Dynamical temperature study for classical planar spin systems

Wira B. Nurdin*, Klaus-Dieter Schotte†
Institut für Theoretische Physik, Freie Universität Berlin
Arnimallee 14, 14195 Berlin, Germany
(March 22, 2022)

Making use of the Rugh’s micro–canonical approach to temperature we study \(XY\)–spin systems by the strictly energy conserving over-relaxation algorithm. In this micro-canonical simulation the temperature and also the specific heat are determined as averages of expressions easy to implement. The \(XY\)–chain is studied for a test. The second order transition on a cubic lattice and the first order transition on fcc lattice are analyzed in greater detail to have a more severe test about the feasibility of this micro-canonical method.

PACS numbers: 05.50.+q, 75.10.Hk, 75.40.Mg

I. INTRODUCTION

Dynamical simulations of large systems of spins or particles should in principle lead to the same information as statistical simulations generating a canonical ensemble. Although the energy is conserved one can determine the temperature for a system consisting of kinetic and potential energy the temperature by the average kinetic energy. With the recent advance in the understanding of the micro–canonical temperature initiated by Rugh \[1–3\], one can “measure” the temperature and also the specific heat along the trajectory of spin systems where such a decomposition of the energy does not exist. In the case of \(XY\)–spins one could also add the sum over the angular velocities but a dynamical check of statistical mechanics by a common molecular dynamics simulation is not an easy numerical task \[4\]. We think by using spin systems alone one has more efficient means to pursue this program.

Several attempts have been made to establish a strictly micro–canonical approach to study phase transitions \[5,6\]. Here we want to present a study of the planar or \(XY\)–spin systems, making use of a micro–canonical temperature definition discussed recently \[3\] and the “over–relaxation algorithm” \[7,8,11\]. This algorithm has been used to accelerate Monte Carlo simulations for Heisenberg or \(XY\) spins for example. Since it conserves energy it can be taken as a Metropolis step, where steps leading to equal or lower energy are always accepted. The Metropolis procedure leads to thermalisation, whereas the over–relaxation algorithm generates different configurations and thereby improves the convergence. The question we want to address is, can one work alone with the over–relaxation algorithm. Since the temperature can be calculated as an average the Metropolis procedure is not needed for the temperature determination. However, it is not guaranteed whether in a fixed energy simulation one “visits” enough regions of phase space in order to determine the physical observables reliably. More specifically we want to ask: is the finite size analysis the same as for canonical simulations? A closely connected question: is the analysis of a first order transition really different from the standard one using a histogram \[5\] analysis?

For numerical tests we have chosen \(XY\)–spins on a chain and on three dimensional simple cubic (sc) and face centered cubic (fcc) lattices both with nearest neighbour coupling. A second order transition on the sc lattice and the first order one on fcc \[12\] will thus be studied.

II. MICRO–CANONICAL TEMPERATURE FOR CLASSICAL \(XY\)–SPIN SYSTEMS

A. General approach

Instead of three components for the classical Heisenberg system in our preliminary paper \[3\], here we want to study the simpler \(XY\)–spin system where only two components \(\vec{S} = (S^1, S^2)\) have to be taken into account, that is the spin vector is confined to a circle with radius \(S\). No dynamical equation can be written down similar to \(\frac{\partial \vec{S}}{\partial t} = \vec{S} \times \vec{H}\) for the three dimensional vector \(\vec{S}\) in a magnetic field \(\vec{H}\). The energy \(-\vec{H} \cdot \vec{S} = -H S \cos \varphi\) is the same for the two directions \(\pm \varphi\) the vector \(\vec{S}\) can point. Contrary to the three dimensional case, there is no continuous path between these equal energy states at \(\pm \varphi\).

Still we can calculate the size of the phase space \(W\) summing over all contributions with the same energy \(E\). \(W\) corresponds to the density of states in the classical limit. With the entropy \(S\) as a function of energy given by

\[S(E) = \ln W(E)\]

\*E-mail: nurdin@physik.fu-berlin.de, on leave from Physics Department, Hasanuddin University, Makassar.
\†E-mail: schotte@hmi.de
\[ S = \ln W \]  

(Boltzmann’s constant set to unity), the density of states contains all information necessary for a thermodynamic analysis. We want to show that the derivative of \( S \) with respect to the energy is easily accessible.

