_{\mathrm{MCS}}\} \setminus \{X\}_j$ so it "reuses" the measurements of the overlapping regions. This aspect must be taken into account by a correct normalization:

$$\begin{aligned} Y_j &:= \frac{1}{b(B-1)} \sum_{X \notin \{X\}_j} X \\ \mathrm{var}(Y) &= \frac{B-1}{B} \sum_{j=1}^{B} \left(Y_j - \frac{1}{B} \cdot \sum_{k=1}^{B} Y_k \right)^2 \end{aligned}$$

1.4.4. Calculation of critical field $h_c(\beta)$

The critical field $h_c(\beta)$ is defined such it fulfills the equation $\langle M \rangle (\beta, h_c(\beta)) = 0$, i.e. the critical field compensates the influence of the minus boundary on magnetization. We solve this equation numerically by the method of *nested intervals*: Since $\langle M \rangle_\beta (h)$ is a monotonously increasing function answering the effect of external field we simply need to select a value $h_{i+1} = \left(h_i^- + h_i^+\right)/2 \in I_i := \left[h_i^-, h_i^+\right]$ and look if it is negative, positive or (close to) zero. If it is negative, we will set $h_{i+1}^- = h_i^-$ and $h_{i+1}^+ = \left(h_i^- + h_i^+\right)/2$, i.e. we will divide I_i in the middle and take the lower part and continue the procedure on I_{i+1}, if magnetization is positive we will set $h_{i+1}^- = \left(h_i^- + h_i^+\right)/2$ and $h_{i+1}^+ = h_i^+$, i.e. taking the upper part, if magnetization is (close to) zero, we will break the algorithm and have $h_c \approx h_{i+1}$.

Since $h_c(\beta)$ is the value of the inverse function of $h \mapsto \langle M \rangle (\beta, h)$ at $\langle M \rangle = 0$ we derive the errors from $\langle M \rangle$:

$$\begin{aligned} h\left(\langle M\rangle\right) - h_c &= \left(\frac{\partial \langle M\rangle}{\partial h}\right)^{-1}_{h=h_c} \cdot \langle M\rangle \\ &= \left(\beta\sigma^2_{\langle M\rangle}\right)^{-1} \cdot \langle M\rangle \\ \sigma^2_{h=h_c} &= \left(\beta\sigma^2_{\langle M\rangle}\right)^{-2} \cdot \sigma^2_{\langle M\rangle} \\ &= \frac{1}{\beta^2\sigma^2_{\langle M\rangle}} = \frac{1}{\beta\chi} \end{aligned}$$

Since $h_c\left(L,\beta\right) \lesssim 4J/L$ we find the *relative* error of h_c

$$\begin{aligned} \frac{\varepsilon_{h_c}}{h_c} &= \frac{1}{h_c} \cdot \frac{1}{\sqrt{\mathrm{MCS}\,\beta\chi\left(\beta,h_c\right)}} \\ &\gtrsim \frac{L}{4J} \cdot \frac{1}{\sqrt{\mathrm{MCS}\,\beta\chi\left(\beta,h_c\right)}} \end{aligned}$$

If we wish to have a certain ε_{h_c} we need the following N independent Monte Carlo steps

$$N \gtrsim \frac{1}{16J^2} \cdot \frac{1}{\beta\chi\left(\beta,h_c\left(\beta\right)\right)} \cdot \frac{L^2}{\varepsilon^2_{h_c}}$$

1.4.5. Extrapolation

The quality of simulation results essentially relies on an exact estimate of the external field h which is a simulation parameter like β and which must coincide well with the critical field h_c. The only way to receive these important data prior the simulation is to *extrapolate* them from prior simulations of lower system sizes. Thus we need a reliable *interpolation* algorithm. We expect the critical field $h_c\left(L\right)$ to evolve in a law of decay over L. The paper of Kotecký and Medved' suggest the Finite Size Scaling of $h_c\left(L\right)$ to be power-like. In the first order approximation we take the ansatz

$$h_c\left(L\right) \approx D \cdot L^{-\delta} + C$$

To extrapolate the $h_c\left(L\right)$ of interest we hope the triples $\left(L-3, L-2, L-1\right)$ as interpolation input yield a good approximating law. How to interpolate given data technically is discussed in appendix A. Of essential interest is the problem for arbitrary triples $\left(L_1, L_2, L_3\right)$. This flexibility allows us to experiment with the best selections of interpolation inputs but demands a non-explicit iterating calculation, a fixed point iteration.

By the way: Since we have a tool interpolating exponential decay *and* a fast variant of heat bath algorithm we are in the comfort to investigate the exponential behaviour of an accurate measured autocorrelation $A(t)$. My personal hope was to find a method for a more precise calculation of correlation time τ. But the interpolation failes with the ansatz

$$A(t) \quad = \quad A\mathrm{e}^{-t/\tau_a} + B\mathrm{e}^{-t/\tau_b} \ .$$

I recognized that the most accurate samples, which are that for the lowest t, start almost linearly and that this causes the interpolation to calculate degenerated roots or roots of negative radicals. In other words: The ansatz is qualitatively wrong and needs to be refined.

