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Efficiency of the microcanonical over-relaxation algorithm for vector spins analyzing first and second order transitions

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Abstract. We simulate vectorial spin systems solely with the microcanonical over-relaxation algorithm where the temperature is calculated by a formula of Nurdin and Schotte. We show that this procedure is the most efficient local algorithm besides the nonlocal cluster algorithm not only for first order transitions but also for second order ones. A comparison is made with the Metropolis, heat bath, multicanonical and the Creutz's demon algorithms. We study, using these algorithms, the frustrated J_1-J_2 model on a cubic lattice for XY, Heisenberg and $O(4)$ spins. These models have a breakdown of symmetry $Z_3 \otimes SO(N)/SO(N-1)$ for the number $N = 2$, 3, 4 of spin components leading to transitions of first order. We show that they are strongly first order. Then, to test the over-relaxation update for second order transitions, we study a ferromagnet on a cubic lattice and a frustrated antiferromagnet on a stacked triangular lattice. We finally point out the advantages and the flaws of the over-relaxation procedure.

PACS. 05.70.Fh Phase transitions: general studies – 64.60.Cn Order-disorder transformations; statistical mechanics of model systems – 75.10.Hk Classical spin models – 75.10.Nr Spin-glass and other random models

1 Introduction

The common ensemble to study phase transitions of spin systems is the canonical one, where the temperature is fixed and the system can change its energy within a certain limit. This preference is due to the existence of fast and easy to implement algorithms like the local heat-bath and Metropolis algorithms and the non local cluster algorithms. Cluster algorithms have considerably improved the efficiency compared to the ones using local updates but for frustrated spin systems unfortunately they cannot be applied in an efficient way.

We would like to show that with the use of the microcanonical ensemble, where the system is isolated and the energy must be constant, the performance of simulations of vector spin systems can be improved compared to the local canonical algorithms. We use the over-relaxation procedure [1] where a spin is rotated around its local field keeping the energy constant. This algorithm is usually used in canonical Monte-Carlo simulations in combination with a heat bath or Metropolis algorithm to improve the efficiency, see for example [2]. Here we apply the over-relaxation update alone. The temperature is then calculated as an average using the formulation of Nurdin and Schotte [3]. This procedure has two advantages: it is fast and we do not add additional degrees of freedom to calculate the temperature contrary to the usual microcanonical demon algorithm introduced by Creutz [4]. Indeed the last algorithm adds corrections to the calculation of the properties of the spin system.

We will concentrate on the performance of the over-relaxation algorithm for first and second order transitions showing that it compares favorably to the other local algorithms like the Metropolis, heat-bath and multicanonical procedures. We will first introduce the method. Then, using it together with the other algorithms, we will study first order transitions and then demonstrate its usefulness also for second order transitions.

2 Methods: algorithms and microcanonical temperature

2.1 Over-Relaxation (OR)

We assume that Hamiltonians of spin systems have the form:

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij}\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j = -\frac{1}{2} \sum_i \boldsymbol{h}_i \cdot \boldsymbol{S}_i, \qquad (1)$$

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where the sum $\langle ij \rangle$ runs over all mutually interacting spin pairs only once, $\boldsymbol{h}_i$ is the local field acting on the spin $\boldsymbol{S}_i$ at site i, the spin $\mathbf{S}$ is of norm unity, and the factor $1/2$ is due to double counting.

We consider microcanonical schemes as a succession of single-spin updates. When the ith spin is selected for an update, the interaction energy of this spin with the surrounding ones is

$$E_i = -\boldsymbol{h}_i \cdot \boldsymbol{S}_i = -h_i\, x_i \tag{2}$$

and therefore $x_i = \cos\theta_i$ or the angle θ_i between $\boldsymbol{h}_i$ and $\boldsymbol{S}_i$ should not change to keep the energy constant. Under this restriction there remains a freedom for the spin to precess around the local field $\boldsymbol{h}_i$ if the spin has more than two components.