With \( N \) spins of length \( |\vec{S}_i| = 1 \), that is \( \vec{S}_i = (\cos \varphi_i, \sin \varphi_i) \) one has

\[ W = \int \delta(E - \mathcal{H}) \prod_{i=1}^{N} d\varphi_i = \int_{\mathcal{H}=E} \frac{d\Omega_{N-1}}{|\nabla \mathcal{H}|} \]

where the integration is over \( N \) unit circles. However, the integral is restricted to \( 2N-1 \) dimensions by \( \mathcal{H} = E \). This restriction taken into account, one arrives at the second form of the integral with the gradient taken with respect to all \( \varphi_i \) angles [3]. Because the direction of the infinitesimal surface elements \( d\Omega \) normal to the surface of constant energy coincides with the direction of the gradient \( \nabla \mathcal{H} \), one arrives at a second form of the constant energy integral

\[ W = \int_{\mathcal{H}=E} \frac{\nabla \mathcal{H} d\Omega_{N-1}}{|\nabla \mathcal{H}|^2} = \int \Theta(E - \mathcal{H}) \nabla \left( \frac{\nabla \mathcal{H}}{|\nabla \mathcal{H}|^2} \right) \prod_{i=1}^{N} d\varphi_i . \]

Applying Gauss’ theorem this integral can be written as an integral over all phase space with energy lower than \( E \), the restriction given by the Heavyside step function \( \Theta \). The quantity to be integrated is the divergence of a vector field \( X \) with the property that the scalar product of \( \nabla \mathcal{H} \) and \( X = \nabla \mathcal{H}/|\nabla \mathcal{H}|^2 \) is unity [2]. The derivative is then

\[
\frac{\partial W}{\partial E} = \int \delta(\mathcal{H} - E) \nabla \left( \frac{\nabla \mathcal{H}}{|\nabla \mathcal{H}|^2} \right) \prod_{i=1}^{N} d\varphi_i
\]

a constant energy integral like [3] for \( W \). The ratio of these two integrals gives then the inverse temperature

\[
\frac{1}{T} = \frac{\partial W/\partial E}{W}
\]

since \( 1/T = \partial S/\partial E \) with the entropy \( S \) given by [1].

In order to obtain the inverse temperature according to [1] and [3] one has to average the following quantity, called \( 1/T_{xyz} \) for short

\[
\frac{1}{T_{xyz}} = \sum_{i=1}^{N} \partial_i \frac{\partial \mathcal{H}}{\sum_{l}(\partial_l \mathcal{H})^2} ,
\]

where we use the notation \( \partial_i = \partial/\partial \varphi_i \). To compare with the Heisenberg case [3] of a three dimensional vector confined to a sphere one identifies \( \partial_i \partial \varphi_i \) as the third component of the angular momentum operator

\[
\frac{\partial}{\partial \varphi_i} = S_i^3 \frac{\partial}{\partial S_i^3} - S_i^2 \frac{\partial}{\partial S_i^2} \]

used in quantum mechanics, only “\( i \)” is missing. Eq.[3] can then be viewed as a reduced form of a micro-canonical temperature for a Heisenberg spin system with the complete angular momentum operator \( \hat{\mathcal{L}}_i = \vec{S}_i \times \nabla i \)

\[
\frac{1}{T_{xyz}} = \sum_{i=1}^{N} \frac{\mathcal{L}_i \mathcal{H}}{\sum_{l}(\mathcal{L}_l \mathcal{H})^2}
\]

instead of only the third component of \( \hat{\mathcal{L}}_i \) appearing in eq.[3].

For large system sizes \( N \gg 1 \) the quantity to be averaged in [3] can be simplified. The two terms generated by differentiation are

\[
\frac{1}{T_{xy}} = \frac{\sum_{l}(\partial_l \mathcal{H})^2}{\sum_{l}(\partial_l \mathcal{H})^2} + \sum_{i=1}^{N} \partial_i \mathcal{H} \partial_i \frac{1}{\sum_{l}(\partial_l \mathcal{H})^2} ,
\]

where the last one can be neglected since it is only of order \( 1/N \). The reason is the short range of exchange interactions. The Hamiltonian \( \mathcal{H} \) connects a spin \( \vec{S}_i \) only to its neighbors so that the differentiation with respect to \( \varphi_i \) is nonzero for \( l = i \) and \( l \) close to \( i \). As a result the second term scales as \( \propto 1/N \) since a single sum in the numerator is outweighed by a double sum in the denominator. Also for large spin systems neglecting again \( 1/N \)-corrections one can take the inverse of [3] to determine the temperature \( T \) directly as an average of

\[
T_{xy} \approx \sum_{l}(\partial_l \mathcal{H})^2 \sum_{l}\partial_l^2 \mathcal{H} ,
\]

that is \( T = \langle T_{xy} \rangle \).
B. Micro-canonical temperature in simulations

