(Nambu) Monopoles and their “Dirac strings” in thermal artificial magnetic square ices

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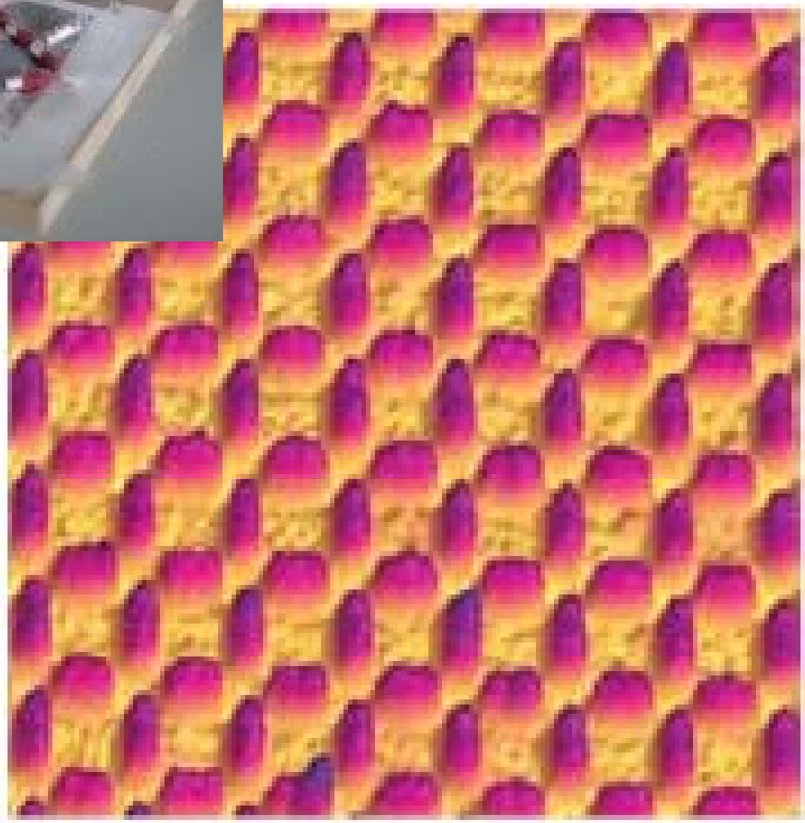
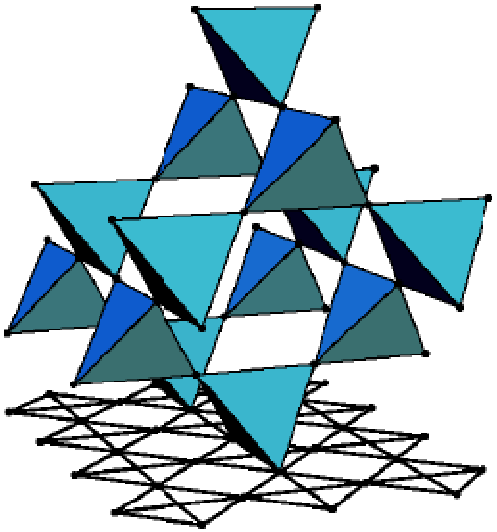
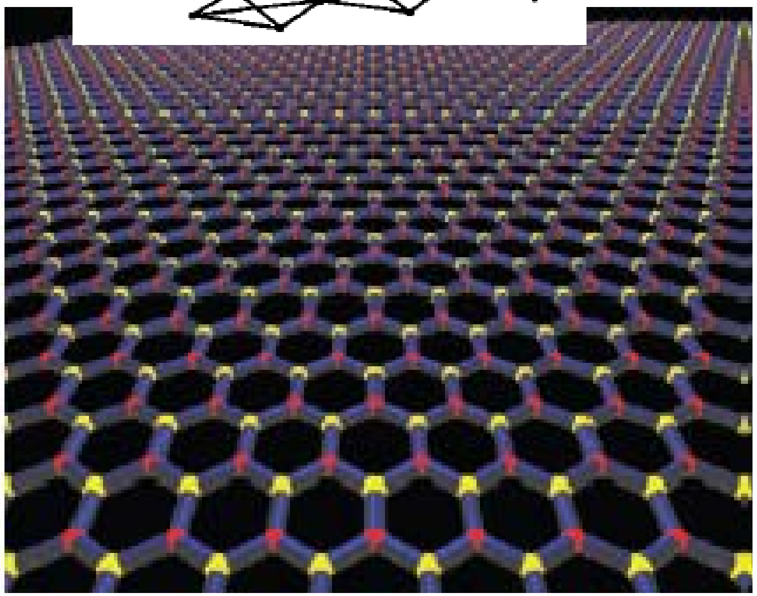
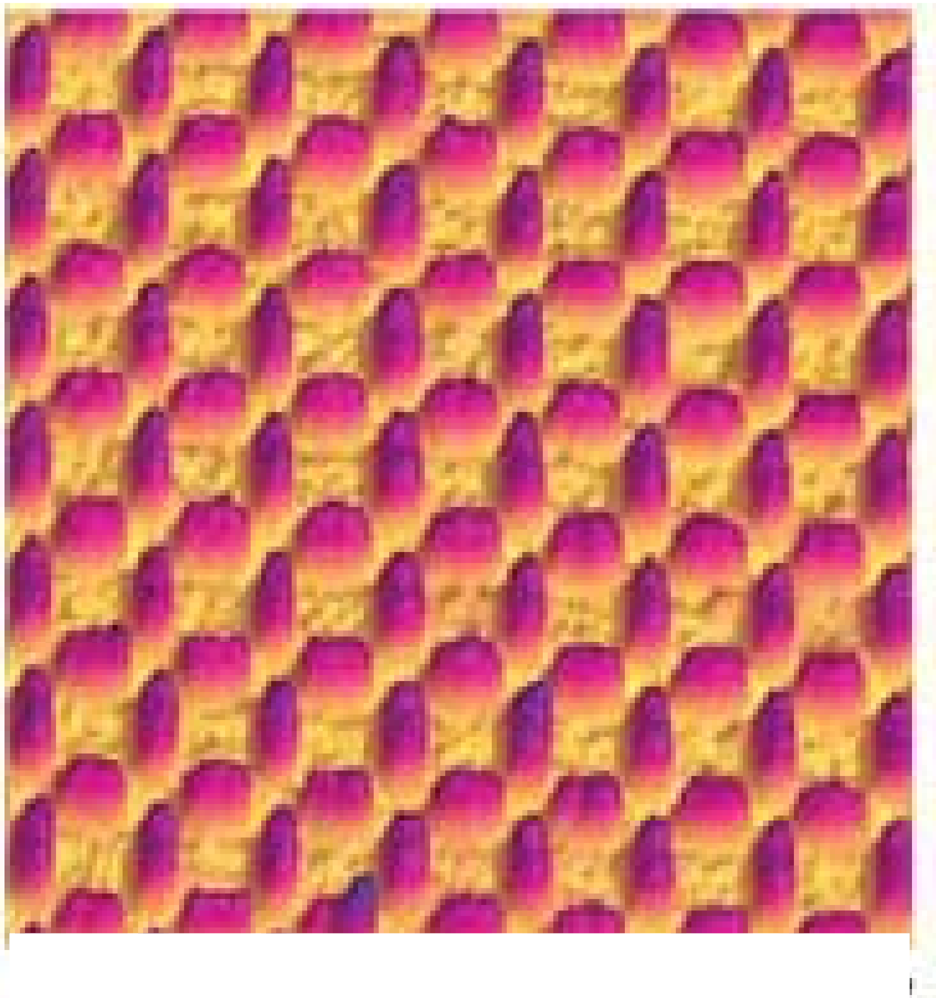
A lot of experimental effort is under way with the objective of constructing dipolar arrays of monodomain nanomagnets. Two-dimensional artificial spin ice arrays of diverse geometries are examples. **They mimic the frustrated spin ice materials.**



