A cluster Monte Carlo method for systems of classical spins with purely dipolar couplings is presented. It is tested and applied for finite arrays of perpendicular Ising dipoles on the triangular lattice. This model is a modification with long-range interactions of the geometrically frustrated Ising antiferromagnet. From measurements of integrated autocorrelation times for energy, magnetization and staggered magnetizations, a high efficiency of the cluster Monte Carlo (MC) algorithm compared to a single-spin-flip algorithm is found. For the investigated model, a finite temperature transition is found which is characterized by a peak in the specific heat and in the staggered susceptibilities.

The progress in the fabrication of very small patterns of ferromagnetic materials opens the fascinating possibility to study experimentally statistical properties of some mesoscopic or exotic magnetic systems. Dipolar couplings between such particles may induce magnetic ordering. These couplings are often only viewed as additional effective anisotropy barriers for the super-paramagnetic relaxation of individual particles. However, such assemblies of ferromagnetic nano-particles are coupled magnetic systems. They should display magnetic phase-transitions for systems with mesoscopic size of individual magnetic moments. Recently, Wirth et al. studied the properties of nanoscale ferromagnetic columns which were grown on substrates in a scanning tunnel-microscope. Magnetic-force microscopic pictures of densely packed columns on a triangular lattice showed typical antiferromagnetic correlations where rows of nearest-neighbour moments point alternatingly up and down.

This paper presents a numerical study on the expected thermodynamics for such assemblies of perpendicular dipoles in two dimensions. Its second aim is the introduction of a cluster Monte Carlo (MC) method for dipolarly coupled systems. For the geometrically frustrated triangular lattice, this method allows efficient statistical sampling down to relatively low temperatures. The coupled system we want to study consists of $i = 1 \ldots N$ Ising spins, $\sigma_i \in \{-1, 1\}$

$$H = \frac{1}{2} \sum_{i,j} \nu(R_{ij}) \sigma_i \sigma_j,$$

where $\nu(R) = g R^{-3}$ are interactions between three-dimensional dipoles describing the coupling between the perpendicular moments of the particles. All the couplings are antiferromagnetic. Length is measured in nearest-neighbour distances. If we restrict the interactions in (1) to nearest-neighbour terms we get an Ising antiferromagnet. The triangular Ising antiferromagnet (TIAFM) is one of the few exactly solved systems with geometrical frustration. It was shown that no long-range order is established at finite temperature, but the system becomes critical at $T = 0$. However, additional interactions may lift the ground-state degeneracy and may induce phase-transitions in such underconstrained systems. Hence, model (1) is interesting in its own right.

Cluster-MC methods for spin models (1) are only efficient in critical regions if the clusters do not percolate already above the critical temperature. The energy of model (1) may be decomposed into two parts

$$H = \sum_{\Delta} V_{\Delta} + \frac{1}{2} \sum_{(i,j) \notin NN} \nu(R_{ij}),$$

where the sum of $V_{\Delta}$ denotes sums of nearest-neighbour interactions in one of the two types of triangular plaquettes (and, with open boundary conditions, some nearest-neighbour interactions along the boundaries also labeled by $V_{\Delta}$). This first part is exactly the TIAFM. The second sum contains the remaining bonds with longer range.

Clusters for the TIAFM can be defined by sampling the sums of energies corresponding to elementary triangular plaquettes. These clusters are the correct critical clusters of the TIAFM percolating at $T = 0$. Applying this cluster definition to the first part of (2) the dipolar system is mapped on a system of clusters which interact through the long-range interactions generated from terms in the second sum of (2). For flipping clusters the usual Metropolis algorithm is used. The algorithm of alternatingly mapping (1) onto interacting clusters via (2) and sampling this mapped system is equivalent to sampling the original system.

We have to show ergodicity and detailed balance to justify the method. The procedure of cluster decomposition may result in deleting all bonds which maps the original system onto itself. Thus, the occurrence of single-spin flips ensuring ergodicity can be checked a posteriori. Detailed balance may be demonstrated by the prescription for general cluster algorithms given by Kandel and Domany, which shows that bonds may be deleted, frozen, or left unchanged to generate systems of interacting clusters equivalent to the original system.

The method is applied for finite arrays of hexagonal shape with $N = 61 \ldots 2977$ spins. The follow-
ing measure for antiferromagnetic correlations is used: Spins are labeled $\sigma_{\mu\nu}$ for sites given by $\mu \mathbf{r}_1 + \nu \mathbf{r}_2$ with nearest-neighbour vectors $\mathbf{r}_{1,2} = (\pm \sqrt{3}/2, 1/2)$. Three types of staggered magnetizations may be calculated by $m^I = 1/N \sum_{\mu\nu} \sigma_{\mu\nu} (-1)^{\mu}$, $m^H = 1/N \sum_{\mu\nu} \sigma_{\mu\nu} (-1)^{\nu}$, and $m^{III} = 1/N \sum_{\mu\nu} \sigma_{\mu\nu} (-1)^{\mu+\nu}$. For the hexagonal arrays, the three types are equivalent. Thus we use the average $m_a = 1/3 \left( m^I + m^H + m^{III} \right)$.