Although there exist no dynamical equations which conserve the energy for $XY$–spin systems, there is a so-called “over–relaxation algorithm” in use to generate spin configurations of equal energy. This algorithm is used in conjunction with the standard Metropolis procedure, see for example [11], to diminish the effects of critical slowing down [8]. The Hamiltonian we want to study is

$$\mathcal{H}_{ex} = -\sum_{ij} J_{ij} \cos(\varphi_i - \varphi_j) ,$$  \hfill (11)

where the sum is over the exchange constants $J_{ij}$ connecting close spins at sites $i$ and $j$. In an equivalent notation this is $\mathcal{H}_{ex} = -\sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$ with $\vec{S}_i = (\cos \varphi_i, \sin \varphi_i)$. The energy $E_i$ contributed by an individual spin $S_i$ is

$$E_i = -\vec{S}_i \cdot \sum_j J_{ij} \vec{S}_j = -\vec{S}_i \cdot \vec{H}_i$$  \hfill (12)

with $\mathcal{H}_{ex} = \frac{1}{2} \sum_i E_i$. To get the total energy $\mathcal{H}_{ex}$ one has to sum over all sites of the lattice and since the exchange interaction appears twice the sum has to be divided by two. The “local” energy $E_i$ depends on the “molecular” field $\vec{H}_i$ generated by the neighbors. It does not change if

$$\vec{S}_i \Rightarrow -\vec{S}_i + 2 \vec{H}_i (\vec{S}_i \cdot \vec{H}_i) / H_i^2 .$$  \hfill (13)

This is the basic step of the “over–relaxation” algorithm which in geometrical terms means a change of $\vec{S}_i$ to its mirror position with the mirror line given by $\vec{H}_i$ as in Fig. 1. In the simulation the spins to be updated are mostly chosen randomly [4].

Using the special form for the Hamiltonian (11) the formula for the temperature (10) simplifies to

$$T_{xy} = -\frac{\sum_i (\partial_i \mathcal{H}_{ex})^2}{2 \mathcal{H}_{ex}} ,$$  \hfill (14)

since summing the second derivative of the Hamiltonian $\mathcal{H}_{ex}$ with respect to all angles $\varphi_i$ one recovers $\mathcal{H}_{ex}$ merely multiplied by $-2$. The easiest way to test the validity of the temperature determination by averaging (14) is to apply the over–relaxation algorithm to a spin chain. However, this algorithm for a linear chain with

$$\mathcal{H}_{chain} = -J \sum_{i=1}^N \cos(\varphi_i - \varphi_{i+1}) \quad \text{and} \quad \varphi_{N+1} = \varphi_1$$  \hfill (15)

would be non ergodic in the case that all exchange constants are equal [4]. In alternating the exchange by $\pm 10\%$ along the chain one has a remedy for this defect easy to implement. The temperature according to (14) for a homogeneous chain is

$$T_{chain} = -\frac{1}{4} \sum_{i=1}^N \left[ J \sum_{\pm} \sin(\varphi_i - \varphi_{i\pm 1}) \right]^2 / \mathcal{H}_{chain} .$$  \hfill (16)

The task is then to check whether for a large chain the canonical relation (14) between energy $E$ and temperature

$$\epsilon = E / N = -J I_1 (J/T) / I_0 (J/T)$$  \hfill (17)

is reproduced. $I_0$ and $I_1$ are modified Bessel function. The specific heat as the derivative $C = dE/dT$ then is

$$C / N = (J^2 + T \epsilon - \epsilon^2) / T^2 .$$  \hfill (18)

We checked that the slight change of the exchange constant $J = 1.0 \pm 0.1$ had no visible effect in Fig. 2. For a comparison using the average value $J = 1$ is sufficient. The temperature and the specific heat for a $XY$–chain determined by the over–relaxation method by varying the energy agree well, as can be seen in Fig. 2, where energy and specific heat are plotted in the conventional way as functions of the temperature. The question how to calculate the specific micro–canonically for $XY$–spin system will be addressed in the next section.

An initial state with a prescribed energy to start the simulation is found in the following way. One solves numerically the differential equations

$$\dot{\varphi}_i = \pm \partial_i \mathcal{H}_{ex} / \tau .$$  \hfill (19)

A change of the angles $\varphi_i$ of the spins involves a change of the total energy, that is $\mathcal{H}_{ex} = \pm (1/\tau) \sum_i (\partial_i \mathcal{H}_{ex})^2$. Depending on the size and sign of the relaxation time $\tau$ in principle starting from randomly chosen orientations $\varphi_i$ of spins any prescribed energy could be reached. Very low energies states, however, can only be found by a succession of energy conserving over–relaxation steps and steps lowering the energy by small amounts using (19).
III. SPECIFIC HEAT OF A XY SPIN SYSTEM