2. Simulation and Evaluation

2.1. General difficulties

Lack of a good algorithm. The most serious difficulty comes with the fact that each standard simulation technique has profound drawbacks: Wolff cluster algorithm is not applicable to systems with a non-vanishing exterior field, Swendsen-Wang cluster algorithm works but does not yield the performance improvement we hoped to achieve. Parallel Tempering fails due to the wide temperature range: to get a good overlap of adjacent histograms the number of parallel simulations must increase and that declines the efficiency of system mixing. Furthermore we need a wide temperature range since there exist a measurable deviation of $h_c(\beta)$ and $h_c(\infty)$ even at $\beta = 4.0$. We decide for $\beta \in (0.0, 2.0)$ as a compromise. Umbrella techniques fail since even for $L = 14$ we have more than 10^5 relevant histogram entries for equally distributed visits but the minus phase is represented by fairly one entry. And we need a good ratio of plus and minus phase to calculate h_c. In my opinion only a cluster algorithm – probably a variation of Swendsen-Wang – may solve our sorrows elegantly.

Unknown simulation parameter $h_c(\beta)$. The simulation must be carried out with an exterior field h very close to actual h_c – which I originally planned to calculate from simulation data – since even if we had an algorithm comparable to Wolff a wrong field would cause bad histogram statistics. The problem enhances as β increases. There exists an exact solution of the limit h_c/L for $L \to \infty$ but this does not help since the asymptotical finite size scaling behaviour is very weak. The only way is to simulate each system size L and to estimate the next field $h_c(L+1)$ e.g. by exponential extrapolation which, in contrast to the whole frustrating situation, is very accurate. Unfortunatly the extrapolation is not reliable for wider ranges of L.

Large histograms. Since we are interested in the magnetical behaviour we need a histogram which seperates the states between coupling energy $K(\sigma) := \sum_{i,j} J_{i,j}\sigma_i\sigma_j$ and magnetization $M(\sigma) := \sum_i \sigma_i$. K ranges between $\pm 2L(L+1)$ and M between

$\pm L^2$. That means our histograms scale in size as $\sim L^4$. Furthermore there are sharpe peaked regions which makes it delicate to decrease the histogram resolution. As mentioned before, h_c has a very sensitive dependence to the peaks close to the pure phases. But the large histograms make calculations considerably long (Swendsen-Ferrenberg reweighting iteration, method of nested intervals to systematically guess h_c) and takes time comparable to the simulation time itself! Fortunatly we only need a high accuracy of the minus phase histogram bin so we ever can choose a resolution grid which reduces the neighbourhood of the minus phase bin to $M = -N$.

Hidden barriers. Since the critical field h_c scales as $\sim L^{-1}$ the energetical contribution of magnetization in the positive droplet phase gets weak in comparison the coupling energy K. This makes many droplet shapes with the same vertical and horizontal diameter close to be equivalent since for given diameters there is a huge class of shapes with "rounded" corners which have the same coupling energy. But using single spin flip algorithms the transition between shapes with different diameters demands whole edge lines to be flipped and for increasing L this becomes increasingly unlike to happen. So even the simulation in the plus phase causes larger correlations.

2.2. The algorithm I took

Finding an appropiate simulation algorithm was a frustrating and time consuming task. I recognized the "great barrier" of rare events between the two magnetization phases in the histogram as the main problem which cannot be circumvented using elabored standard techniques as already mentioned. My uncountable fruitless trials had this in mind: single spin updates make the system undergo a random walk through the (M, K) histogram, i.e. locally jumping to "nearest neighbour" bins at each update. But what we need are *far* jumps between the two phases. Cluster algorithms carry out many far jumps and this is the main effect of decorrelating the simulation.

Out of desperation for the time running out I decided to give it a last try with a very inelegant method. I equipped the parallel tempered heat bath algorithm with a *whole system flip update*. My hope was that this approach would decorrelate the cool end of the parallel tempered chain and that this cool end would feet the middle of the chain with further uncorrelated states. Since the ground state consists of the two pure magnetized phases (if $h = h_c$, of course) this is reasonable but not perfect because for large but finite β the system lies above the ground state where the minus and plus phase are not

symmetric in their distribution: while the minus phase is strongly peaked at $M = -N$ the plus phase has a smoother bulk reaching its maximum at a $M < +N$.

What I did not expect was the considerable improvement for systems of moderat sizes up to $L \approx 24$. Since the whole system flips this improvement also decorrelates the hidden barriers in the plus phase which I explained above.

Unfortunately, this idea came nearly too late. I simulated the problem on my work station only because I felt the time to demand computation time on the busy computer cluster was to short and I needed to hurry up scraping together my results and documenting them. I decided it would be better to invest the remaining time in completing this document. At the end I simulated systems of sizes $L = 7$, 8, 9, 10, 11, 12, 13, 14, 15, 16, 18, 20, 22 and 24 each with 22 parallel replica and 10^6 sweeps per replica. The temperatures β are chosen such that $\beta_i/\beta_{i+1} = \text{const}$ while i is the parallel simulation index with given β_i and $h_i \approx h_c(\beta_i)$. The temperatures ranges in $\beta \in [0.25, 2.0]$. In order to get an estimate of the critical field $h_c(\beta, L)$ I extrapolated it from three previous measurements of $h_c(\beta)$ with the ansatz $h_c(\beta, L) = g \cdot L^\gamma + c$. For the small lattices $L = 7$, 8 and 9 I used extrapolates from exact enumerated lattices $L = 3, \ldots, 6$.

2.3. Evaluation

As mentioned earlier the additional whole-system-flip has an essential impact on the simulation velocity. Figure 2.1 shows the dependence of temperature and the system size. Without the additional system flip the autocorrelation time would grow exponential over β. The bulk in the middle might be reduced using a dynamic adapting distribution of the β_i as proposed in [3].