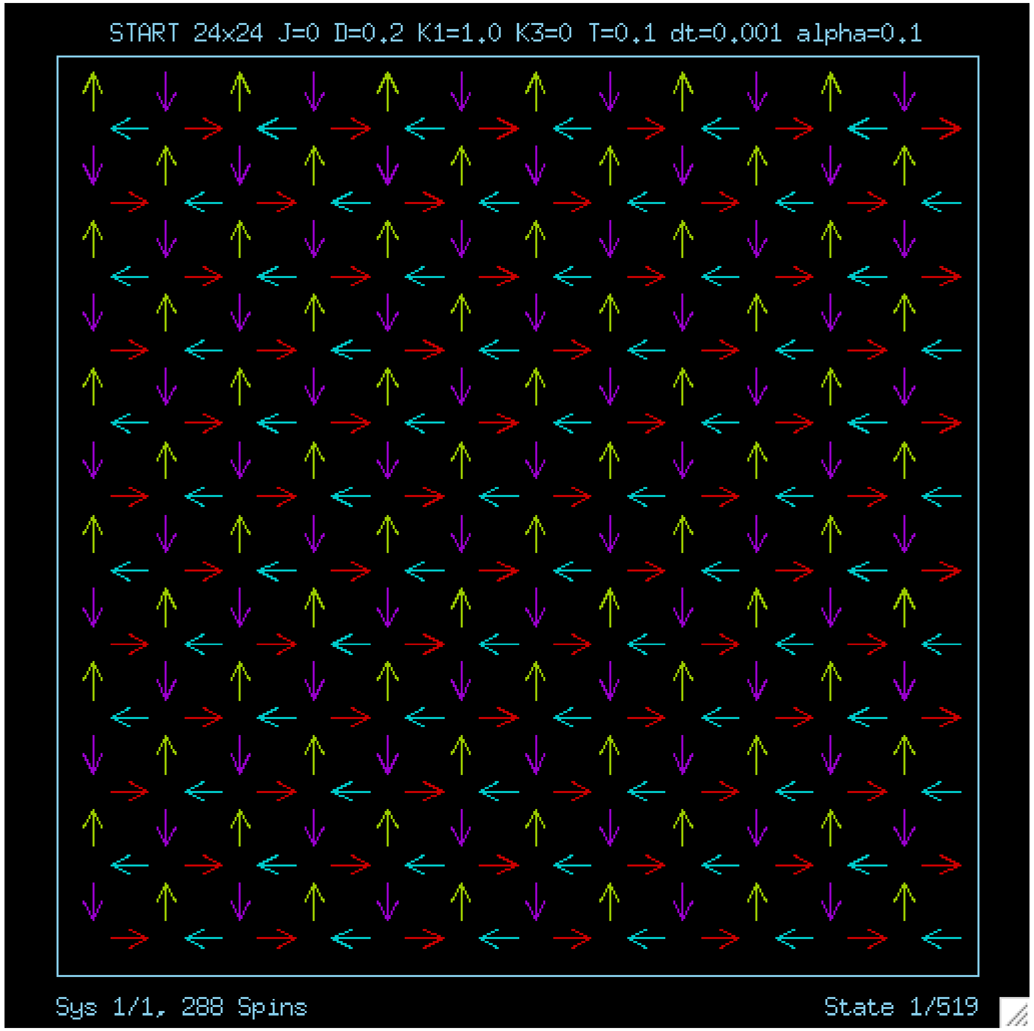




In this talk I would like to present some results about the **thermodynamics** and also, some preliminary calculations about the **dynamics** of these **artificial materials.**



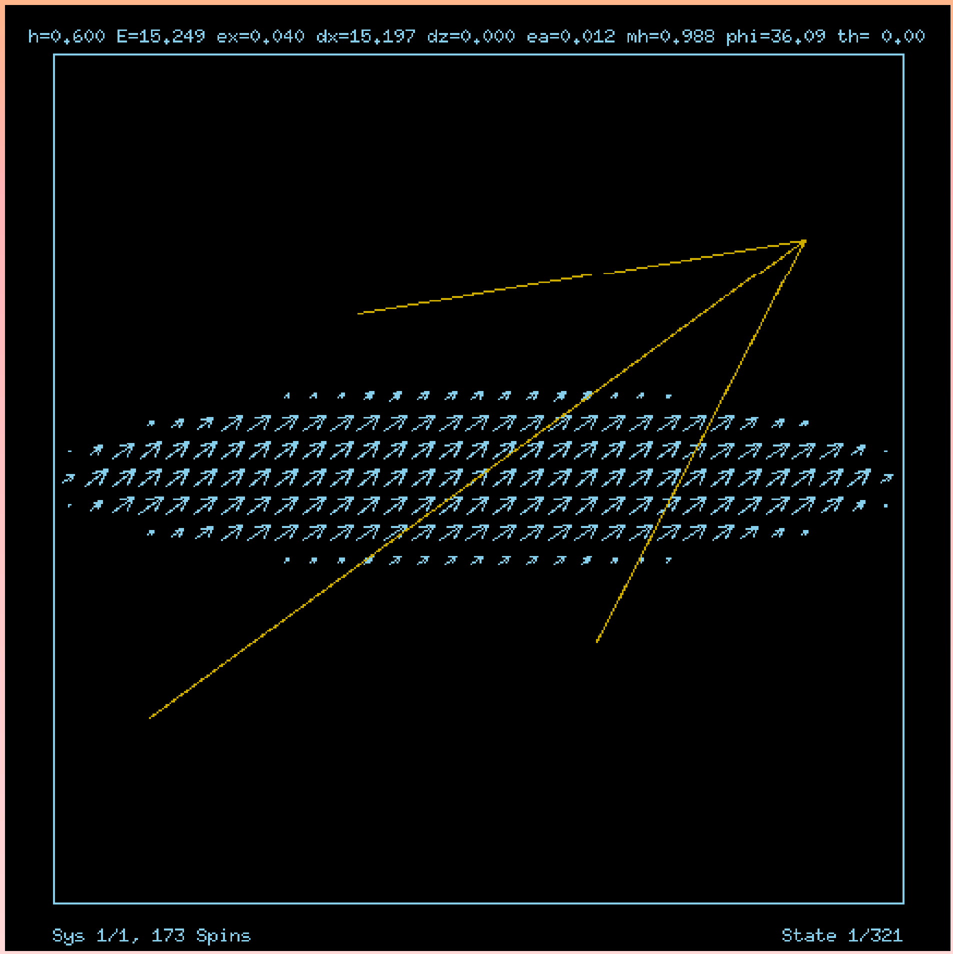
Nature ***439****, 303 (2006)***).**

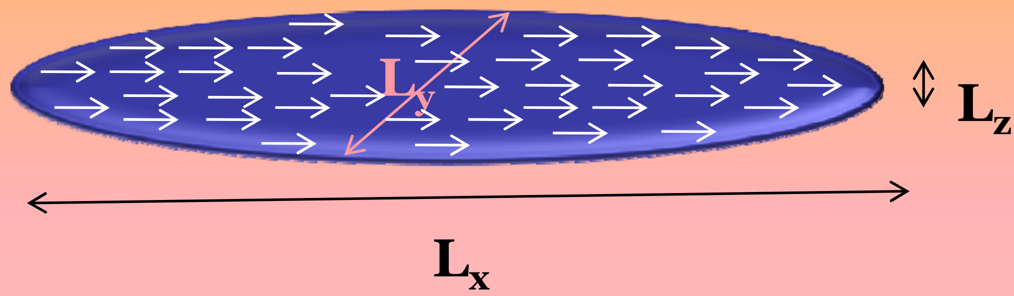


We use two approaches to study these artificial materials:

1. First, the internal structure of the islands is neglected, by considering the magnetic islands as point-like dipoles. The islands have an Ising-like behavior!!!

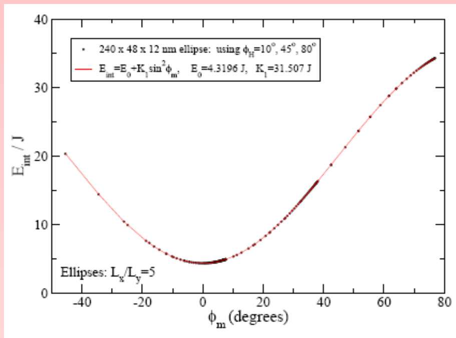
2. The internal structure of the islands is taken into account. We should consider the dynamics of all spins inside each island !!!



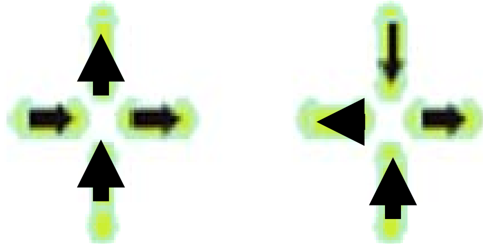


Minimal energy: spins of the island atoms point out along the longest axis (here, the x-axis).

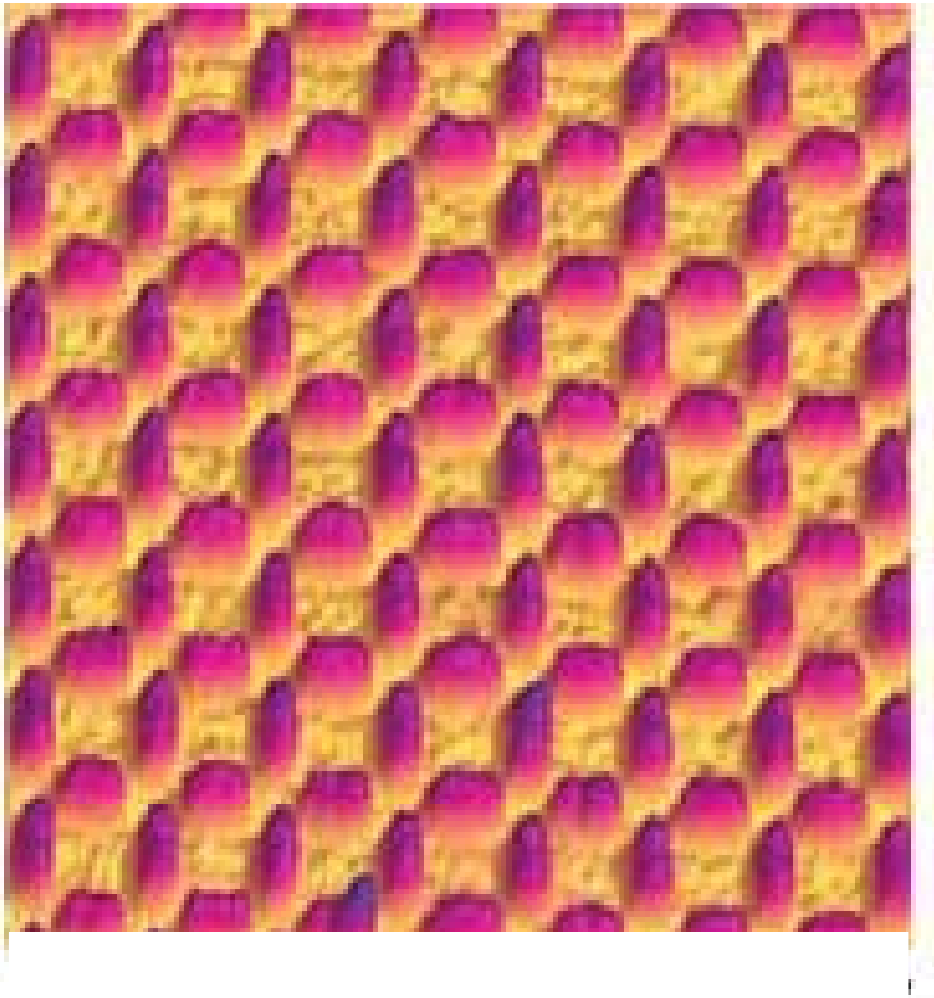
Energy increases as the spins of the island atoms start to point out along any other direction (see graphic).