A. Specific heat for the XY-chain

In taking the derivative of the entropy $S$ with respect to the energy $E$ one obtains the inverse temperature. The second derivative with respect to the energy will then determine the inverse of the specific heat. Formally the first derivative defines the inverse temperature by the divergence of a vector $\vec{X}$

$$\vec{X} = \left( \partial_1 \mathcal{H}, \partial_2 \mathcal{H}, \cdots \partial_N \mathcal{H} \right) / \sum_{i=1}^{N} (\partial_i \mathcal{H})^2$$

(20)

according to (3) written as $1/T = \sum_i \partial_i X_i$. This standard form of $\vec{X}$ can be changed. One can modify $\vec{X}$ as long as the scalar product between $\vec{X}$ and $\nabla \mathcal{H}$ does not change, that is

$$\sum_{i=1}^{N} X_i \partial_i \mathcal{H} = 1 .$$

(21)

To get the volume of phase space with (3) correctly, (21) is the only condition (2). In a “hydrodynamic” picture this means that the flow in phase space $\vec{X}$ across $\mathcal{H} = E$ should be the same as the “natural” flow given by (3) which is perpendicular to the $\mathcal{H} = E$ surface. The constraint (21) leaves enough room for choices better fitted to specific heat calculations as will be shown.

For a chain a variant to $\vec{X}$ is

$$\vec{X}' = \left( 0, \partial_2 \mathcal{H}, 0, \partial_4 \mathcal{H}, \cdots, 0, \partial_N \mathcal{H} \right) / \sum_{i=1}^{N/2} (\partial_i \mathcal{H})^2 ,$$

(22)

and one easily checks that the normalisation (21) is still valid. In the following it is assumed that $\mathcal{H}$ is of the exchange type restricted to nearest neighbors like (11) or specifically (13) for the one dimensional case. The inverse temperature is then given by an expression similar to (8) for $1/T$ is helpful for an easier numerical calculation.

For the temperature determination the inverse of (23) without the $1/N$–correction is sufficient, that is we take

$$\mathcal{T} = - \sum_{j=1}^{N/2} \left( \partial_{2j} \mathcal{H} \right)^2 / \mathcal{H}$$

(24)

and determine the temperature by $T = \langle \mathcal{T} \rangle$. The energy $\mathcal{H}$ or $E$ in the denominator is obtained by summing up the second derivatives, that is $\sum_{i=1}^{N/2} \partial_i^2 \mathcal{H} = -\mathcal{H}$. The derivative of $\mathcal{T}$ with respect to temperature consists of two contributions

$$\frac{dT}{dE} = \frac{1}{C} = \left\langle \sum_{i=1}^{N/2} \partial_{2i} \mathcal{H} \frac{\partial_{2i} \mathcal{H}}{\sum_j (\partial_{2j} \mathcal{H})^2} T \right\rangle - \left\langle T \right\rangle \left\langle \frac{1}{\mathcal{T}} \right\rangle$$

$$= 1 - \frac{T}{E} - T \left\langle \frac{1}{\mathcal{T}} \right\rangle + 2T \left\langle \frac{\sum_{i=1}^{N/2} (\partial_{2i} \mathcal{H})^2 \partial_{2i} \mathcal{H}}{\left[ \sum_j (\partial_{2j} \mathcal{H})^2 \right]^2} \right\rangle .$$

(25)

The first has its origin in the direct energy dependence of the temperature average of $\sum_i \partial_i (X_i' \mathcal{T})$. The second term comes from the energy dependence of the normalization necessary for the temperature average. The definition (23) leads to the first two terms in the expanded form of the next line whereas the two last terms are generated by using (23) for $1/\mathcal{T}$. With

$$\frac{1}{\mathcal{T}} = \frac{1}{\mathcal{T} + \Delta \mathcal{T}} = \frac{1}{\mathcal{T}} - \frac{\Delta \mathcal{T}}{\mathcal{T}^2} + \frac{(\Delta \mathcal{T})^2}{\mathcal{T}^3} - \cdots$$

(26)
and $\Delta T = T - T$ the ‘1’ in \( [23] \) disappears and only terms $\propto 1/N$ remain. This is to be expected since the reciprocal of the specific heat behaves as $dT/dE \propto 1/N$. One notices that the inverse of the specific heat depends on the temperature fluctuation. As a further simplification the averages of the last term of \( [24] \) can be taken separately for the denominator and the numerator by neglecting $1/N^2$ corrections. Further the average of the denominator is simply $(E T)^2$ since $\langle \sum_j (\partial_j \mathcal{H})^2 \rangle = TE$ according to \( [24] \). The difference to the true average would result again in a $1/N^2$ correction and can therefore safely be neglected.