The simplest and most efficient way to implement microcanonical updates corresponds to

$$\boldsymbol{S}_i \longrightarrow -\boldsymbol{S}_i + 2\,\boldsymbol{h}_i(\boldsymbol{h}_i \cdot \boldsymbol{S}_i)/h_i^2, \tag{3}$$

which means that the spin $\boldsymbol{S}_i$ is flipped to the most distant direction from the initial one preserving the angle with the local field $\boldsymbol{h}_i$. We call this scheme "OR" to distinguish it from the more general "OR+rotation" or "OR+R" update where the rotation angle around a local field is chosen at random. In the former and simpler OR-procedure no random numbers are necessary. Depending on the spin dimension N the increase in time consumption of an OR+R update as compared with that of an OR update varies from a factor 2 for a Heisenberg spin to a large factor for a spin with many components.

For XY spins it has been shown [5] that with OR alone not all possible states could be reached and a multi-spin algorithm should be used instead. We think that the Heisenberg case is less problematic since these spins have an additional component. Still for calculating critical exponents it could be wise to apply one OR+R step for every 5 or 10 OR steps.

Another problem is the way to scan the lattice to avoid ergodicity problems. One should not implement a sequential OR-update since collective motions in the spin system could be generated which statistically have no weight [5]. As a compromise we divide the lattice into mutually non-interacting sublattices and update one sublattice after the other. The order of addressing the spins in one sublattice does not matter. Another way to circumvent this problem would be to change the order of updates statistically. To do this economically one should generate about 100 different orders for the spins before a simulation starts. After visiting all spins of the lattice the order is changed to another of the prefabricated ones. Using the simpler way of sequentially updating the different sublattices we did not encounter any problems.

2.2 Microcanonical temperature

With the microcanonical method the entropy of a system is obtained, and the microcanonical temperature could in principle be calculated by numerically differentiating the entropy. However, this method gives noisy results, and is difficult to apply in practice.

Nurdin and Schotte [3] have given a more useful and explicit expression for the microcanonical temperature for a Heisenberg spin system. If the Hamiltonian has the standard form (1), the inverse of the microcanonical temperature is given by the average of

$$\frac{1}{\mathcal{T}} = \frac{-4\,\mathcal{H}}{\sum_i |\boldsymbol{h}_i \times \boldsymbol{S}_i|^2} \tag{4}$$

over a microcanonical ensemble. A generalization to N dimensional spin vectors would be

$$\frac{1}{\mathcal{T}} = \frac{-2\,(N-1)\,\mathcal{H}}{\sum_i \sum_{k<l} \left| h_i^k\, S_i^l \,-\, h_i^l\, S_i^k \right|^2} \tag{5}$$

where the sum over all $\binom{N}{2}$ possible vector product components has to be taken besides the sum over all lattice spins i. We prove in the appendix that this formula can be simplified by restricting the sum to $l = k+1$ with $N+1 \equiv 1$ for l. Using this generalization the three dimensional formula (4) with $-4\,\mathcal{H}$ in the numerator will be valid for all dimensions. For $N = 2$ only one term contributing twice appears, whereas for $N \geq 2$ always N terms have to be calculated. In both formulas (4) and (5) additional terms $\propto 1/N_s$ are left out, where N_s is the number of spins. Besides the practical point to neglect these rather cumbersome corrections, the micro-canonical temperature with its rather curious behavior for a few degrees of freedom contained in the full expression will certainly not be relevant for large spin systems studied here.

We will now describe shortly Creutz's demon algorithm and the multicanonical algorithm in the form we will use later to compare with the over-relaxation algorithm. For the description of canonical Metropolis and heat-bath algorithms especially for the efficiency of those simulation techniques we refer to [6].

2.3 Creutz's demon algorithm

In demon algorithm of Creutz [4] another degree of freedom called a demon is added, and the sum of energies of the system and of the demon is kept constant. To some extent the condition of energy conservation is relaxed. Because of the tendency to increase the entropy in the joint system, the spin system is more likely to take energy from the demon than to give it back, which means that the demon energy will not be large. In order to update a configuration of spins, a new direction for a spin is chosen at random and it will be accepted as long as the demon's energy does not become negative.