The two-dimensional (2D) magnetic square lattice was the first artificial spin ice (see *Nature* ***439*, *303 (2006)*).**



$$H_{SI} = Da^3 \sum_{i \neq j} \left[\frac{\vec{S}_i \cdot \vec{S}_j}{r_{ij}^3} - \frac{3(\vec{S}_i \cdot \vec{r}_{ij})(\vec{S}_j \cdot \vec{r}_{ij})}{r_{ij}^5} \right]$$



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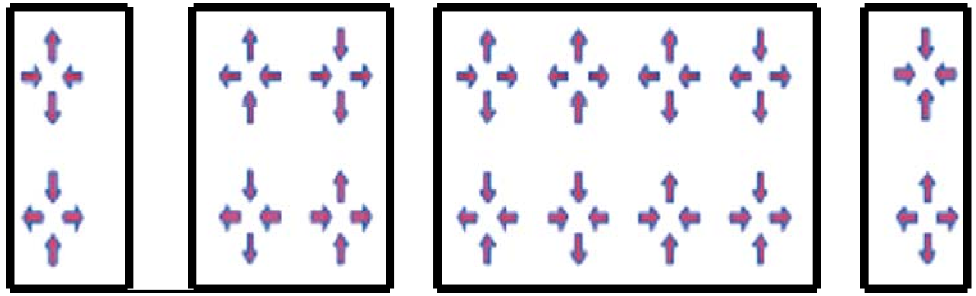
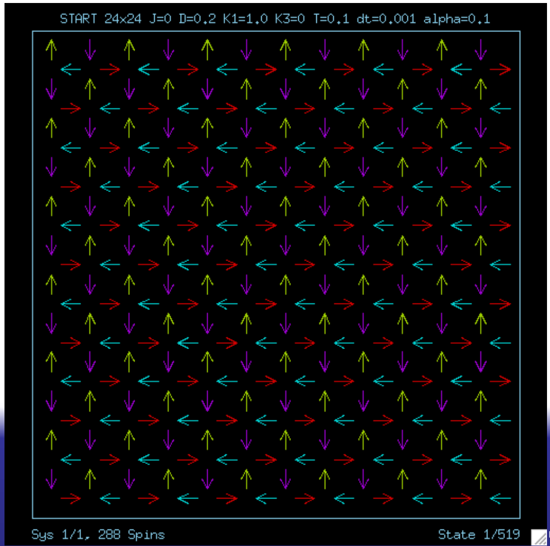
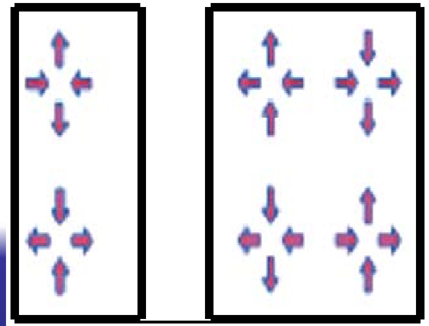


Ice rule: the 6 bonds are not equivalent.

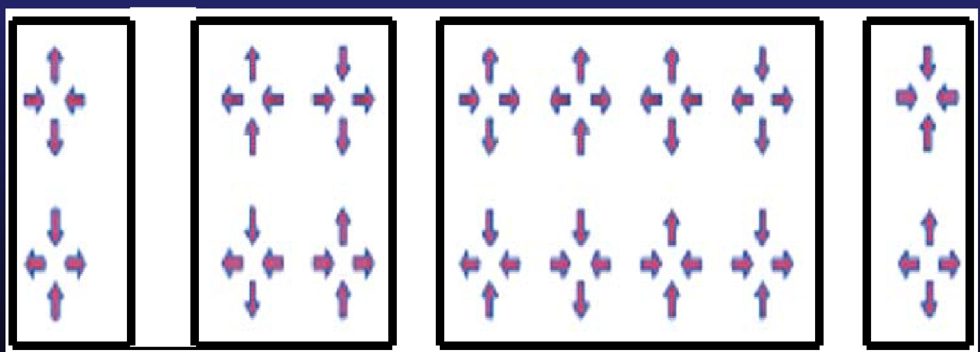
In each vertex, the ice rule dictates that 2 spins point inward and 2 point outward. However, differently from the 3d spin ice, in 2d, not all spins can be equidistant. Then, the six bonds between the four islands belonging to a vertex are not all equivalent.

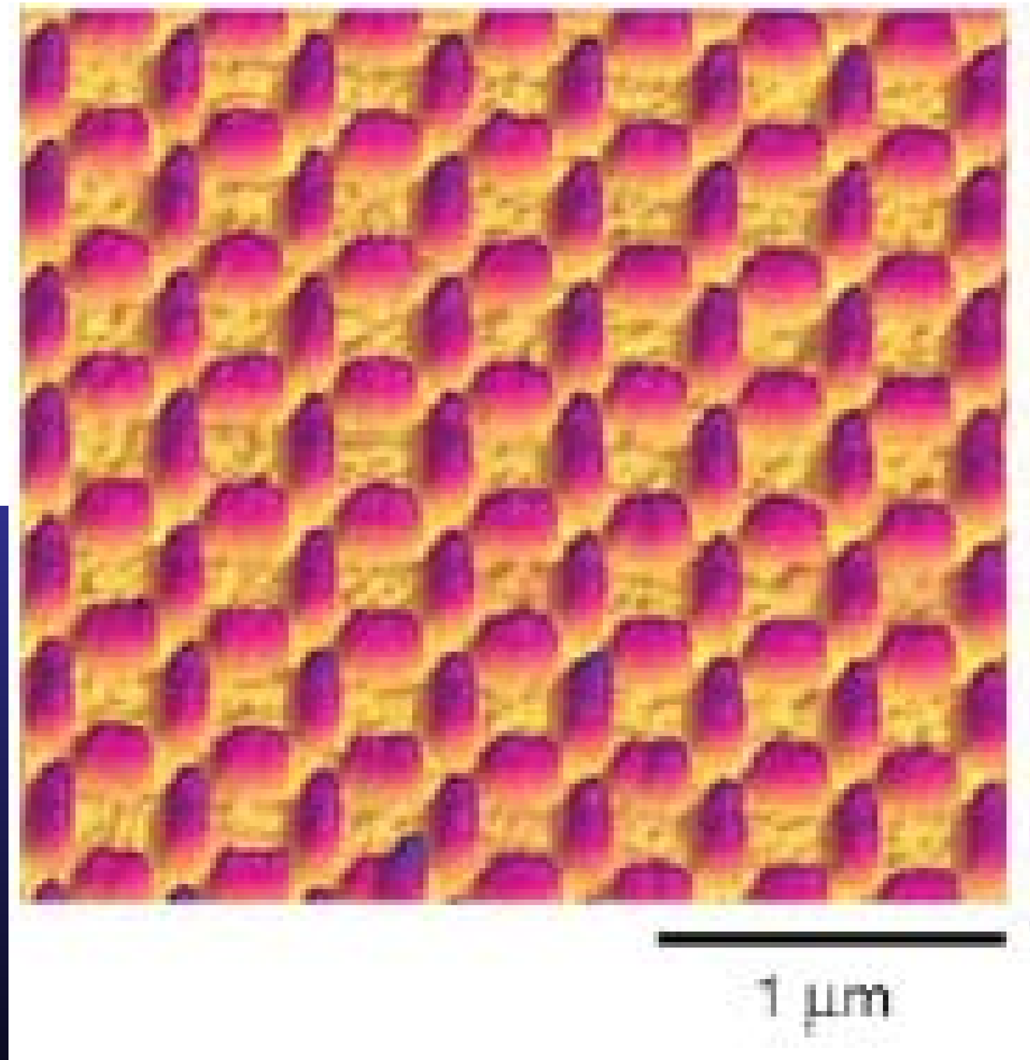
Indeed, considering the two topologies that obey the ice rule, topology 2 has about four times more energy than topology 1.