Taking the simplifications into account, the specific heat is then

$$
\frac{1}{C} = \frac{T/TE}{1/N} - \langle (\Delta T)^2 \rangle/T^2 + 2 \frac{\langle \sum_{j=1}^{N/2} (\partial_j \mathcal{H})^2 \partial_j^2 \mathcal{H} \rangle}{T E^2} \quad (27)
$$

No further simplifications are possible. In the last term appears the local energy $-\partial_j^2 \mathcal{H}$ besides the square of the “torque” $(\partial_j \mathcal{H})^2$ used for the temperature determination. To get an understanding of the average of these two quantities let us define a local energy deviation $\Delta \mathcal{H}_{2j} = -\partial_j^2 \mathcal{H} - 2\gamma \mathcal{H}/N$. The $\gamma$ value is determined by splitting the average of \( [27] \) into two parts

$$
\langle \sum_{j=1}^{N/2} (\partial_j \mathcal{H})^2 \partial_j^2 \mathcal{H} \rangle = - \langle \sum_{j=1}^{N/2} (\partial_j \mathcal{H})^2 \Delta \mathcal{H}_{2j} \rangle - \frac{2\gamma}{N} \langle \sum_j (\partial_j \mathcal{H})^2 \mathcal{H} \rangle = \frac{2\gamma}{N} T E^2 .
$$

such that the first term depending on the local energy fluctuations should vanish. The average of the second term is $\propto T E^2$ according to \( [24] \). The inverse of the specific heat \( [27] \) is then

$$
\frac{1}{C} = \frac{T}{TE} + \frac{4\gamma}{N} - \frac{\langle (\Delta T)^2 \rangle}{T^2} \quad (29)
$$

which at low temperatures with $T/(-E) \ll 1$ should reduce to

$$
\frac{1}{C} \approx \frac{4}{N} - \frac{\langle (\Delta T)^2 \rangle}{T^2} ,
$$

a form derivable (see appendix) for a chain of harmonic oscillators with the temperature fluctuation $2/N$ so that $C_{osc} = N/2$. At low temperatures one expects $\gamma = 1$, since the $XY$-spin chain should have the same specific heat as a harmonic oscillator chain.

To get the specific heat of the $XY$–chain shown in Fig. 2 relation \( [27] \) has been used. At low temperatures the specific heat for one spin is $1/2$ as expected.

**B. Specific heat for the $XY$–lattice systems**

The strategy to calculate the specific heat for a chain can also be used for two or three dimensional lattices. For square and simple cubic lattices a decomposition in two sublattices analogously to the even odd decomposition for the chain can be made. A spin is even or odd if the sum of its coordinates $(i, j, k)$ is even or odd.

The point is that the no nearest neighbor “bond” $\vec{S}_i \cdot \vec{S}_j$ appears twice in different components which is the case for the vector $\vec{X}$ defined by \( [22] \). As a consequence only local energy and temperature terms have to be averaged.

For a chain and a simple cubic lattice starting from all “even” or all “odd” sites all the interactions $\vec{S}_i \cdot \vec{S}_j$ are taken into account and $\sum_{i=1}^{N/2} \partial_{i,l} \mathcal{H} = -\mathcal{H}$ for $l = \text{even, odd}$ so that renumbering the spins \( [22] \) can be used without further changes. As an example we show in Fig. 3 the specific heat of the $XY$–model on a simple cubic lattice obtained this way. Only close to the critical region differences between the canonical simulation using the Metropolis method and the micro–canonical simulation are visible.

In the general case, for a face centered cubic lattice as an example, slight changes have to be made. The fcc lattices can be thought to consist of four sublattices, one simple cubic lattice and three additional ones shifted in the three direction $(1, 1, 0), (1, 0, 1)$ and $(0, 1, 1)$ to the centers of the faces of a cube. If one picks out one of these simple cubic lattices one can take over all the equations from the last section for the chain, only the energy connected to that sublattice is no longer a constant since is not the total energy. With $M^3$ of lattice points of the simple cubic lattice, that is $N = 4 M^3$ the total number the spins, the temperature analogous to \( [24] \) is

$$
\mathcal{T}_i = - \sum_{i=1}^{N/4} (\partial_{i,l} \mathcal{H})^2 / \mathcal{H}_i \quad \text{with} \quad T = \langle \mathcal{T}_i \rangle , \quad (31)
$$

where the summation takes into account all angles $\varphi_{j,l}$ of one of the cubic sublattices with number $l = 1, 2, 3$ or 4. The partial energy is $\mathcal{H}_i = - \sum_{i=1}^{N} \partial_{i,l}^2 \mathcal{H}$. In a sense one has four thermometers which should of course give the same temperature. Similarly one can calculate the specific heat starting from one sublattice. We studied the anti-ferromagnetic transition on a fcc lattice (see section V), but the specific heat calculation with formulas similar to \( [27] \) did not give stable results in the neighborhood of the first order transition because of the singular nature of the specific heat.
In principle the scaling behavior close to a second order phase transition should be the same for a canonical ensemble and for a micro-canonical ensemble. So one expects for a micro-canonical ensemble close to the critical energy that the “measured” temperature should dependent on the size of the system. This corresponds to the size dependence of the energy for a canonical ensemble at the critical temperature \( T_c \).