To improve this Metropolis-like update method we apply here the better heat bath scheme. A spin $\boldsymbol{S}_i$ is selected for an update by requiring that the joint energy E_0

$$-\boldsymbol{h}_i \cdot \boldsymbol{S}_i + E_d = -h_i\, x_i + E_d \equiv E_0, \tag{6}$$

should be constant. If one demands that the demon energy E_d should be positive, then the new x_i value can only be chosen in the region $\max[-1, -E_0/h_i] \leq x_i \leq 1$. Thereby we avoid spin directions which are to be rejected.

The temperature T is usually defined by the average of the demon energy, since it is distributed proportionally to $\exp(-E_d/T)$. We note that the value E_d has a lot of dispersion. The demon as a thermometer represents only a tiny subsystem whereas using the spin temperature formula (4) the temperature of a whole system is "measured". Moreover in contrast to Ising case at least one random number is needed for each step which also slows down the simulation compared to the OR procedure.

2.4 Multicanonical method

The multicanonical method [7] for first-order phase transitions has been successful in alleviating an exponential growth of the tunneling time between free energy minima to an algebraic one. The basic idea is to sample the mixed phase configurations with the same statistical weight as the configurations of the pure phases.

The multicanonical algorithm is efficient in the sense that a relevant energy range can be covered in a single run, but with the proviso that a sufficiently good approximation for the density of states can be obtained in a reasonable time. However, it slows down severely with increasing system sizes connected with the problem of a widening energy range to cover, since the method is only a random walk in energy. The characteristic time of this algorithm in units of scans of a lattice is expected to behave optimally like $\sim L^d$. In actual implementation with a succession of single-spin updates, the performance of the algorithm is usually worse.

The close connection between the micro-canonical and the multi-canonical method of analyzing first order transition can be found in reference [8].

3 Models and numerical results

3.1 First order transition: J_1-J_2 antiferromagnet on a cubic lattice

We consider a Heisenberg model on the simple cubic lattice with the Hamiltonian

$$H = \sum_{\langle ij \rangle} J_1 \, \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \sum_{\langle\langle ij \rangle\rangle} J_2 \, \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \qquad (7)$$

where the sums $\langle ij \rangle$ and $\langle\langle ij \rangle\rangle$ run over nearest neighbors and next-nearest neighbors pairs, respectively. Both interactions $J_1 > 0$ and $J_2 > 0$ are positive or antiferromagnetic. Energy and temperature will be measured in units of J_1. The numerical simulations are performed for systems of size $L \times L \times L$ with periodic boundary conditions. The lattice will be divided into eight cubic sub-lattices for the OR-updates. This way, a sequential update is possible as described in Section 2.1.

For $0 < J_2 < J_1/4$ the ground state has a simple antiferromagnetic structure. For $J_2 > J_1/4$ the ground state has an additional degeneracy, besides the possibility of a global rotation. However, by the mechanism of "order by disorder" collinear states are selected in the ordered phase. What remains are three different ways to choose directions in the cubic lattice where the spins are parallel. Each collinear state starting with an antiferromagnetic configuration on a square lattice is completed by stacking this spin order on top of each other. The breakdown of symmetry between high and low temperatures will be of the type $Z_3 \otimes SO(N)/SO(N-1)$ with Z_3 the three state Potts symmetry and $SO(N)/SO(N-1)$ the usual breakdown of symmetry for ferromagnets for spins with N components. For more details see for instance the review article of one of the authors [9,10].

This breakdown of symmetry is therefore identical to those found in hcp, fcc, stacked triangular lattice with second neighbor interactions which also have strong first order transition for XY and Heisenberg spins (see [9] and references therein). One hypothesis advanced in the last reference is that for any N the transition will be of first order because of the same breakdown of the Z_3 symmetry (threefold degeneracy) which should always lead to a first order transition in three dimensions. For J_1-J_2 model on a cubic lattice this was checked for Heisenberg spins only [11]. We show here that it is also true for XY and $O(4)$ spins.