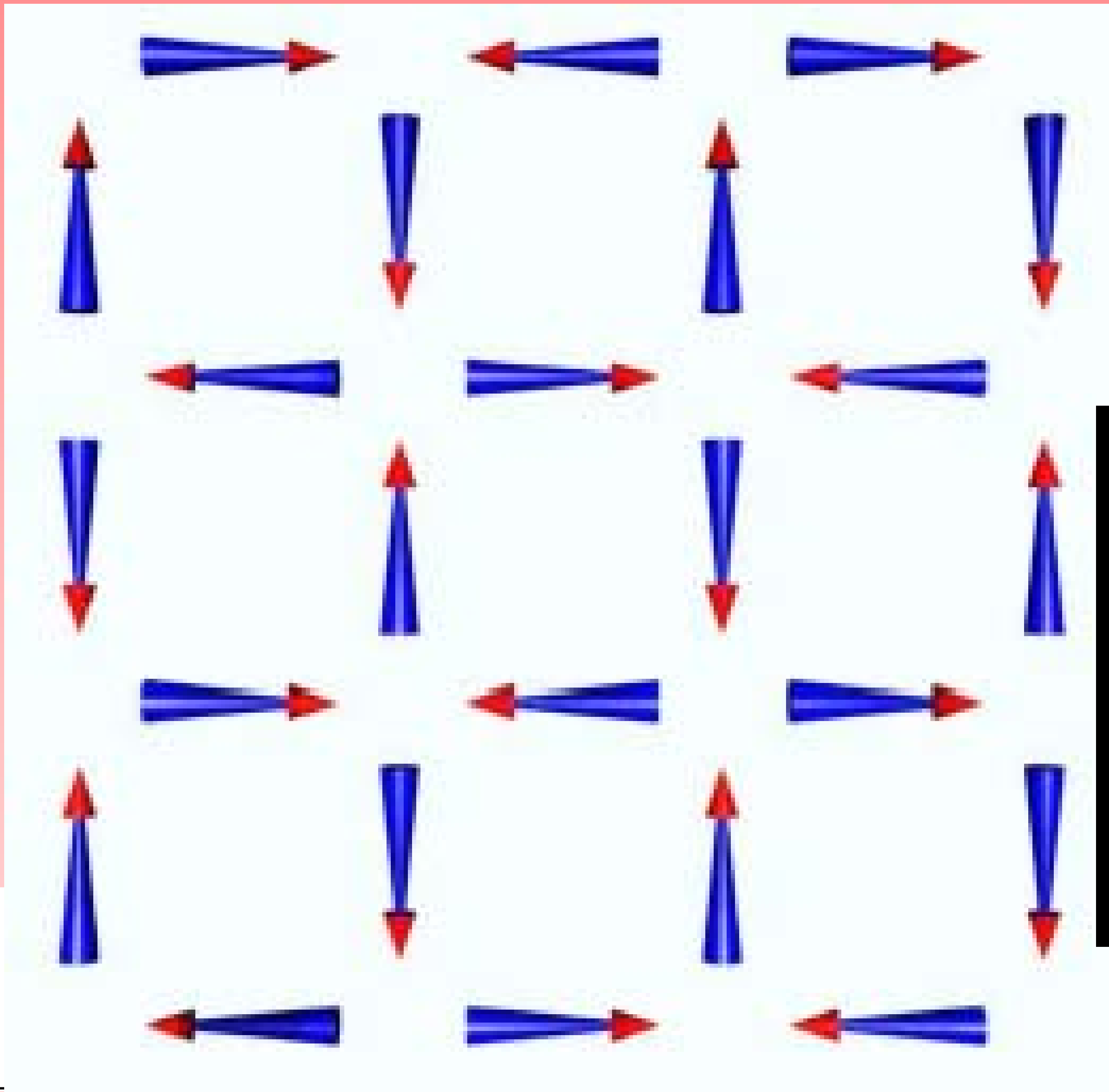


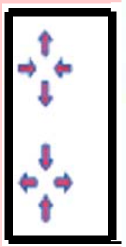
Topology 1, Topology 2

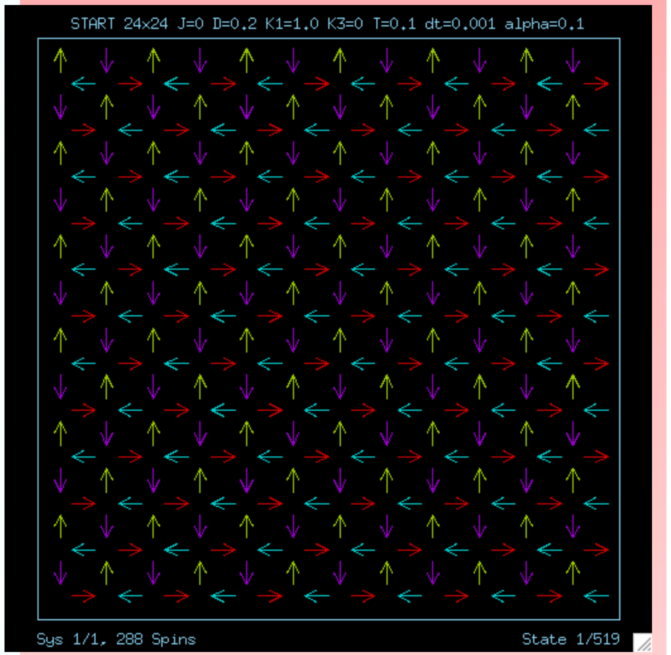


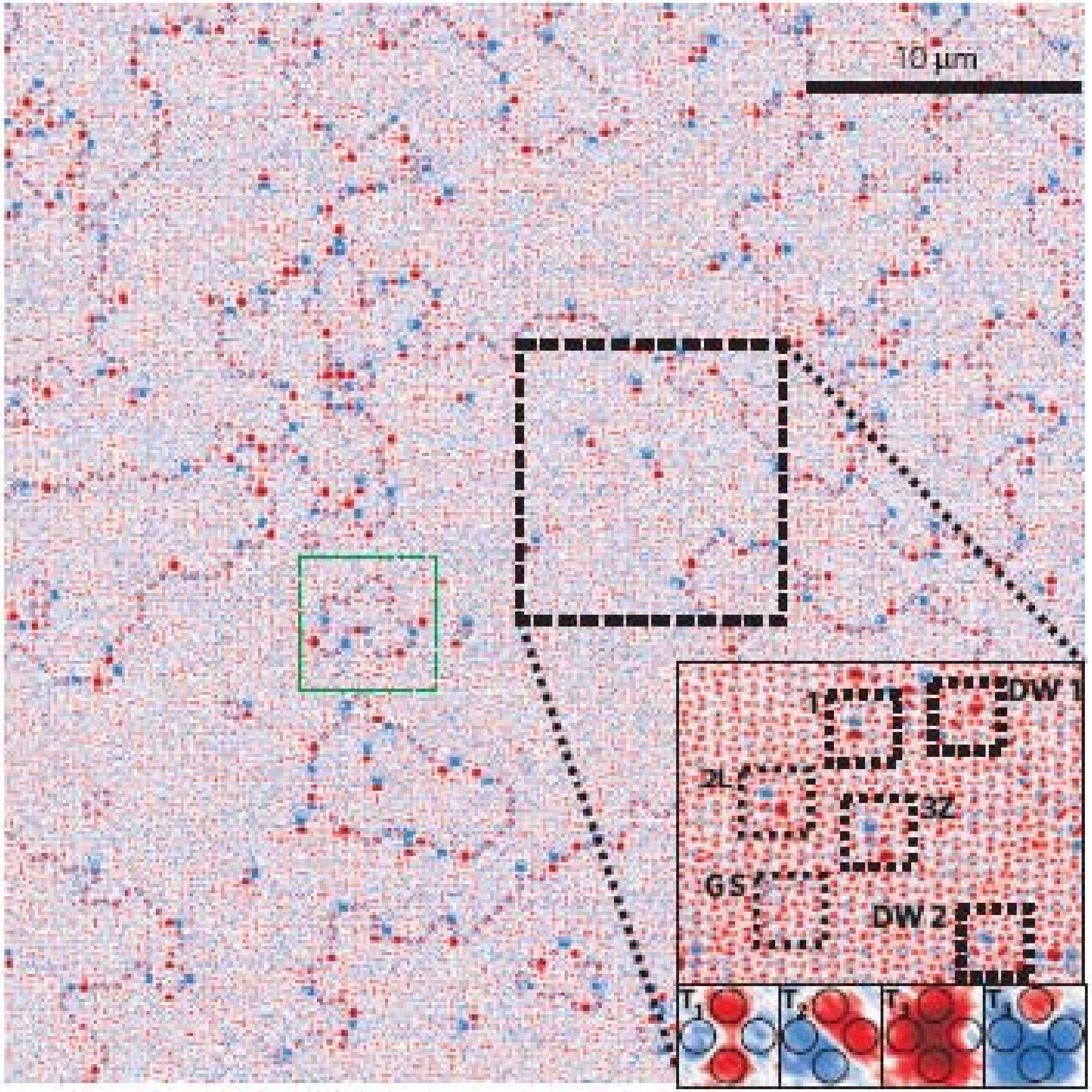


Below we show the configuration of the ground state. Clearly, it obeys the ice rule (all vertices with topology 1).