The correlation length \( \xi \) grows like \( \xi \propto \xi_0/|T - T_c|^\nu \) for a temperature close to the critical temperature \( T_c \). This length \( \xi \) cannot become larger than the size \( L \) of a finite system. In a micro-canonical simulation at the critical energy \( E_c \) this finite size effect should be directly visible. Since the system size takes the role of the correlation length, the recorded temperature \( T_L \) should deviate from its critical value \( T_c \) according to

\[
T_L = T_c + T_1 L^{-\nu},
\]

that is by rewriting \(|T_L - T_c| \propto L^{-\nu}\) as an equation. In Fig. 4 the size dependence of the critical temperature is plotted and one sees that the temperature defined as an average of \( T_L \) reproduces the expected effect.

We took as the critical temperature \( E_c = 0.989 \) found by Schultka et al. In the temperature scaling analysis we should recover the temperature these authors started with that is the value \( T_c = 2.2017 \) determined by Janke. This is actually the case, since we find \( T_c = 2.202 \).

For a canonical system where the temperature is fixed by its critical value \( T_c \), the critical energy \( E_c \) has finite size corrections. Loosely speaking one has \(|E - E_c| \propto |T - T_c|^{1-\alpha}\) in the neighborhood of the critical point. The linear dependence between energy changes \( E - E_c \) and temperature changes \( T - T_c \) is modified to a power law dependence by the specific heat exponent \( \alpha \). With this modification the finite size correction of the critical energy follows in close analogy to (32)

\[
E_L = E_c + E_1 L^{-(1-\alpha)/\nu}\]

from \(|E_L - E_c| \propto L^{-(1-\alpha)/\nu}\). The relation (33) has been used to determine the critical energy \( E_c \). For an XY–system practically the same exponent for the micro-canonical scaling according to (32) or the canonical one using (33) can be taken, since \( \alpha \) is very small in aXY system. Actually in (33) a correction term \( E_2 L^{-(1-\alpha)/\nu} \) has been added to (32). In the analysis of (32) the corresponding correction is also needed, as can be seen in Fig. 4.

We test the over-relaxation algorithm by studying the dynamical scaling behavior \( T_L \). To use this procedure one should start with a configuration as far as possible from equilibrium with an energy fixed to its critical value. We take a random configuration for the spins as a starting configuration. It turns out to have an energy close to equilibrium.

The magnetization \(|\vec{M}|\) exhibits more clearly the power law dependence, since no constant term must be subtracted. It should depend on the update steps \( t \) like

\[
|\vec{M}| \propto t^{\gamma/(2z)}.
\]

This corresponds to \( \langle \vec{M}^2 \rangle \propto L^{\gamma/\nu} \) or \( \langle |\vec{M}| \rangle \propto L^{\gamma/2\nu} \), valid for finite size scaling with the exponent \( \gamma \) for the susceptibility. The rule of transcription is simply that one should replace \( L \) by \( t^{1/2} \). Since \( \eta \) is small we take 1 for the ratio \( \gamma/(2\nu) = 1 - \eta/2 \).

We used two slightly different ways for the implementation of the over-relaxation algorithm. The first one consists of choosing randomly the spins to be updated. The second method uses a sequential update. The lattice is partitioned into two sublattices corresponding to the up and down sublattices of an anti-ferromagnet. Since the interaction is only between nearest neighbors the numbering of the spin used for the sequential update does not matter. First the the spin vectors sitting on the up-spin sites are updated and then the others. Technically one decides whether an index is even or odd before one starts with the over-relaxation. A spin is an even or odd one if the sum of its coordinates \((i, j, k)\) is even or odd.

Taking the results of the simulation depicted in Fig. 5 one notices that with \( z_{\text{seq}} = 1 \) and \( 1/0.58 \approx 7/4 \) the sequential update is the more efficient algorithm. However, to be more on the safe side concerning ergodicity one might prefer the random update with \( z_{\text{ran}} = 1/0.42 \approx 7/3 \). Since always half the total number of spins are “turned around” the greater efficiency of the sequential update might be connected to the nonlocal nature of the update reminiscent of the very efficient cluster algorithms.
V. FIRST-ORDER PHASE TRANSITIONS

The micro-canonical technique can be shown to be most suitable in simulating first order transitions. A $XY$-spin model having such a transition is an anti-ferromagnet on the fcc-lattice. For simplicity we take only the interaction between nearest neighbors. This model has been analysed by Diep and Kawamura [12] using standard Monte Carlo techniques. There the first order nature of the transition for $XY$ and Heisenberg spins was shown. Especially for an Ising model the frustrated anti-ferromagnetic order on a fcc-lattice leads to a strong first order transition [6,19]. For the vector spins this phenomenon is less pronounced.