2.3.1. Finite Size Scaling of the critical field

The scaling of the normed critical field $B_0(\beta, L) := h_c(\beta, L) \cdot L$ is very slow. Figure 2.2 shows the measured results and gives an overview of the further scaling in which we assume a power law $B_0(\beta, L) = D(\beta) \cdot L^{-\delta(\beta)} + B_0(\beta, L \to \infty)$ which interpolates the measurements of $L = 18$, 22 and the explicit known limit $L \to \infty$. As we conclude from the plot even very large systems of sizes $L = 2^{7 \ldots 10}$ do not approximate the infinite size limit very well.

Even the power law has a slow scaling. Figure 2.3 shows the parameters D and δ of

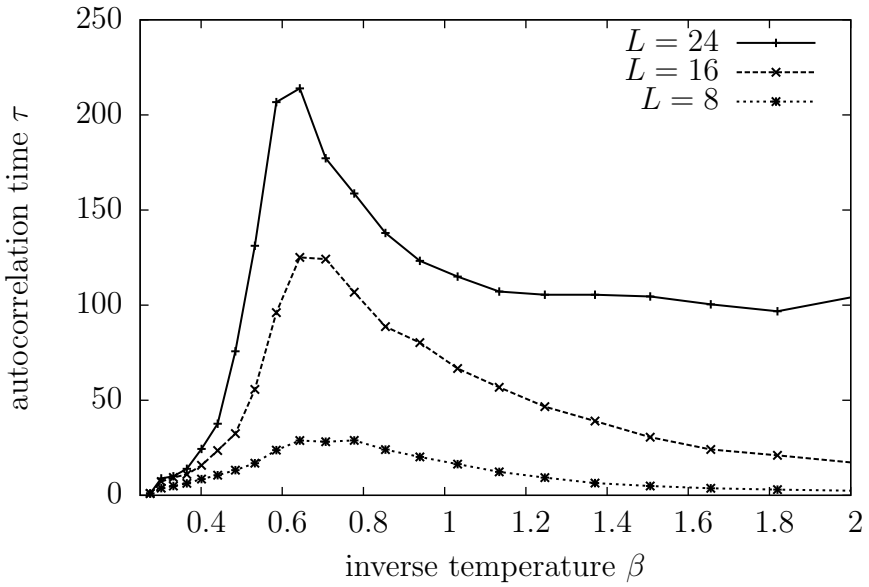

Fig. 2.1.: *Autocorrelation times in dependence of L and β for parallel tempered heat bath algorithm with a whole-system-flip-proposal each sweep.*

interpolations in dependence of the measurements we took: Reliable fits are possible e.g. for triples $(L, 16, \infty)$ with $L = 2, \ldots, 8$. While $D_{L,16,\infty}$ suggests an explicit approximation for $L \to \infty$ the shape of $\delta_{L,16,\infty}$ obeys a less obvious expression.

2.3.2. Finite Size Scaling of magnetization and susceptibility

The finite size scalings of magnetization and susceptibility in the formulas of Kotecký and Medved' have a dependency on the unknown $h_\chi(L)$, i.e. the critical field defined by the maximal value of $\chi_L(h)$. If we approximate $h_\chi(L) \approx B_0/L$ as done in their paper we expect systematical deviations of the explicit estimates from the actual measured quantities.

As we can see in figure 2.4 the magnetization $m_L(h)$ is qualitatively well reproduced by the complete explicit formulas, except for the systematical shift along the h axis due to the wrong critical field estimate. But as in the case of critical field estimates the explicit result shows a significant, systematical deviation as temperature β tends to β_c. Further, the convergence is weaker close to the critical point and stronger in the cold phases.

The accordance of explicit and measured result gets quite more obvious for the susceptibilities $\chi_L(h)$ which are peaked at the critical field $h = h_c$, cf. fig. 2.5 . Again we find