In order to observe the first order character of the phase transition more clearly, we choose for the ratio J_2/J_1 the low value 0.26. In Figure 1a, b, c we show the result for the OR for the energy as function of the temperature for XY, Heisenberg and $O(4)$ spins. When the size L becomes large enough the energy-temperature relation exhibits an "S"-shape typical for first order transitions. We note that for microcanonical simulations only one temperature is determined for each energy and the problem of canonical simulations does not arise where two stable states of different energies can exist at a temperature. The size of the bend in the "S" decreases slowly as function of the number of spin components N but we do not think that the first order transition will become a second order one for large N. This work is therefore in favor of a first order transition in the breakdown of symmetry $Z_3 \otimes SO(N)/SO(N-1)$ for any N in three dimensional case.

We will now compare the efficiency of the algorithms. The local canonical ones are extremely inefficient because of the presence of, at least, two stable phases separated by a region of very low probability. These simulations suffer therefore from an extremely strong slowing down and their autocorrelation time τ will have an exponential size dependence. We compare three algorithms where this defect is absent or less strong: the microcanonical over-relaxation and Creutz's demon algorithms, and the multicanonical algorithm. For the microcanonical algorithms the autocorrelation time τ is obtained by integrating the autocorrelation function of magnetization [2]. For the multicanonical algorithm, a characteristic time τ_{Mu} is defined as the

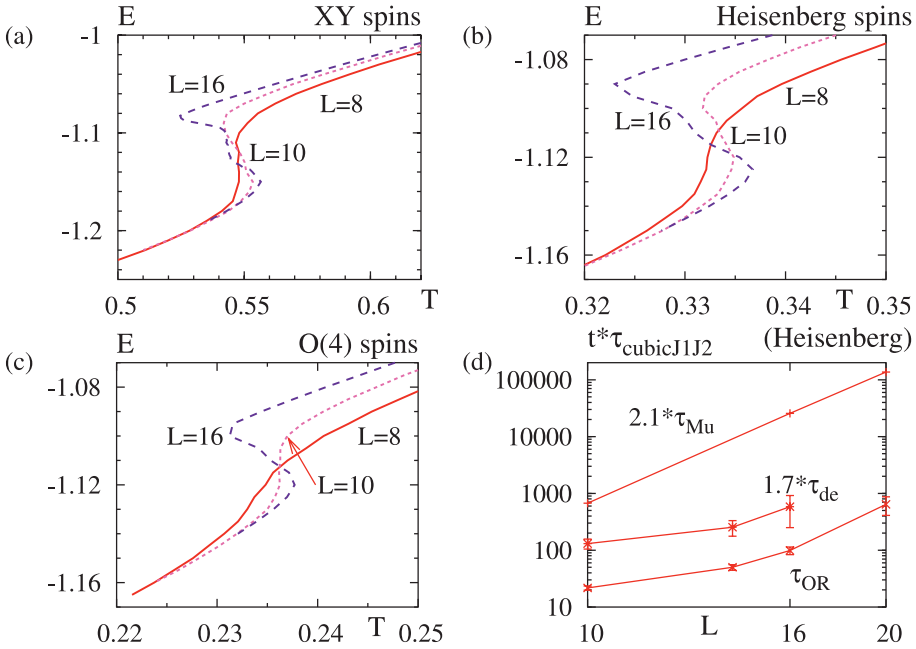

Fig. 1. Size dependence of the energy-temperature relation of the OR procedure for the J_1-J_2 antiferromagnet on a cubic lattice. a) for XY spins, b) for Heisenberg spins, c) for O(4) spins. The three plots show the "S" shape characteristic of a strong first order transition. d. Autocorrelation time (magnetization) for Heisenberg spins multiplied by the time consumption of one step for the demon algorithm or the over-relaxation algorithm (put to 1) for comparison. "τ_{Mu}" correspond to the tunneling time for the multicanonical algorithm. The over-relaxation is by far the most efficient algorithm to study first order transition.

tunneling time which is the number of Monte Carlo steps it takes for the system at T_c to travel from one peak to the other.

The results are plotted in Figure 1d for Heisenberg spins. The autocorrelation time is multiplied by the time one step of each algorithm takes putting $t_{\rm OR} = 1$. In our heat bath implementation the demon algorithm is 1.7 times slower than the OR one and the multicanonical algorithm by a factor of 2.1. We plotted the result for the OR and demon algorithm at $E = -1.09$ which shows the strongest size dependence. For another energy like at $E = -1.11$ there is almost no size dependence visible.