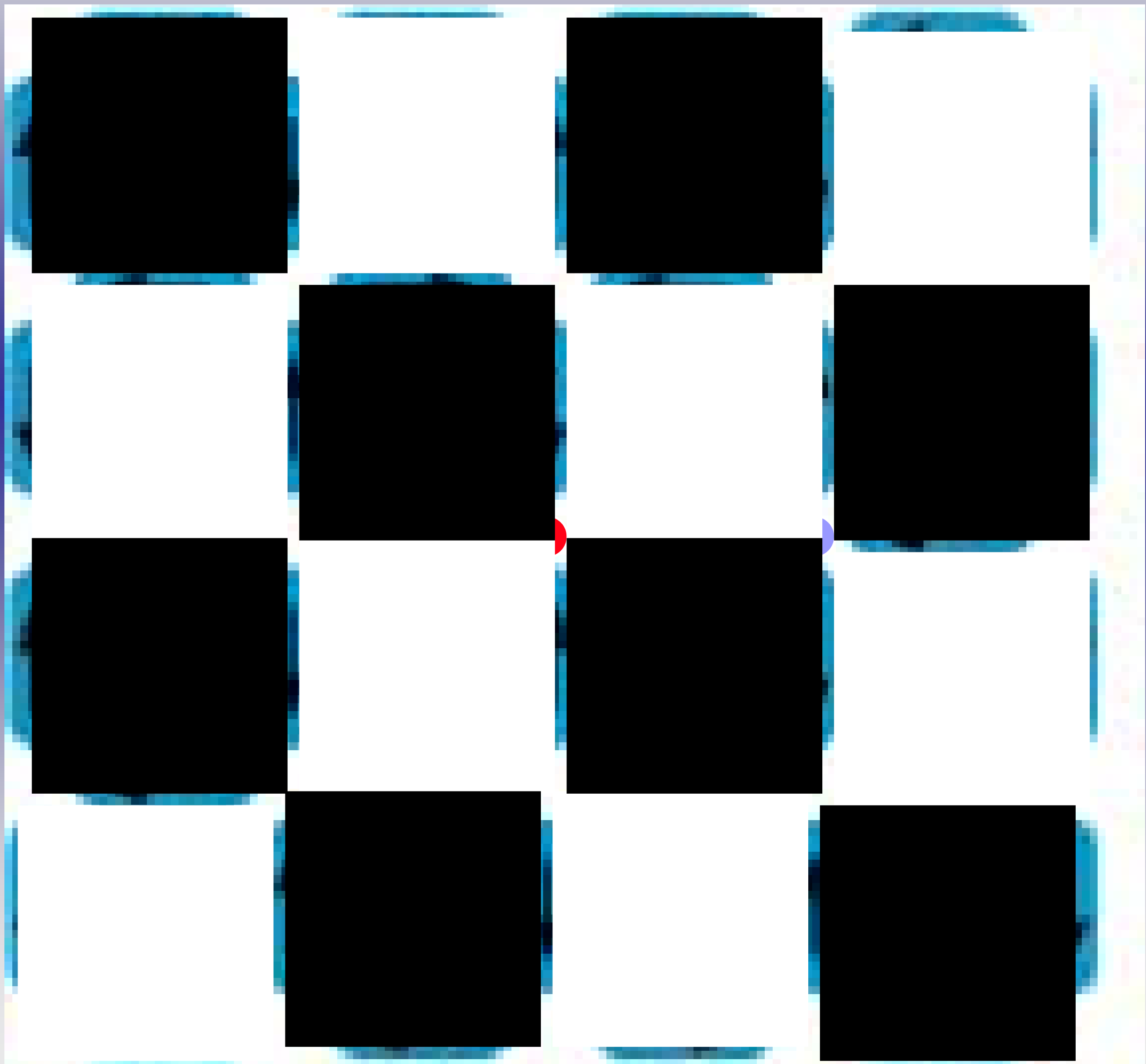




This ground state was not obtained experimentally until 2010 (**Morgan *et. al.*, Nature Phys. 7, 75 (2011)**).

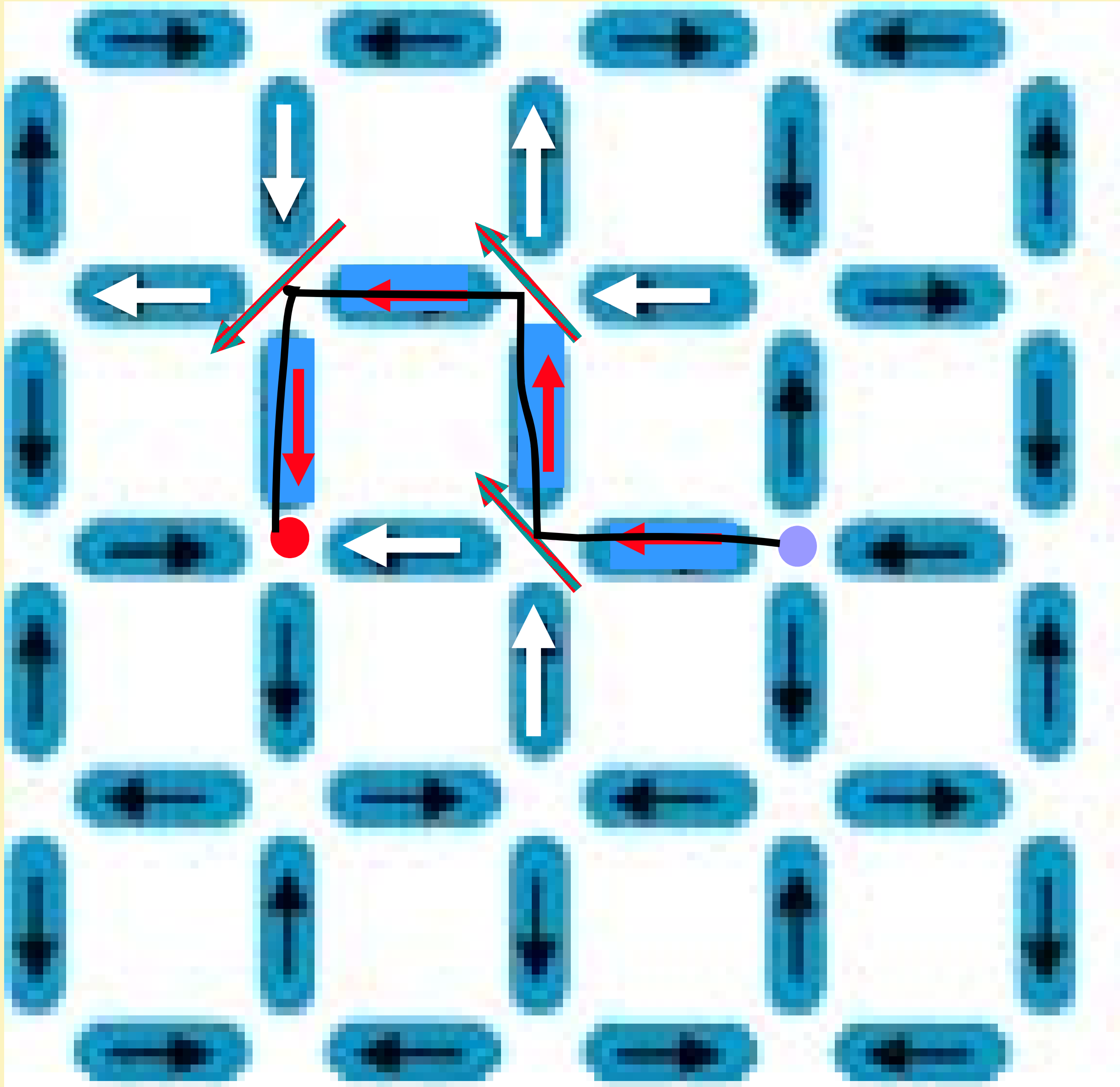
It was solved by allowing the magnetic islands in the artificial spin ice to interact as they are gradually formed at room temperature. As a result, the system can be effectively thermalized, allowing it to find its predicted ground state.

The ground state looks like a checkerboard. The effective magnetic charge in each vertex is naturally zero.

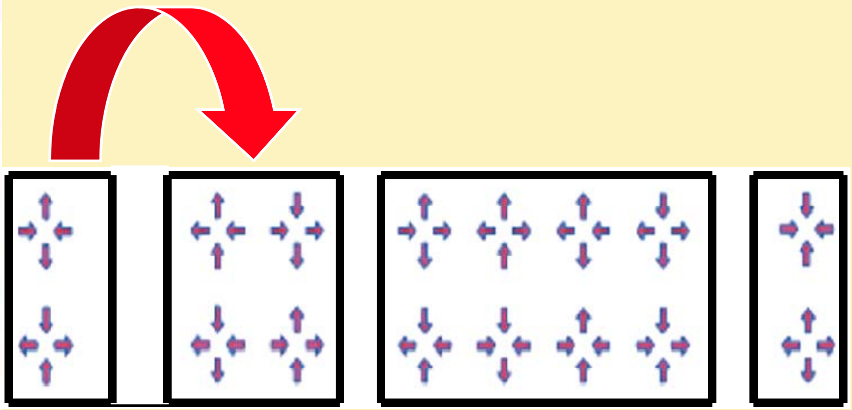


The most elementary excitation involves inverting a single spin (violating the ice rule) to generate localized dipole magnetic charges (blue and red circles with a red arrow in between).

The simplest excitations are then 2 neighbor vertices, one of them in the 3-in, 1-out (red) state and the other in 3-out, 1-in (blue) state.