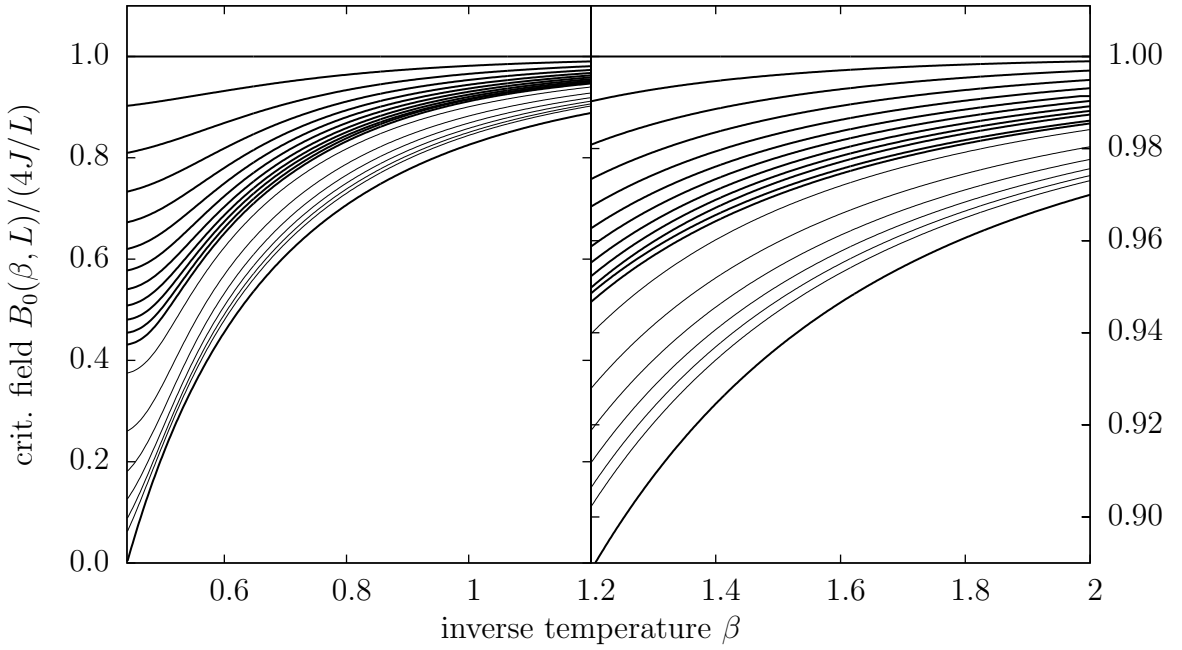

Fig. 2.2.: *Plot of critical field for different sizes L. The thick lines show calculation from measurements for $L = 2, 4, 6, ..., 24$ and the explicit $L \to \infty$. The thin lines show interpolations for $L = 32, 64, 128, 512, 1024$.*

systematical shifts due to the inaccuracy of the estimation $h_\chi(L) \approx B_0/L$. A closer look reveals the right tails of the measurement peaks a bit stronger than the left ones while the explicit peaks have a symmetric shape.

We conclude our visual comparison: *the semi-explicit formulas of magnetization and susceptibility are substancially better than the more simple estimate of the external field*. Since these relations incorporate the unknown $h_\chi(L)$ they do not provide an explicit expression unless this unknown term is replaced by the worsening B_0/L.

It remains the question of quantitative accuracy of the semi-explicit estimations. To have the measured data comparable with the explicit, we calibrate our measurements to a relative field $\eta := h - h_c(L)$. The measurement plots over η would show the same centering arrangement as the explicit data with B_0/L as critical field estimate. The residues $R_L^{(i)}(h)$ for $i = 1, 2$ are summands and thus they are the difference of the explicit and the actual quantities. Kotecký and Medved' state that these residues decreases with increasing L and are constrained by a power law $CL^{-\delta}$ where $\delta \in (0, 1/4)$ can be chosen arbitrarily and C is sufficiently big. Unfortunately, the power law is so weak that the available range of L

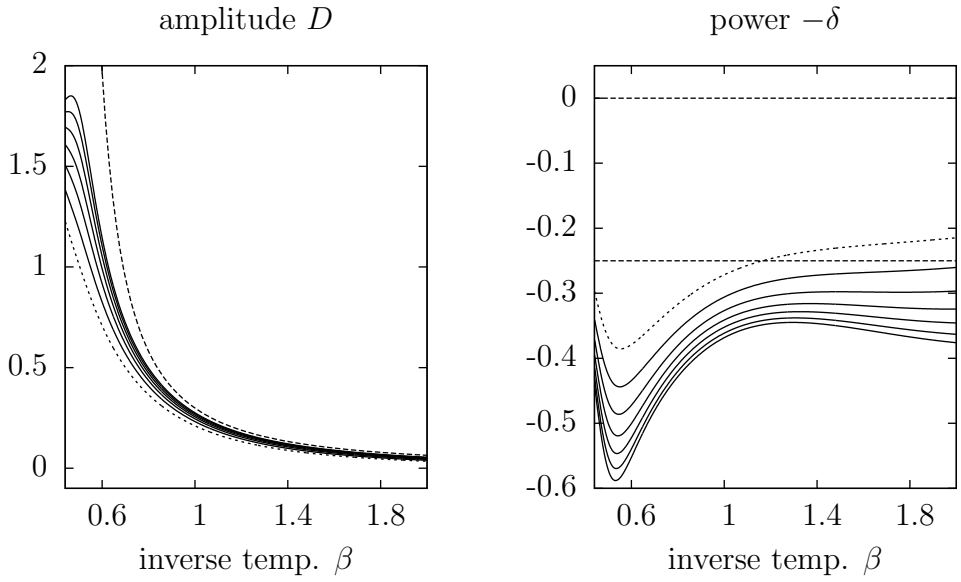

Fig. 2.3.: *Interpolation parameters D and $-\delta$ for $h_c = DL^{-\delta} + B_0/L$. Considered for triples $(L, 16, \infty)$, $L = 2, ..., 8$. ($L = 8$ is dotted to distinguish it from others). Left: the dashed line is the function $(4(\beta - \beta_c))^{-3/2}$ which might be the limit $L \to \infty$. Right: the dashed lines present the interval $(0, 1/4)$.*

is to small to have an effect which is large enough to see more than statistical fluctuation.

2.4. Conclusion

Conclusion on algorithmic strategy. The parallel tempered heat bath algorithm equipped with an whole-system-spin-flip proposal marks a first goal of the gained "far jumps" in the histogram walk but nevertheless it is not as efficient as needed. I guess that finally a multi-magnetic umbrella technique would yield results of comparable quality. Further steps must be made to improve this idea. Such certain flip algorithm must do more than simply flip the whole system. Probably, there is a method which relates "cold" positive droplets with the negative phase and makes transitions between these two areas more likely to happen.

