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Microcanonical Simulation on the First Order Phase Transition of the XY Antiferromagnet on the Stacked Triangular Lattice

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The nature of the phase transition of antiferromagnetic vector spin models on the stacked triangular lattice (STA) has been an issue of debate.[1)] In order to account for the coplanar non-collinear order in the ground state one needs two vector fields in a Ginzburg–Landau–Wilson Hamiltonian. The field theoretical renormalization group analysis shows that there is a threshold value N_c for the number of spin component N, and for $N > N_c$ the transition is of second order belonging to a new "chiral" universality class, while for $N < N_c$ the chiral fixed points ceases to exist in the real parameter space and the transition is of first order. According to a recent estimate based on a Monte Carlo renormalization group study, $3 < N_c < 8$.[2)] Therefore a first order transition is expected for the physically relevant XY and Heisenberg spin systems.

The phase transition of the XY or Heisenberg STA is of very weak first order and is said to be of "almost second order" with large (but finite) correlation lengths due to a slow velocity region in the renormalization group flow. Monte Carlo simulations on systems with moderate size appear to show second order transitions with pseudo-critical behavior. Strong first order transitions were found for variants of the model on which a constraint of local rigidity was imposed which still belong to the same universality class as the original STA.[1)] Recently the first order nature of the phase transition in XY antiferromagnet on the stacked triangular lattice (XY-STA model) was demonstrated directly by canonical Monte Carlo simulations[2,4)] on large systems, in which the energy probability distribution shows a double peak structure near the transition temperature. The purpose of the present paper is to show the first order transition of the XY-STA model by applying a novel technique: a microcanonical method.

To distinguish a weak first order transition from a second order one can be difficult, especially if the energy jump, the characteristic of a first order transition, is tiny as is the case for frustrated spin systems.[1)] Limited to accessible system sizes one may analyze the different power law behavior of the maximum of specific heat or susceptibility, with an exponent equal to three for a first order transition and less than three for a second order transition. The obvious solution to increase the size of the system runs into difficulties for the canonical simulations (at constant temperature) because of the growing autocorrelation times. Also the histogram method is then restricted to smaller intervals of temperature shrinking as the inverse power of the system size.

In this short note we will show that the microcanonical simulations (at constant energy) can help to solve the problems encountered in canonical simulations. The method has been tested for strong first order transitions and also for second order ones.[3)] Before presenting the method and the results we have to describe the model we study. It is given by the usual Hamiltonian

$$H = \sum_{\langle ij \rangle} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \tag{1}$$

where $\boldsymbol{S}_i$ denotes a XY (two-component) spin with $|\boldsymbol{S}_i| = 1$ defined on the lattice site i of the stacked triangular lattice, and the sum is over all the nearest neighbor pairs $\langle ij \rangle$. We set $J_{ij} = J_{\parallel} = 1$ (antiferromagnetic) for intra–plane nearest neighbor pairs and $J_{ij} = J_{\perp} = -3/4$ for inter–plane nearest neighbor pairs following ref. 2. We simulate rectangular systems which contain $L_x \times L_y \times L_z$ spins, imposing periodic boundary condition for all three directions, with $(L_x, L_y, L_z) = (84, 96, 84)$ and $(126, 144, 126)$, that is the same sizes as in ref. 2. We obtained qualitatively similar results for systems with $J_{\parallel} = -J_{\perp} (> 0)$ and $L_x = L_y = L_z$.

The simplest way to sample over the microcanonical ensemble is to apply the over-relaxation algorithm, in which each spin is updated in the way:

$$\boldsymbol{S}_i \longrightarrow -\boldsymbol{S}_i + 2\boldsymbol{h}_i(\boldsymbol{h}_i \cdot \boldsymbol{S}_i)/|\boldsymbol{h}_i|^2. \tag{2}$$

In other words, the spin $\boldsymbol{S}_i$ at site i is flipped to its mirror image with respect to $\boldsymbol{h}_i = -\sum_j J_{ij} \boldsymbol{S}_j$ which is the local field acting on $\boldsymbol{S}_i$. Under the update (2) the local energy $E_i = -\boldsymbol{h}_i \cdot \boldsymbol{S}_i$ is invariant. This procedure is the most efficient local algorithm having the smallest autocorrelation.[3)]

Following Nurdin and Schotte[5,6)] the microcanonical temperature can be calculated as an average over the microcanonical ensemble for vector spin systems. For XY spins the inverse of the microcanonical temperature is given as an average of

$$\frac{1}{\mathcal{T}} = \frac{-2H}{\sum_i |h_i^x S_i^y - h_i^y S_i^x|^2}. \tag{3}$$

To generate the microcanonical ensemble a two-site microcanonical updating together with the over-relaxation algorithm was applied from time to time to resolve the issue of non-ergodicity of the over-relaxation.[7)] In order to keep the interaction energy $E_0 = -h_j x_j - h_l x_l$ of two spins at j and l (nearest neighbor ones excluded) fixed, by changing $x_j = \boldsymbol{h}_j \cdot \boldsymbol{S}_j/|\boldsymbol{h}_j|$ and x_l, one has also to satisfy a detailed balance condition. The two spins are updated as follows: 1) Choose x'_j uniformly in the range $[\max(-1, (-E_0 - h_l)/h_j), \min(1, (-E_0 + h_l)/h_j)]$ and let $x'_l = (-E_0 - h_j x'_j)/h_l$. 2) Accept the transition $(x_j, x_l) \to (x'_j, x'_l)$ with probability $\min([(1 - x_j^2)(1 - x_l^2)(1 - x'^2_j)^{-1}(1 - x'^2_l)^{-1}]^{1/2}, 1)$.