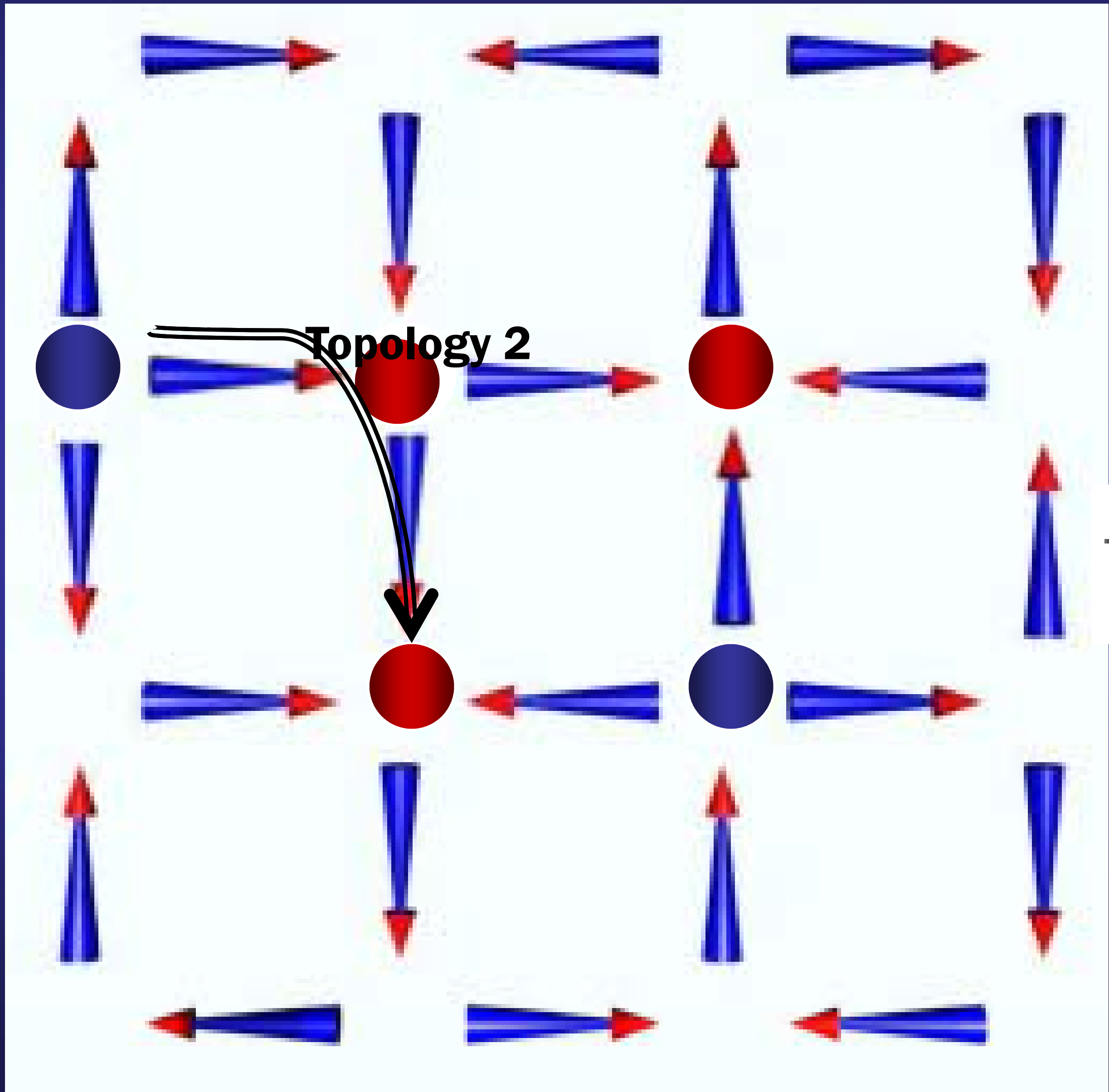


In principle, blue and red charges could be separated without further violation of the ice rule. However, it just happens if the topology is changed along a line of vertices connecting the two charges. It costs energy!



These effective magnetic charges interact through a potential given by ((arXiv:0809.2105 (2008), JAP **106**, 063913 (2009)):