Conclusion on the explicit approach of Kotecký and Medved'. The theory has a quite good accordance to the measurements when we consider the semi-explicit expression for magnetization and susceptibility. The theory surely is mathematical consistent but lacks useful statements for temperatures close to the critical temperature and it is

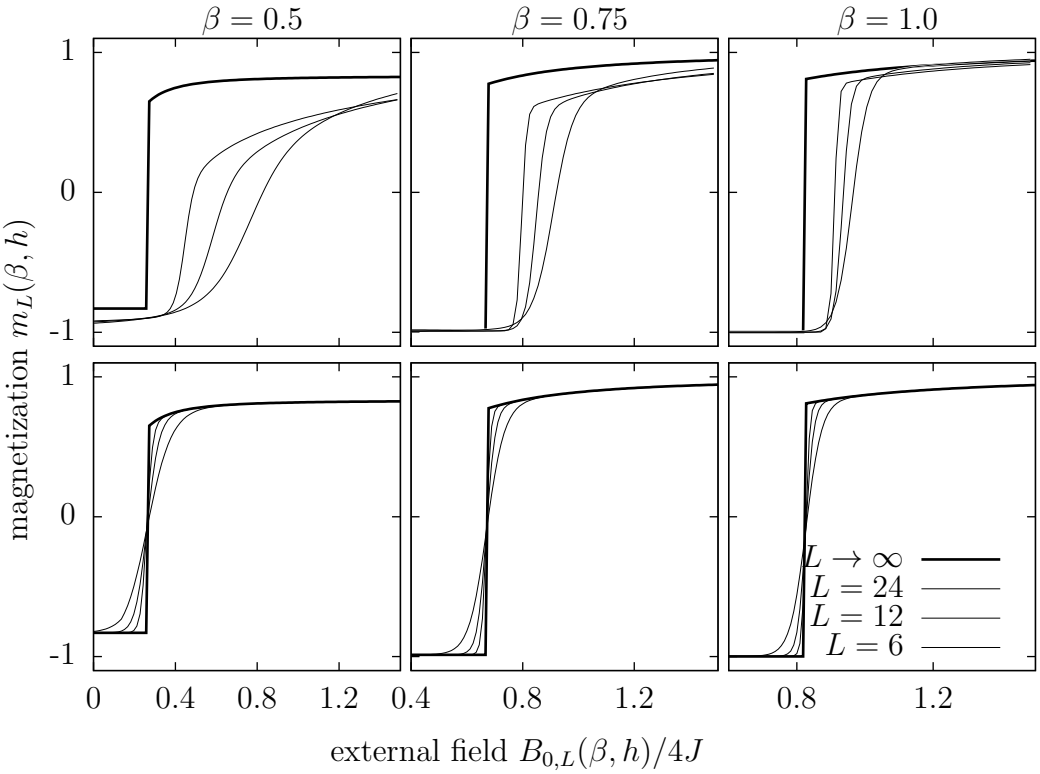

Fig. 2.4.: *Comparison of magnetization finite size scaling between actual measurements and explicit results with approximation* $Lh_\chi(L) = B_0$

insufficient predicting the external field.

Personal Conclusion. The whole situation of this work is highly unsatisfactory. I guess there is no point in my life where I had undertaken a task with such an amount of ambitious dedication and diligence. And never I had such a bad ratio of effort to result. But this should not be an accusation, not for me and not for somebody else. At the beginning of my studies on this topic *I* decided to find a reliable simulation technique and not to stop untill I had found something. It turned out to be a true sophisticated challenge. I risked to fail and now I pay for it with a suboptimal result. But what are the alternatives?

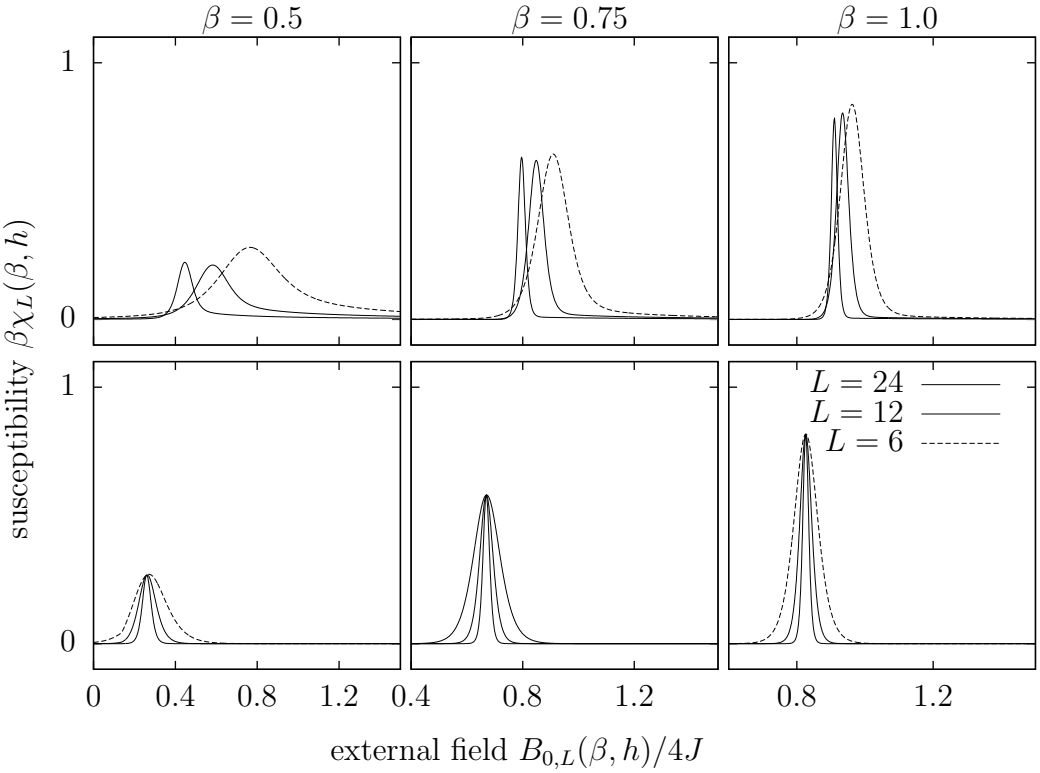

Fig. 2.5.: *Comparison of susceptibility finite size scaling between actual measurements and explicit results with approximation* $Lh_\chi(L) = B_0$

Acknowledgement

At this point now it is a pleasure to thank my dear sister Ulrike and Philip Dowerk for their patient und friendly support. While I typed this diploma thesis in the last minutes running me out you helped me saving time in answering technical questions on all that documentory stuff while your proof reading rescued me from some stilistic curiosities. Lots of thanks!