In Fig. 1 we show the results of the microcanonical simulations for the microcanonical temperature as a function of energy. For the larger system with $126 \times 144 \times 126$ spins there is an energy range where the microcanonical inverse

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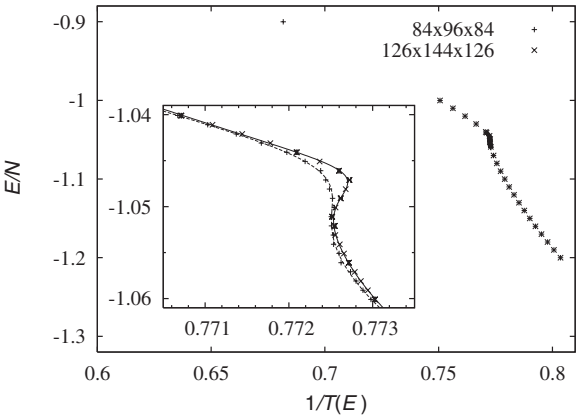

Fig. 1. The inverse of the microcanonical temperature as a function of energy per spin. Microcanonical simulations were performed for systems with size $84 \times 96 \times 84$ and $126 \times 144 \times 126$. The first order nature of the transition and finite size effects can be seen.

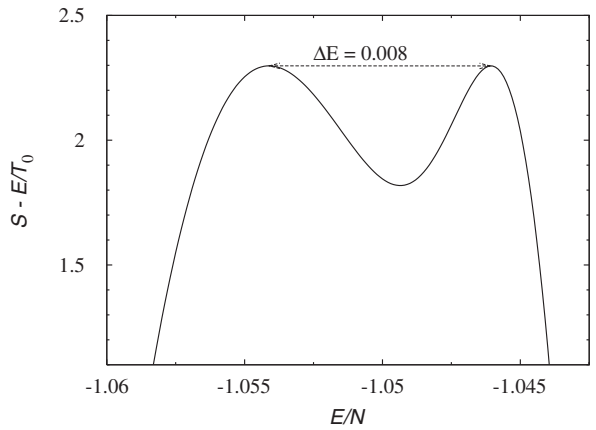

Fig. 2. The equal height construction using eq. (4) to determine the transition temperature $1/T_0 = 0.7726$ and the latent heat 0.008 indicated by the arrow.

temperature is no longer a monotonically decreasing function of energy. The "S" shape clearly indicates that the transition is of first order. The lines are plotted using a fit functions.[8)]

The autocorrelation time for the biggest size is about 300 Monte Carlo steps per spin in the mixed phase region, while far from that region it is more than an order of magnitude smaller. By comparison the same quantity is more than 12000 in canonical simulations.[4)] Therefore the microcanonical simulations is more than 40 times more efficient and this ratio will increase as function of the size because the autocorrelation time is exponential in the canonical simulations but follows only a power law in the microcanonical ones.[3)]

In Fig. 2 we show the integral

$$\int_{E_0}^{E} \left(\frac{1}{T} - \frac{1}{T_0} \right) \mathrm{d}E = \mathrm{const} + S(E) - \frac{E}{T_0} \qquad (4)$$

where the value of $1/T_0 = 0.7726$ has been chosen to get equal height peaks. We note that the value of the critical temperature T_0 is quite sensitive to the form of the fit functions but the fourth decimals is a safe estimate corresponding to the temperature Itakura found.[2)] We can also read off the difference of energy between the maxima which gives the latent heat L at the transition temperature. We get $L = \Delta E = 0.008$ which is similar to the one found in canonical simulations.[2)] The exponential of the function plotted in the Fig. 2 corresponds to the histogram of the canonical simulations.[9)]

In conclusion with microcanonical simulation we were able to define clearly the order of the phase transition. We want to stress that the method is much more efficient than the canonical simulations concerning the speed but also to calculate other quantities like the critical temperature, the entropy and the latent heat. We could try to apply the same method to Heisenberg spins on STA. However, it was estimated that the first order transition could only be seen when the linear size of the system is larger than 800,[2)] which is beyond the reach of the present day computer resources, also for our microcanonical method.

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$$1/T(E) = f_0 + \frac{c(E_0 - E)^2}{1 + \exp[(E - E_1)/\epsilon]} - \frac{a(E_1 - E)}{1 + \exp[(E - E_1)/\epsilon]}$$
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