$$V(R,X) = q/R + bX + c,$$

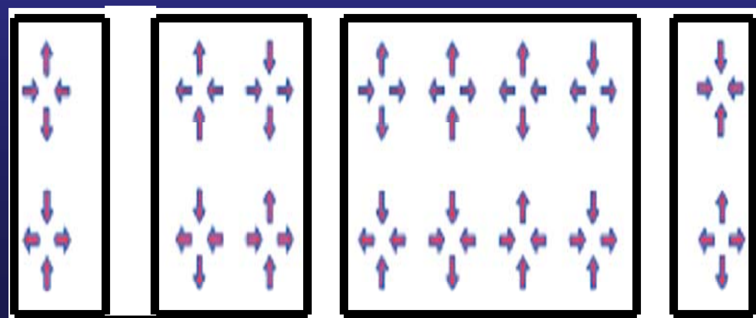


where

$$q \approx -4Da,\ b \approx 10D/a \text{ and } c \approx 23D$$

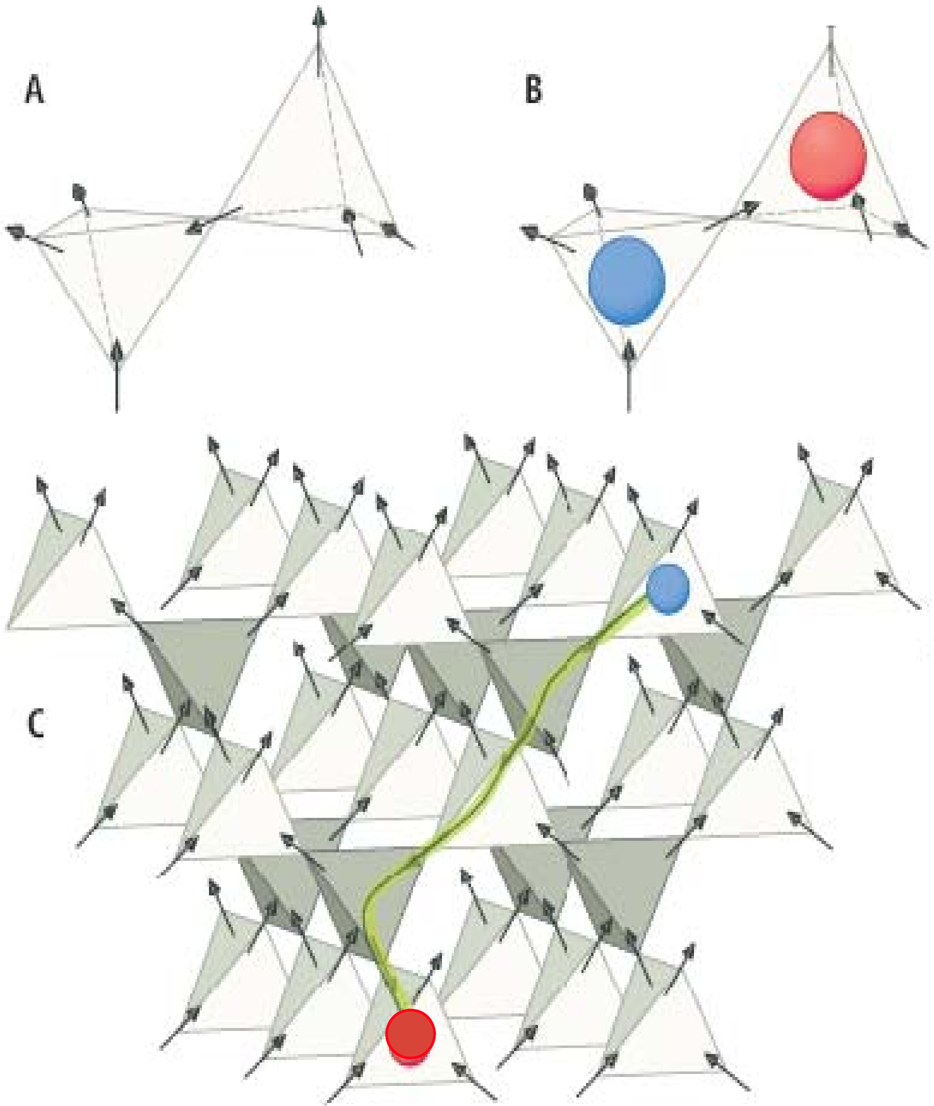
a is the lattice spacing

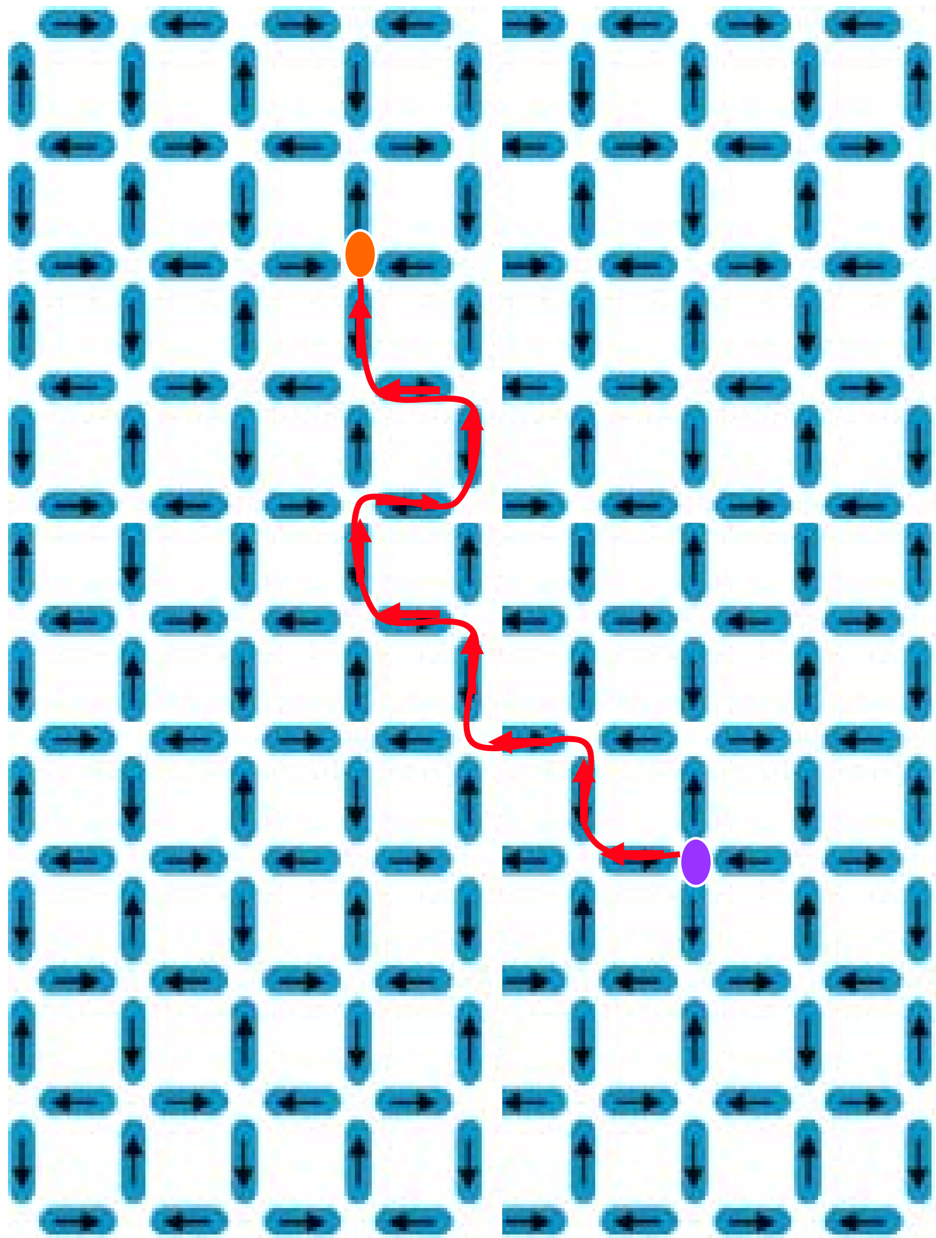
$$-\mu_0 Q_M^2 / 4\pi R \rightarrow |Q_M| = \sqrt{4\pi |q| / \mu_0}$$



Differently from the usual 3d spin ice, the string connecting the charges in the 2d case is energetic, with a nonzero tension. The string energy is then proportional to the string length X, $V(R,X)= q/R + bX + c$.

$$|Q_M| = \sqrt{4\pi|q|/\mu_0}$$

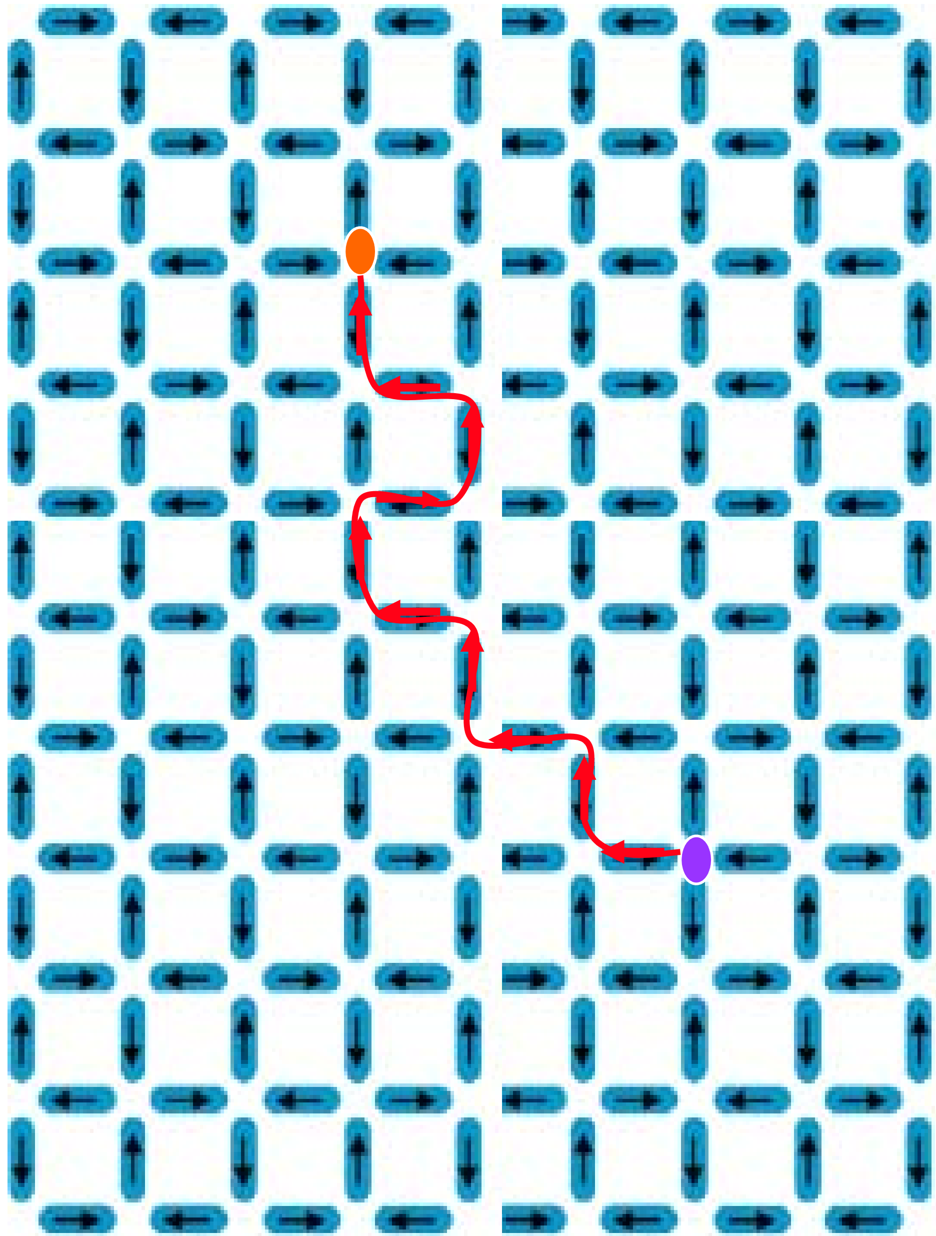




This picture bears in mind that these excitations are, to some extent, similar to **Nambu monopoles & strings!**

See Y. Nambu, Phys. Rev. D 10, 4202 (1974):

1. The end points of the string behave like particles with charge g, which leads to a Yukawa interaction.
2. The string has energy! For a sufficiently long string, the string energy is dominant.
3. The string is oriented, i.e., has an intrinsic sense of polarization, like a magnet.