A. Mathematical considerations on extrapolation of decay

Problem. For a certain function of the type

$$f(t) \;=\; Ae^{at} + Be^{bt} + Ce^{ct} + \ldots \quad \underset{t\to\infty}{<} \quad \infty$$

we only know a finite set of of key-value pairs ("points") $f_1 = f(t_1)$, $f_2 = f(t_2)$, $f_3 = f(t_3)$, ... from which we like to reconstruct f, i.e. the parameters $a, A, b, B, c, C, \ldots$

Case I (2 points given). A function $f(t) = A \cdot a^t$ with given values $f_0 = f(t_0)$ and $f_1 = f(t_1)$ has parameter $a = \sqrt[t_0-t_1]{f_0/f_1}$ and $A = f_0/a^{t_0}$.

Case II (3 points given). Let

$$f(t) \;=\; A \cdot a^t + B$$

for unknown A, a, B and let $f_i = f(t_i)$ be given for $i = 1, 2, 3$. With elementary transformations we yield the solution

$$\begin{aligned} a &= \frac{f_3 - f_2}{f_2 - f_1} \\ A &= \frac{f_2 - f_1}{a^{t_1}(a-1)} \\ B &= f_0 - Aa^{t_0} \end{aligned}$$

Case III (4 points). Let

$$f(t) \;=\; A \cdot a^t + B \cdot b^t$$

for unknown A, a, B, b. Let $f(t_i) = f_i$ be known for $t_i = i = 0, 1, 2, 3$ and let $f_i f_{i+2} \neq f_{i+1}^2$, i.e. $f(t)$ is a true bi-exponential and not $\sim \mathrm{e}^{ct}$. We isolate the coefficients

$$\begin{aligned} A(i) &= \left(f_i - Bb^{t_i}\right) a^{-t_i} \\ B(i) &= -\frac{f_{i+1}a^{-t_{i+1}} - f_i a^{-t_i}}{(a/b)^{t_{i+1}} - (a/b)^{t_i}} \end{aligned}$$

using two adjacent pairs $(t_i, f_i), (t_{i+1}, f_{i+1})$. Of course $A(0) = A(1) = A(2) = A(3)$ and $B(0) = B(1) = B(2)$. With $c = a/b$ and $C(i) := f_{i+1}a^{-t_{i+1}} - f_i a^{-t_i}$ we conclude from $B(i) = B(i+1)$ that

$$\begin{aligned} r\left(c^{t_i} - c^{t_{i+1}}\right) &= \left(c^{t_{i+1}} - c^{t_{i+2}}\right) \ , \ r := C(i+1)/C(i) \\ 0 &= c^{t_{i+2}} - (r+1)\, c^{t_{i+1}} + r c^{t_i} \\ 0 &= c^2 - (r+1)\, c + r \cdot 1 \\ \Longrightarrow c &\in \{1, r\} \end{aligned}$$

Since we are not interested in $a = b \Leftrightarrow c = 1$ the solution $c(i) = r = C(i+1)/C(i)$ is the only relevant. Again we have $c(0) = c(1)$ and we conclude

$$\begin{aligned} C(1)^2 &= C(0)\, C(2) \\ \left(f_2 a^{-2} - f_1 a^{-1}\right)^2 &= \left(f_1 a^{-1} - f_0 a^0\right)\left(f_3 a^{-3} - f_2 a^{-2}\right) \\ 0 &= \left(f_1 f_3 - f_2^2\right) a^{-4} + \left(f_1 f_2 - f_0 f_3\right) a^{-3} + \left(f_0 f_2 - f_1^2\right) a^{-2} \\ 0 &= q + 2pa + a^2 \ , \ p = \frac{1}{2} \cdot \frac{f_1 f_2 - f_0 f_3}{f_0 f_2 - f_1^2} \ , \ q = \frac{f_1 f_3 - f_2^2}{f_0 f_2 - f_1^2} \\ a &= -p \pm \sqrt{p^2 - q}. \end{aligned}$$

Since we could have done the same calculation for b instead of a – swapping A, a and B, b causes no change in $f(t)$ – we conclude that the above formula also represents b. We

choose

$$\begin{aligned} a &= -p + \sqrt{p^2 - q}\ ,\ \ p := \frac{1}{2} \cdot \frac{f_1 f_2 - f_0 f_3}{f_1 f_3 - f_2^2} \\ b &= -p - \sqrt{p^2 - q}\ ,\ \ q := \frac{f_0 f_2 - f_1^2}{f_1 f_3 - f_2^2} \\ B = B(0) &= \frac{f_1 - f_0 a}{b - a} \\ A = A(0) &= f_0 - B. \end{aligned}$$