The temperature for a large range of energies has been determined and the region between 1.35 and 1.55 was scanned more carefully. The energies are all positive and therefore all temperatures negative since we kept the convention of the preceding sections that the ferromagnet has the lowest energy and the exchange constant $J = -1$.

In the inset of Fig. 6 the S-shape of the energy versus temperature dependence clearly indicates the first order nature of the transition.

We want to analyse in greater detail the data for the largest lattice with $4 \times 24^3$ spins. The idea is to use Maxwell’s equal area construction to determine the transition temperature. A direct approach is not advisable since the statistical errors for the temperature changes are quite large. A better way is to determine first the entropy [5,6]. With the energy density $\epsilon = E/N$, the entropy density $s = S/N$, the reciprocal temperature $\beta = 1/T$ and $\beta = \partial s/\partial \epsilon$ one obtains the entropy by integrating

$$\frac{1}{N} \ln P = s - \epsilon \beta_c = \int_{\epsilon_0}^{\epsilon} d\epsilon (\beta - \beta_c). \tag{36}$$

The logarithm of the density of states $W$ as the entropy is changed by subtracting $E/T$, that is $P = W \cdot e^{-E/T}$. This probability $P$ depicted in Fig. 7 has the double peak form of the histograms one obtains by counting the frequency an energy $E$ occurs in a Monte Carlo simulation. The peaks must have equal height at the transition temperature corresponding to Maxwell’s equal area rule.

The temperature we find by this procedure is $T_c = 0.7397$. However, in looking at the insert of Fig. 6 a considerable size dependence. The energy difference between the two maxima $\Delta \epsilon = 0.13$ gives an estimate for the latent heat. One can also read off from Fig. 7 the difference in the logarithm of the probabilities $\ln P_{\text{max}} - \ln P_{\text{min}} \approx N \times 0.0005$, that is for $\ln P$ at the peaks and for the minimum between the peaks. Since the cluster has $N = 4 \times 16^3$ spins the ratio $P_{\text{min}}/P_{\text{max}} \approx e^{-8}$ or $10^{-4}$ is already too small for a standard Monte Carlo simulation. In upgrading the weights by using the “multi-canonical” method this low probability problem is circumvented. With the micro-canonical procedure no modification seems to be necessary here. However, first order transitions are beset of hysteresis phenomena, they are bound to occur also in micro-canonical simulations.

VI. CONCLUDING REMARKS

We confirmed that the temperature calculation as averages given by (10) and (14) give reliable results. The severe tests were (a) the size dependence of the temperature for a second order transitions and (b) the non monotonic dependence of the temperature on the energy in the neighbour-hood of a first order transition. Further we wanted to demonstrate that efficient micro-canonical simulations for vector spins are feasible making use of the over relaxation algorithm. However, since the histogram technique is missing, the critical energy cannot be determined precisely by Binder’s cumulant technique [22]. For first order transitions the method appears suitable.

The inverse of the specific heat as the derivative of the temperature with respect to energy is linked to averages of fluctuations. They are far more complicated than the energy fluctuation one has to calculate for the specific heat in the canonical ensemble. Nevertheless we could show that the specific heat can be calculated micro-canonically. That the temperature definition is not unique is the essential point of Rugh’s micro-canonical temperature definition [3]. This freedom of choice was essential for finding manageable expressions.

A. Acknowledgment

We thank W. Janke for pointing to the close similarity between a micro canonical and canonical analysis of first order transitions. We are thankful D. Loison for showing us the use of the over-relaxation algorithm.
VII. APPENDIX

A. Micro canonical Specific heat for a harmonic oscillator chain

The concept used for the micro canonical temperature and the specific heat determination is best be illustrated for a set of harmonic oscillators. We take a one dimensional example with the potential energy

\[ V = \frac{1}{2} \sum_{i} (x_i - x_{i+1})^2 \quad \text{and} \quad x_{N+1} = x_1 \]

for a chain of coupled oscillators. Following the procedure for the spin chain of section III a vector \( \vec{X} \) is defined by

\[ \vec{X} = -\left(0, F_2, 0, F_4, \cdots, 0, F_N\right) / \sqrt{\sum_{i=1}^{N/2} F_{2i}} \]

where the expressions \( F_n = -\partial V / \partial x_n \) mean the forces acting on the n-th particle. Obviously Rugh’s condition for the “flow” \( \vec{X} \), namely \( -\sum_{i} F_i X_i = 1 \) holds, since only even components appear in the scalar product. The minus sign comes from the definition of the forces \( F_i \) as negative derivatives.