We observe that the OR algorithm is almost 10 times better than the demon algorithm. The comparison is even more in favor of the OR algorithm when one compares with the multicanonical algorithm which is for large size two order of magnitude slower. We should remark, however, that only one simulation is necessary for the multicanonical procedure to extract properties of the system for a larger range of temperature or energy. In contrast the micro-canonical simulations must be repeated for each energy. However the OR simulation is so much faster than the multicanonical one therefore is still better, in particular considering that the autocorrelation time τ_{OR} is more or less constant as a function of the system size if the energy deviates little from the energy of transition $E = -1.09$.

In conclusion, the over-relaxation is the most efficient algorithm for studying first order transition. Moreover it is very easy to apply, in particular compared to the multicanonical method.

3.2 Second order transitions for ferromagnets and frustrated Heisenberg antiferromagnets

We study two models with a second order phase transition. The first one is a Heisenberg model with a ferromagnetic interaction between nearest neighbor spins on a simple cubic lattice given by the Hamiltonian (1) with $J > 0$. The second model is an antiferromagnet on a stacked triangular lattice with nearest neighbor interactions $J < 0$. The ground state of this frustrated system has a 120° structure [9]. No cluster algorithm exists for this case and the fastest canonical algorithm is a heat-bath procedure [6].

The cubic ferromagnet has a genuine second order phase transition and its critical temperature is 1.4432 [12]. The stacked triangular antiferromagnet shows "almost second order transition" which, for the sizes considered here, resembles a true second order transition [9]. The critical temperature is about 0.96.

In Figure 2a results of the microcanonical and canonical methods for the cubic ferromagnet are shown. The same temperature-energy relation are obtained as expected except for finite size effects not visible at this scale.

In Figures 2b and d the temperature dependence of the autocorrelation time τ are shown for the magnetization of the ferromagnet on a cubic lattice of size $L = 10$ and of the antiferromagnet on a triangular lattice of size $L = 12$. We observe for both models that the micro-canonical OR is faster than the other algorithms. For the cubic ferromagnet (Fig. 2b) the gain is about 2.5 compared to the demon algorithm, 3 compared to the heat bath and 7 compared to the Metropolis algorithm. These numbers do not