Case IV (5 Points). The problem

$$\varphi(t) = Aa^t + Bb^t + C$$

with five given values $\varphi_i = \varphi(t_i)$, $t_i = 0, \ldots, 4$ reduces to the above case III by setting

$$f_i := \varphi_i - \varphi_{i+1}\ ,\ \ i = 0, \ldots, 3$$

and we then yield verbatim solution for a and b. The coefficients are calculated as

$$\begin{aligned} B &= \frac{af_0 - f_1}{(b-a)(b-1)b^{t_0}} \\ A &= \frac{bf_0 - f_1}{(a-b)(a-1)a^{t_0}} \\ C &= \varphi_0 - Aa^{t_0} - Bb^{t_0}. \end{aligned}$$

Case V (6 points). Let

$$f(t) = Aa^t + Bb^t + Cc^t$$

and let $f_i := f(t_i)$ for $t_i = i = 0, \ldots, 5$ be given. We isolate the coefficients

$$\begin{aligned} A(i) &= f_i a^{-t} - Bd^{t_i} - Cg^{t_i}\ ,\ \ d := b/a, g := c/a \\ B(i) &= \frac{\varphi_i - C\gamma_i}{\delta_i}\ ,\ \ \gamma_i := g^{t_{i+1}} - g^{t_i}, \delta_i := d^{t_{i+1}} - d^{t_i}, \varphi_i = f_{i+1}a^{-t_{i+1}} - f_i a^{-t_i} \\ C(i) &= \frac{\varphi_i \delta_{i+1} - \varphi_{i+1}\delta_i}{\gamma_{i+1}\delta_i - \gamma_i \delta_{i+1}} = \frac{D_i}{\gamma_{i+1} - \gamma_i d}\ ,\ \ D_i := \varphi_i d - \varphi_{i+1} \end{aligned}$$

and it holds that $A(0) = \ldots = A(5)$, $B(0) = \ldots = B(4)$ and $C(0) = \ldots = C(3)$. Thus we get from $C(i) = C(i+1)$

$$\begin{aligned} D_{i+1}(\gamma_{i+1} - \gamma_i d) &= D_i(\gamma_{i+2} - \gamma_{i+1} d) \\ D_{i+1}(g - d) &= D_i g(g - d) \\ g(i) = g &= D_{i+1}/D_i \end{aligned}$$

and it holds $g(0) = g(1) = g(2)$. With $g(i) = g(i+1)$ and $d = b/a$ we have

$$\begin{aligned} D_{i+1}^2 &= D_i \cdot D_{i+1} \\ (\varphi_{i+1} d - \varphi_{i+2})^2 &= (\varphi_i d - \varphi_{i+1})(\varphi_{i+2} d - \varphi_{i+3}) \\ 0 &= \left(\varphi_{i+1}^2 - \varphi_i \varphi_{i+2}\right) d^2 + (\varphi_i \varphi_{i+3} - \varphi_{i+1}\varphi_{i+2})\, d + \left(\varphi_{i+2}^2 - \varphi_{i+1}\varphi_{i+3}\right) \\ 0 &= d(i)^2 + \frac{\varphi_i \varphi_{i+3} - \varphi_{i+1}\varphi_{i+2}}{\varphi_{i+1}^2 - \varphi_i \varphi_{i+2}} \cdot d(i) + \frac{\varphi_{i+2}^2 - \varphi_{i+1}\varphi_{i+3}}{\varphi_{i+1}^2 - \varphi_i \varphi_{i+2}}. \end{aligned}$$

Solving this equation, setting $d(0) = d(1)$ and evaluating this as a polynomial over a with a computer algebra system we yield a polynomial of degree 8 which separates into two irreducible factors of degree 3 and 5. The smaller polynomial has the form ($\Gamma_{ijk} := f_i f_j f_k$)

$$\begin{aligned} 0 = {} & (+\Gamma_{135} - \Gamma_{225} - \Gamma_{144} + \Gamma_{234} + \Gamma_{234} - \Gamma_{333}) + \\ & (-\Gamma_{035} + \Gamma_{125} + \Gamma_{044} - \Gamma_{134} - \Gamma_{224} + \Gamma_{233})\, a + \\ & (+\Gamma_{025} - \Gamma_{115} + \Gamma_{124} - \Gamma_{034} + \Gamma_{133} - \Gamma_{223})\, a^2 + \\ & (-\Gamma_{024} + \Gamma_{114} + \Gamma_{033} - \Gamma_{123} - \Gamma_{123} + \Gamma_{222})\, a^3 \end{aligned}$$

Once again we argue that changing the roles of A, a with B, b and C, c yields the same polynomial. That means the solution of this polynomial represents a, b, c and with the

Cardan Formula, casus irreducibilis, we get the solving algorithm

$$\begin{aligned}
n &:= -\Gamma_{024} + \Gamma_{114} + \Gamma_{033} - \Gamma_{123} - \Gamma_{123} + \Gamma_{222} \\
\alpha &:= \left(+\Gamma_{025} - \Gamma_{115} + \Gamma_{124} - \Gamma_{034} + \Gamma_{133} - \Gamma_{223}\right)/n \\
\beta &:= \left(-\Gamma_{035} + \Gamma_{125} + \Gamma_{044} - \Gamma_{134} - \Gamma_{224} + \Gamma_{233}\right)/n \\
\gamma &:= \left(+\Gamma_{135} - \Gamma_{225} - \Gamma_{144} + \Gamma_{234} + \Gamma_{234} - \Gamma_{333}\right)/n \\
-3p &:= \beta - \alpha^2/3 \\
-2q &:= 2\alpha^3/27 - \alpha\beta/3 + \gamma \\
\omega &:= \arccos\left(q \cdot p^{-3/2}\right)/3 \\
a &= -2\sqrt{p}\cos\left[\omega + \pi/3\right] \\
b &= +2\sqrt{p}\cos\left[\omega\right] \\
c &= -2\sqrt{p}\cos\left[\omega - \pi/3\right] \\
C = C\left(0\right) &= \frac{\left(f_1 - f_0 a\right)b - \left(f_2 - f_1 a\right)}{\left(c-a\right)\left(c-b\right)} \\
B = B\left(0\right) &= \frac{f_1 a^{-t_1} - f_0 a^{-t_0} - C\left(g^{t_1} - g^{t_0}\right)}{d^{t_1} - d^{t_0}} \\
A = A\left(0\right) &= f_0 - B - C
\end{aligned}$$