The inverse temperature defined as the divergence of \( \vec{X} \) is then

\[ \frac{1}{T'} = -\sum_{i=1}^{N/2} \frac{\partial F_{2i}}{\sum_{j=1}^{N/2} F_{2j}} = \sum_i \frac{\partial^2 V}{\sum_j F_{2j}^2} - 2 \sum_i \frac{F_{2i}^2 \partial^2 V}{\left[\sum_j F_{2j}^2\right]^2} \]

with \( \partial F_{2i} = \partial / \partial x_{2i} \). Since the second derivative of the chain potential is \( \partial^2 V / 2 \) one gets finally

\[ \frac{1}{T'} = \frac{N}{\sum_{j=1}^{N/2} F_{2j}^2} \]

that is the expression one has to average to obtain the inverse temperature.

Neglecting the finite size corrections we determine the temperature by averaging the quantity

\[ T = -\frac{1}{N} \sum_{j=1}^{N/2} F_{2j}^2 \]

The specific heat \( C \) is then given by

\[ \frac{1}{C} = \frac{d}{dE} \langle T \rangle = \sum_{i=1}^{N/2} \frac{\partial F_{2i}}{\sum_{j=1}^{N/2} F_{2j}^2} \langle T \rangle + \langle T \rangle \frac{1}{T'} \]

\[ = 1 + \langle T \rangle \frac{1}{T'} \]

Using the expansion (26) for the reciprocal temperature the last equation for the inverse of the specific heat reduces to

\[ \frac{1}{C} = \frac{4}{N} - \frac{\langle (T - \langle T \rangle)^2 \rangle}{\langle T \rangle^2} \]

in the limit for \( N \gg 1 \). This is eq. (30) used for a comparison with the specific heat formula (28) of the XY-spin chain. The last term of (33) is the temperature fluctuation. Its size must be \( 2/N \) since the specific heat of \( N \) oscillators is \( C = N/2 \). One could determine this temperature fluctuation for an oscillator chain analytically, since \( V \) and \( T \) are quadratic forms, but this technical detail would be of little interest.

The last formula has the same structure as the specific heat formula of Lebowitz, Percus and Verlet [21] for a system of interacting particles. There the total conserved energy is the sum of the kinetic and the potential energy. From the fluctuations of the kinetic energy \( K \) (proportional to the fluctuations of the temperature) the specific heat \( C \) can be determined in the micro canonical simulation with the help of

\[ \langle (K - \langle K \rangle)^2 \rangle / \langle K \rangle^2 = \frac{2}{3N} - \frac{1}{C} \]

where the average of the kinetic energy for \( N \) particles “measures” the temperature by \( \langle K \rangle = 3N T/2 \). For the oscillator chain discussed here only the potential energy was considered (see (A.1)) and the partition of the energy is between even and odd sites.
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FIG. 1. Over-relaxation update: Mirroring $S$ at the local molecular field $H$ produces $S'$. 
FIG. 2. Specific heat and temperature per spin as a function of temperature for $XY$–chain of 16 spins. The lines represent the canonical relations (14) and (15).
FIG. 3. Specific heat of a $24^3$ cubic lattice, circles canonical and triangles micro-canonical simulations. Near $T_c \approx 2.20$ canonical ($2 \cdot 10^5$ steps) and micro-canonical results ($2 \cdot 10^6$ steps) differ.
FIG. 4. The temperatures (+) for the critical energy $E_c = 0.989$ as a function of the lattice size $L$. One finds from the fit (upper curve) $T_c = 2.2013$ and $\nu = 0.6709$ using eq.(32) and adding $T_2 L^{-2/\nu}$ necessary to correct the deviation from scaling for small $L$. 
FIG. 5. $|M|$ for clusters of size $24^3$, $32^3$ and $48^3$ as a function of sequential updates starting from disorder at the critical energy. Also shown is the linear size dependence of $|M|$ used for the scaling plot in the insert. Not shown is the update with randomly chosen spins for $32^3$ with an almost linear relation between $|M|/L$ and $(\text{steps})^{0.42}/L$. $|M|$ has been averaged a few thousand times.
FIG. 6. Results of microcanonical simulations for fcc lattices with linear dimension 8, 12, 16 and 20. The energy is plotted as a function of the temperature. The inset shows the S-form of the energy in the vicinity of $T_c \approx 0.75$. 
FIG. 7. Relation between energy density $\epsilon$ and probability $P(\epsilon) = e^{\epsilon - \beta\epsilon}$ for the antiferromagnet on a fcc lattice of size $16^3$ according to [36]. Equal height of the two peaks selects the best critical temperature.