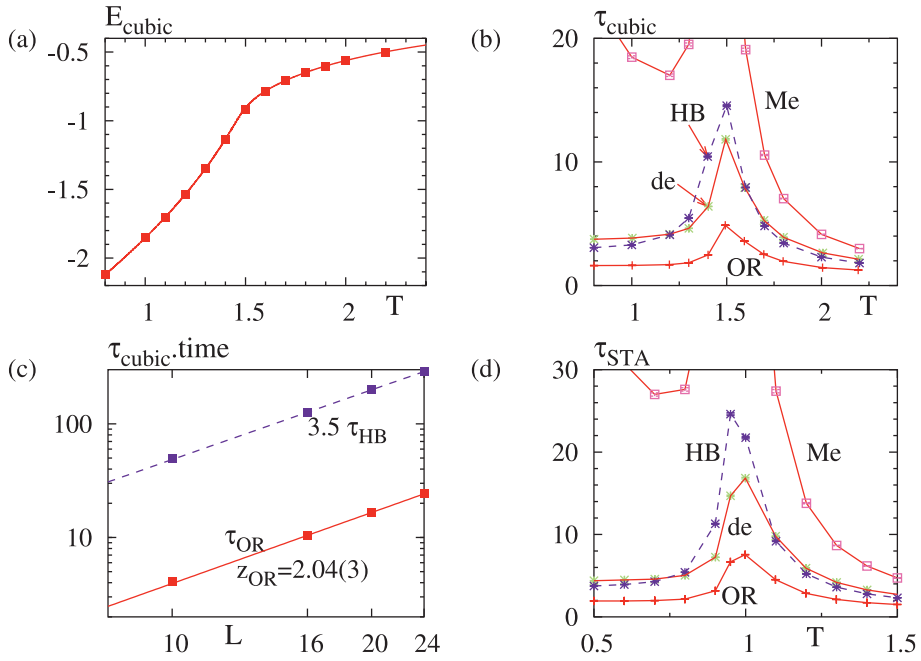

Fig. 2. a) Cubic ferromagnet: Energy-temperature relation for the over-relaxation (line) and for the Metropolis (points) procedure. The errors are smaller than the symbols. b) Cubic ferromagnet: Autocorrelation time τ (magnetization) for size $L = 10$. Me=Metropolis, HB=Heat Bath, de=Creutz's demon, OR=Over Relaxation. c) Cubic ferromagnet: τ multiplied by the time consumption of one step for the heat bath and the over-relaxation procedures (put to 1) as function of the size L. The dynamical exponent $z_{\rm OR} = 2.04(3)$ is similar to the one of the heat bath. The over-relaxation is almost ten times more efficient than the heat bath. d) Stacked triangular antiferromagnet: Autocorrelation time τ (magnetization) for size $L = 12$. The OR algorithm has similar properties for non frustrated and frustrated magnets.

take into account that the OR implementation runs faster than the other algorithms, about three times faster than the heat bath for example. Similar conclusions hold for frustrated lattice as can be seen by comparing Figure 2d with Figure 2b.

In Figure 2c we show for the cubic ferromagnet the size dependence of the autocorrelation time τ at T_c, or at the critical energy E_c for microcanonical simulations, obtained in the log-log scale by fitting to the form $\tau = \tau_0 \cdot L^z$. For this purpose the critical energy E_c was estimated by extrapolating E_L to $L \to \infty$ using the scaling relation

$$E_L = E_c - a\, L^{-(1-\alpha)/\nu}, \tag{8}$$

where E_L is a canonical average of the energy at T_c for a finite lattice of size L. We adopted the values found in the literature for T_c and for the critical exponents α and ν, and estimated the critical energy to be about -0.989. The dynamic critical exponent z obtained is 2.04(3) for the OR procedure, similar to the one for the heat bath algorithm.

Therefore, for a second order transition the OR is the fastest local algorithms and could be used to calculate the critical exponents [13]. However the OR procedure has a disadvantage compared to the canonical ones: results cannot be resummed for another energy. Therefore many more simulations for different energies are necessary. Since the OR is about ten to twenty times faster than the heat bath it could still be better depending on the model studied.

3.3 Spin glasses

We tried to apply this method to the spin glasses. However the microcanonical over-relaxation seems not be adapted to these systems and we found that the exchange algorithm [14] coupled with a canonical heat bath has a much better performance [6].

4 Conclusion

We wanted to show that the over-relaxation procedure is the fastest of the local algorithms, cluster algorithms excluded. Especially well adapted to study first order transition it could be also of use to study second order transitions. We hope that this publication will increase the interest in this method and further its use.

Appendix: Micro-canonical temperature for O(N) spins

In a molecular dynamics simulation for a system of classical particles one takes usually the kinetic energy as a measure for the temperature. For a system of three component spins $\boldsymbol{S}_i$ we use together with the over-relaxation simulation the average of expression (4) to determine the

temperature. The spin temperature formula (4) written as

$$\mathcal{T}_{O(3)} = -\frac{\sum_i \dot{\boldsymbol{S}}_i^{\,2}}{4\,\mathcal{H}} , \tag{A.1}$$

shows clearly its analogy to the particle temperature $\mathcal{T}_{part} = m\sum_i \dot{\boldsymbol{x}}_i^2 \,/(3\mathcal{N})$, where the number of particles $\mathcal{N}$ is the normalizing factor instead of the energy $\mathcal{H}$ for the spin system given by (1). The squares of the velocities $\dot{\boldsymbol{S}}_i$ or $\dot{\boldsymbol{x}}_i$ appear in both cases. For spin systems one would have to integrate

$$\dot{\boldsymbol{S}}_i = [\boldsymbol{S}_i \times \boldsymbol{h}_i] , \tag{A.2}$$

where $\boldsymbol{h}_i = -\nabla_i \mathcal{H}$ is the local field (equivalent to the definition in (1)) acting like a magnetic field on the spin $\boldsymbol{S}_i$. However, the over-relaxation algorithm as a "stroboscopic" molecular dynamics simulation is better suited to calculate thermodynamic entities as shown in preceding sections.