Problem. Given a function

$$f\left(t\right) = g \cdot G^t + c$$

from which we know $f_i = f\left(t_i\right)$ for some $t_0 < t_1 < t_2 \leqslant \infty$ and g, G, c are unknown and shall be calculated. We isolate G and formulate a fixed point equation whose contractive form depends on f it it is a decay $(0 < G < 1)$ or a growth $(G > 1)$.

$$\begin{aligned}
\alpha &:= \frac{f_0 - f_1}{f_1 - f_2} = \frac{G^{t_0} - G^{t_1}}{G^{t_1} - G^{t_2}} = \frac{1 - G^{t_1 - t_0}}{G^{t_1 - t_0} - G^{t_2 - t_0}} \quad \text{or} \quad \frac{G^{t_0 - t_2} - G^{t_1 - t_2}}{G^{t_1 - t_2} - 1} \\
\left(\alpha + 1\right) G^{t_1 - t_0} &= 1 + \alpha G^{t_2 - t_0}, \text{ with } G < 1 \text{ for decay} \\
\text{or} \quad \left(\alpha + 1\right) \bar{G}^{t_2 - t_1} &= \alpha + \bar{G}^{t_2 - t_0}, \text{ with } \bar{G} := G^{-1} < 1 \text{ for growth} \\
\text{decay: } x_1 = \varphi_1\left(x_1\right) &:= \frac{1 + \alpha x_1^{s_1}}{\alpha + 1}, \text{ with } 0 < x_1 := G^{t_1 - t_0} < 1,\ s_1 := \frac{t_2 - t_0}{t_1 - t_0} > 1 \\
\text{growth: } x_2 = \varphi_2\left(x_2\right) &:= \frac{\alpha + x_2^{s_2}}{\alpha + 1}, \text{ with } 0 < x_2 := \bar{G}^{t_2 - t_1} < 1,\ s_2 := \frac{t_2 - t_0}{t_2 - t_1} > 1
\end{aligned}$$

Ever it holds $\alpha > 0$ for decay and growth. To proof contractivity we use the following

Lemma. For $0 < a, b < 1$ and $p > 1$ we have $|a^p - b^p| \leqslant |a - b|$. *Proof.* We know that $p \mapsto a^p$ is a decreasing function since $0 < a < 1$; we yield $a = a^1 > a^p$ and $b > b^p$. Without loss of generality $a \geqslant b$. So there is a $c \in (0, 1)$ such that $a \cdot c = b$ and from this follows $b^p = a^p c^p \leqslant a^p c^0 = a^p$. Finally we get $|a^p - b^p| = a^p - b^p \leqslant a - b = |a - b|$.

Lemma (contractivity). For decay φ_1 and for growth φ_2 is contractive.

Proof. Let $x, y \in (0, 1)$. $\lambda := \alpha / (\alpha + 1) < 1$ and $\mu := 1 / (\alpha + 1) < 1$ ever hold. The above lemma yields

$$\begin{aligned} |\varphi_1(x) - \varphi_1(y)| &= \left| \frac{\alpha}{\alpha + 1} \right| \cdot |x^{s_1} - y^{s_1}| \leqslant \lambda |x - y| \\ |\varphi_2(x) - \varphi_2(y)| &= \left| \frac{1}{\alpha + 1} \right| \cdot |x^{s_2} - y^{s_2}| \leqslant \mu |x - y| . \end{aligned}$$

From Banach's fixed point theorem we conclude that for decay φ_1 and for growth φ_2 has one and only one fixed point x_1 or x_2, respectively. From them we calculate the constants G, g and c.

$$\begin{aligned} G &= x_1^{1/(t_1 - t_0)} = x_2^{-1/(t_2 - t_1)} \\ g &= \frac{f_0 - f_1}{G^{t_0} - G^{t_1}} \\ c &= f_0 - g G^{t_0} \end{aligned}$$

Problem. Given a function

$$f(t) = g \cdot t^{\gamma} + c$$

from which we know $f_i = f(t_i)$ for some $0 < t_0 < t_1 < t_2$ and g, γ, c are unknown and shall be calculated. We reformulate f to transform this problem to that one previously discussed.

$$\tilde{f}(\tilde{t}) := f\left(t = \mathrm{e}^{\tilde{t}}\right) = g \cdot (\mathrm{e}^{\gamma})^{\tilde{t}} + c$$

With $\tilde{t}_i = \log(t_i)$ and $\tilde{f}_i = f_i$ we yield $g = \tilde{g}$, $\gamma = \log\left(\tilde{G}\right)$ and $c = \tilde{c}$.

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Leipzig, den January 29, 2013

Christoph Vogelsberg

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Christoph Vogelsberg