Here, our algorithm is first used in the Swendsen-Wang (SW) form by deleting/freeze bonds for all plaquettes of a randomly chosen type. It turns out that after mapping onto the system of interacting clusters best performance was achieved by attempts to flip just one (randomly chosen or the largest) cluster. Integrated auto-correlation times for energy, magnetization, and for the staggered magnetizations $m^I$...$m^{III}$ were calculated as measure of efficiency by a self-consistent windowing method. Independent isothermal runs were started from slowly cooled and relaxed configurations. For sizes $N = 61 \ldots 469$ between several $10^4$ and $10^5$ cluster-MC sweeps (MCS, i.e., attempted cluster moves), for the two larger sizes only $10^3$...$4$ MCS could be performed. As expected, the autocorrelations for the magnetization decay rapidly at all temperatures. The autocorrelations for energy are similar to those of the staggered magnetizations. Thus, we only show the average integrated auto-correlation time $\tau_a$ for the staggered magnetizations in Fig. 1(a) and compare it to runs with the single-spin-flip Metropolis algorithm for the two smallest system sizes. Fig. 1(b) shows the average size $<c>$ of flipped clusters. The strong increase of $<c>$ towards low temperature means that all spins are increasingly correlated. This transition becomes sharper with larger $N$. The size distribution of flipped clusters always consists of a rapidly decreasing part starting with single-spin flips. For low temperatures and small system sizes clusters with size close to $N$ are found also.

Still, the corresponding $\tau_a$ does not grow dramatically. For $N > 469$ we could measure $\tau_a$ only down to $T/g \simeq 0.19$, where it becomes essentially independent of $N$ while $<c> \simeq 2$. The single-spin-flip algorithm yields far larger $\tau_a$ which in a critical region should grow with system size as $\tau_a \propto N^{z/2}$ with $z \simeq 2$. This comparison demonstrates the efficiency of this cluster-MC.

However, the numerical cost of the SW-algorithm scales as $N \tau_a$. Therefore, a Wolff-type algorithm was implemented for further production runs shown below. Only a single cluster is grown starting from a randomly chosen plaquette. The performance of this algorithm is similar to the SW-algorithm but the numerical effort is smaller. Its numerical cost scales as $<c> \tau_a$.

Cluster-MC runs with several $10^5$ MCS were performed for $N \leq 721$. For $N > 1519$ serious problems in the critical region $T/g \leq 0.18$ arise. Cycling temperature displays hysteresis of the energy. Measurements could be done for runs with only few $10^4$ MCS in the critical region with $N \geq 1519$. Here, configurations both from cooling and heating were first relaxed for longer times before start of measurements to ensure that they are close to equilibrium. Sampling was performed for energy per spin $E$, specific heat $C = \langle E^2 \rangle - \langle E \rangle^2/T^2$, the staggered magnetizations, the corresponding susceptibilities $\chi^X = \langle (m^X)^2 \rangle - \langle m_X \rangle^2 / T$ and the fourth-order Binder cumulant $U^X = 1 - \langle (m^X)^4 \rangle /\langle 3 \langle (m^X)^2 \rangle^2 \rangle$ ($X = I, II, III$). Using the histogram method by Ferrenberg and Swendsen, these various quantities were evaluated as functions of temperature in the critical region. Results are shown in Figs. 2 and 3. The diverging peak in the specific heat (Fig. 2(b)) indicates the presence of a transition at or closely below $T/g \simeq 0.18$. Similarly, the peak for the average staggered susceptibility $\chi_a$ shows that the transition (Fig. 3(a)) is related to antiferromagnetic ordering. Near $T/g \simeq 0.18$, $m_a$ steeply increases reaching values $\sim 0.3$ to 0.4 (not shown here). However, the average Binder-cumulant $U_a$ for the various system sizes does not provide a clear indication for a continuous transition by a unique crossing of $U_a(T)$-curves for the different system sizes at one critical temperature (Fig. 3(b)). The transition might be first order instead as indicated by the observed hysteresis when cycling temperature. Then the apparent correlation of system sizes $N < 1000$ corresponds only to the size of typical nuclei of the low-temperature phase. On the other hand, the behaviour of the $U_a(T)$-curves which seem to merge below $T/g = 0.18$, is consistent with usual observations at a Berezinskii-Kosterlitz-Thouless-transition and a line of critical points at low temperature. Possibly, the peak in the specific heat is only a precursor of this transition, or two transitions are present.

In conclusion a cluster-MC method is presented which may be used for dipolarly coupled spin-systems. It works by generating interacting clusters from sampling of short-range interactions. It is shown to be efficient for the specific case of Ising dipoles on the triangular lattice. This success relies on the ability to define clusters for this geometrically frustrated system which percolate only at $T = 0$. However, the method can be generalized to various other systems with long-range interactions, including systems with continuous spins. The investigation of the exact nature of the finite-temperature transition found with this MC-method remains a task for the future.

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FIG. 1. (a) Average integrated autocorrelation time for staggered magnetizations (see text) versus temperature. Symbols correspond to independent isothermal runs. Comparison between Metropolis single-spin-flip and cluster algorithm. For the largest size $N = 2977$, only one run at $T/g = 0.190$ is shown (big circle). (b) Corresponding average cluster sizes $<c>$ for different system sizes.

FIG. 2. (a) Energy per spin (b) specific heat in the region of the transition temperature of Ising dipoles on hexagonal triangular–lattice arrays with various sizes $N$. 

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FIG. 3. (a) Average staggered susceptibility $\chi_a = 1/3 (\chi^I + \chi^H + \chi^H)$. (b) Corresponding average fourth-order Binder cumulant in the critical temperature region.