To obtain a generalization of (4) or (A.1) for spins with more than three components we have to go back to the definition of the entropy $S(E)$ given by the integral over all "phase space" V, where the energy E is constant

$$\exp(S) = \int \delta(E-\mathcal{H})\, dV . \tag{A.3}$$

Formally written with a δ-function. This is an integral over the constant energy surface O

$$\exp(S) = \oint\limits_{\mathcal{H}=E} \vec{X}\, d\vec{O} = \int \theta(E-\mathcal{H})\, \mathrm{div}\vec{X}\, dV . \tag{A.4}$$

Which can be transformed using Gauss' formula to an integral over the part of phase space with $H \leq E$ indicated by Heaviside's step function θ. The vector of the surface element $d\vec{O}$ and of the gradient of the energy "grad $\mathcal{H}$" are parallel. The simplest form for $\vec{X} = \mathrm{grad}\,\mathcal{H}/|\mathrm{grad}\,\mathcal{H}\,|^2$ corresponds to the condition that the weight to sum over the constant energy surface is $1/|\mathrm{grad}\,\mathcal{H}|$, which gives the standard formula for the density of states.

The more flexible form of (A.4) with a vector field is due to Rugh [15] who notices that for the "flow" in phase space $\vec{X}$ only the restriction

$$\mathrm{grad}\,\mathcal{H} \cdot \vec{X} = 1 \tag{A.5}$$

is necessary. This means that $d\vec{O}$ and $\vec{X}$ need not be parallel, but the "flow" $\vec{X}$ across the constant energy surface should be the same. With the temperature definition

$$\frac{1}{T} = \frac{dS}{dE} . \tag{A.6}$$

one gets by taking the logarithm of (A.4) from the last term on the r.h.s. by differentiating with respect to the energy E a ratio of equal energy integrals

$$\frac{dS}{dE} = \int \delta(E-\mathcal{H})\, \mathrm{div}\vec{X}\, dV \Big/ \int \delta(E-\mathcal{H})\, dV . \tag{A.7}$$

Since $dS/dE = 1/T$ one can now read off Rugh's formula

$$\frac{1}{\mathcal{T}} = \mathrm{div}\,\vec{X} \tag{A.8}$$

the average of which gives according to (A.6) the inverse of the temperature T. For a particle system one puts $\vec{X}_{part} = m\,(\boldsymbol{0}, \boldsymbol{p}_1, \ldots \boldsymbol{0}, \boldsymbol{p}_{\mathcal{N}})/\sum_{i=1}^{\mathcal{N}} \boldsymbol{p}_i^2$ and checks that (A.4) is valid, since all entries for the particle coordinates $\boldsymbol{x}_i$ have been put to zero. Using (A.6) one obtains $1/\mathcal{T}_{part} \approx 3\mathcal{N}\,m/\sum_{i=1}^{\mathcal{N}} \boldsymbol{p}_i^2$. This form is valid for large particle numbers $\mathcal{N}$, where the differentiation of the kinetic energy in the denominator $\vec{X}$ would give only $\mathcal{O}(1/\mathcal{N})$ contributions [15].

What is now the flow $\vec{X}$ for a Hamiltonian of the Heisenberg type given by equation (1)? For three dimensional spins the flow $\vec{X}$ is given by the following formula.

$$\boldsymbol{X}_i = \frac{\boldsymbol{S}_i \times [\boldsymbol{S}_i \times \boldsymbol{h}_i]}{\sum_i |\boldsymbol{S}_i \times \boldsymbol{h}_i\,|^2} . \tag{A.9}$$

Instead of a $6\mathcal{N}$ dimensional vector it is a $3\mathcal{N}$ vector consisting of a collection of three dimensional ones $\boldsymbol{X}_i$ like $\boldsymbol{S}_i$. With $\mathrm{grad}\,\mathcal{H} = (\nabla_1, \ldots \nabla_{\mathcal{N}})\,\mathcal{H} = -(\boldsymbol{h}_1, \ldots \boldsymbol{h}_{\mathcal{N}})$ one checks easily (A.4), that is for the sum one obtains $\sum_i(-\boldsymbol{h}_i)\cdot\boldsymbol{X}_i = 1$. With (A.9) one has another essential restriction $\boldsymbol{X}_i \cdot \boldsymbol{S}_i = 0$, since the length of a spin vector $\boldsymbol{S}_i$ is fixed. This differs from a particle systems, where the coordinates are usually not constrained.

The transposition of (A.8) to the N-component spins $(S_i^1, \ldots S_i^N)$ with the molecular field $(h_i^1, \ldots h_i^N)$ at site i is not complicated, using $\boldsymbol{S}_i \times [\boldsymbol{S}_i \times \boldsymbol{h}_i] = \boldsymbol{S}_i(\boldsymbol{S}_i \cdot \boldsymbol{h}_i) - \boldsymbol{h}_i(\boldsymbol{S}_i \cdot \boldsymbol{S}_i)$

$$X_i^k = \sum_{l=1}^{N} S_i^l(S_i^k h_i^l - S_i^l h_i^k) \Big/ \sum_i \sum_{k<l} (S_i^k h_i^l - S_i^l h_i^k)^2 . \tag{A.10}$$

In the denominator the contributions of the $\binom{N}{2}$ different terms of the torque in N dimensions $D_i^{kl} = S_i^k h_i^l - S_i^l h_i^k$ should be summed only once. Since $\sum_i \sum_{k=1}^{N}(-h_i^k)X_i^k = 1$ and $\sum_{k=1}^{N} S_i^k X_i^k = 0$ one can proceed to find an expression for the temperature using (A.7), that is

$$\sum_i \sum_{k=1}^{N} \frac{\partial X_i^k}{\partial S_i^k} \approx (N-1) \sum_i \sum_{l=1}^{N} S_i^l h_i^l \Big/ \sum_i \sum_{k<l} (S_i^k h_i^l - S_i^l h_i^k)^2 .$$

Only the numerator of (A.9) has been differentiated to obtain a formula for the the thermodynamic limit

$$\left(\frac{1}{\mathcal{T}}\right)_{O(N)} = \frac{-2\,(N-1)\,\mathcal{H}}{\sum_i \sum_{k<l} (S_i^k h_i^l - S_i^l h_i^k)^2} \tag{A.11}$$

where $\sum_i \sum_{l=1}^{N} S_i^l h_i^l = -2\,\mathcal{H}$ according to (1) has been used as a simplification to obtain (5).

Another generalization of the three dimensional ansatz (A.9) to higher dimensions is

$$\tilde{X}_i^k = \sum_{\pm} S_i^{k\pm1}\big(S_i^k h_i^{k\pm1} - S_i^{k\pm1} h_i^k\big) \Big/ \sum_i \sum_k \left(S_i^k h_i^{k+1} - S_i^{k+1} h_i^k\right)^2 , \quad \text{(A.12)}$$

that means only N special components of the torque $D_i^{k,k+1} = S_i^k h_i^{k+1} - S_i^{k+1} h_i^k$ instead of all $\binom{N}{2}$ components are taken into account. As before the nonsensical index $N+1 \equiv 1$. Still $\sum_{k=1}^{N} S_i^k \tilde{X}_i^k = 0$ and also (A.4) is valid as before. For the temperature using (A.7) one obtains

$$\sum_i \sum_k \frac{\partial X_i^k}{\partial S_i^k} \approx \sum_i \sum_k \sum_{\pm} S_i^{k\pm1} h_i^{k\pm1} \Big/ \sum_i \sum_k (S_i^k h_i^{k+1} - S_i^{k+1} h_i^k)^2$$

so that corresponding to (4)

$$\left(\frac{1}{\mathcal{T}_{mod}}\right)_{O(N)} = \frac{-4\,\mathcal{H}}{\sum_i \sum_k (S_i^k h_i^{k+1} - S_i^{k+1} h_i^k)^2}. \quad \text{(A.13)}$$

Both formulas (A.11) and (A.13) are the same and equivalent to the known ones for $N = 2$ and 3. For $N \geq 4$ one would prefer (A.13) as we have done here for $N = 4$, since it will be less time consuming in a micro-canonical simulation. However, one should check with the results a permutation of the indices 1, 2, ... N would give.

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