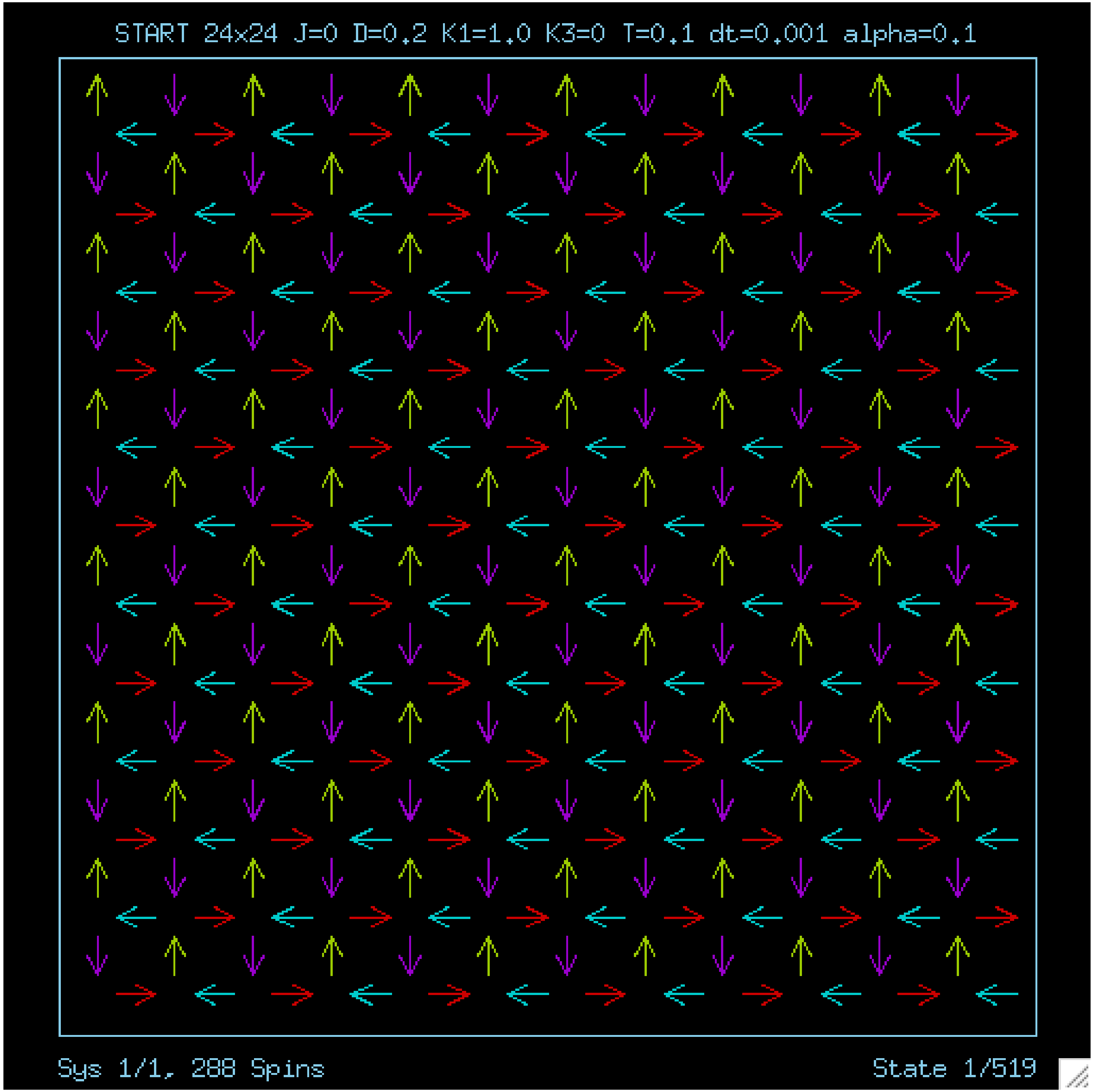


Nambu also argued that there are very likely classical dumbbell-like solutions for the Weinberg-Salam model describing a monopole-anti-monopole pair connected by a string-like tube of neutral weak Z0 flux).

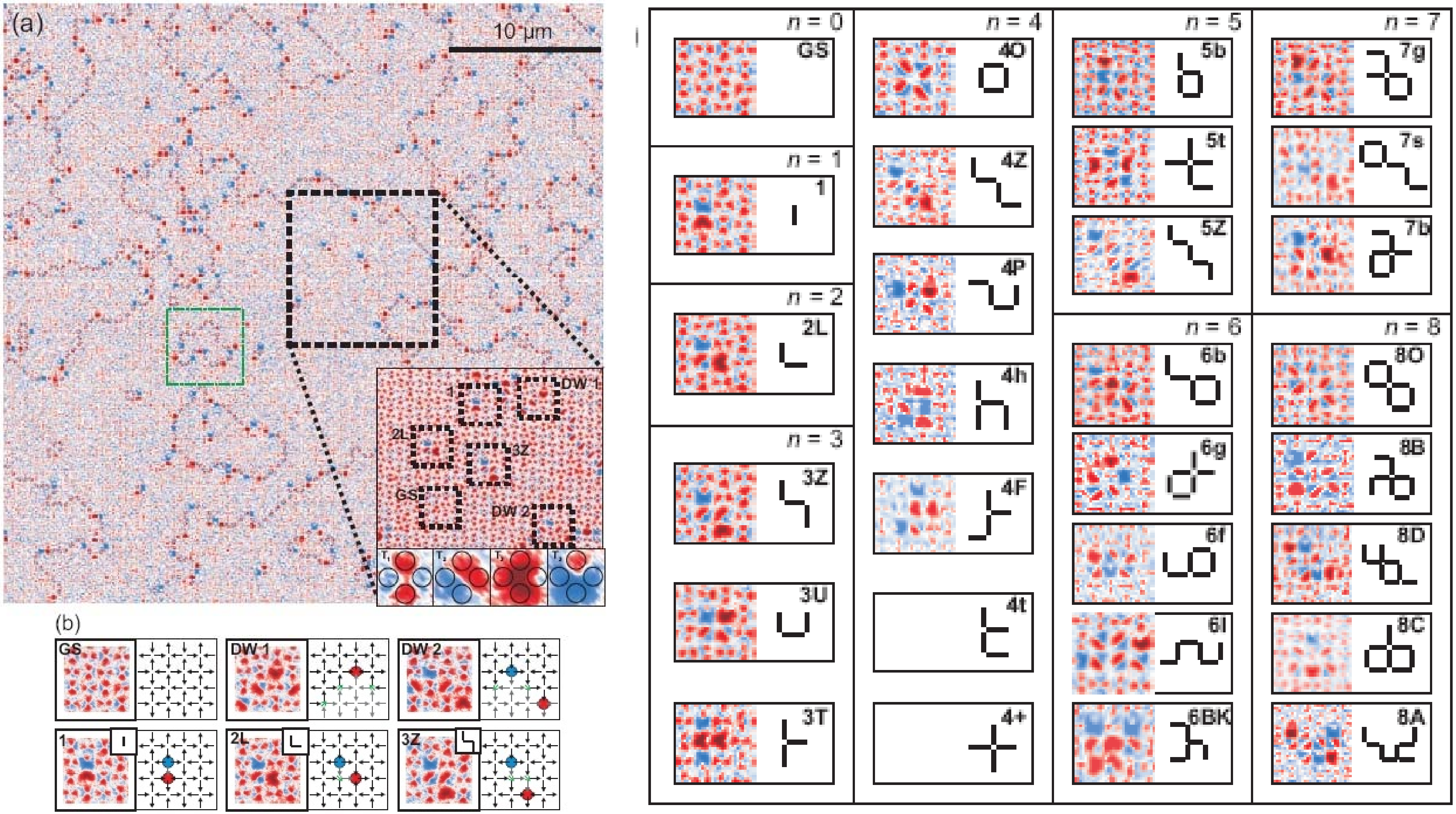
See also Y. Nambu, Nucl. Phys. B 130, 505 (1977).

However, it is not clear whether a description in terms of, for example, **Dirac monopoles** (fractionalized objects) is truly viable in artificial square spin ice systems.

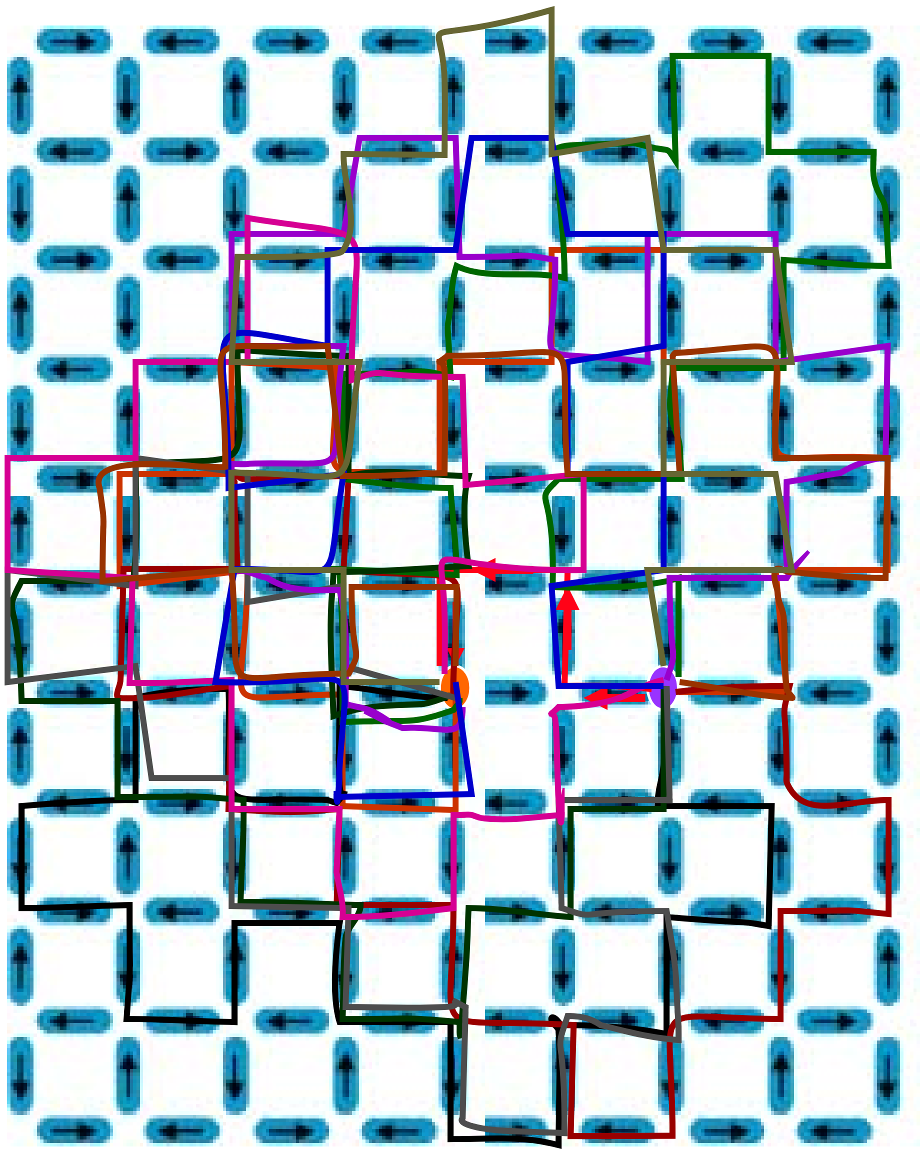
Here we would like to know something about the possibility of "breaking" the string...



These monopoles were identified as small localized departures from the ground state at frequencies that follow the Boltzmann law (**Nature Phys. 7, 75 (2011)**). Excitations 1 and 4O are the first and second excited states respectively.

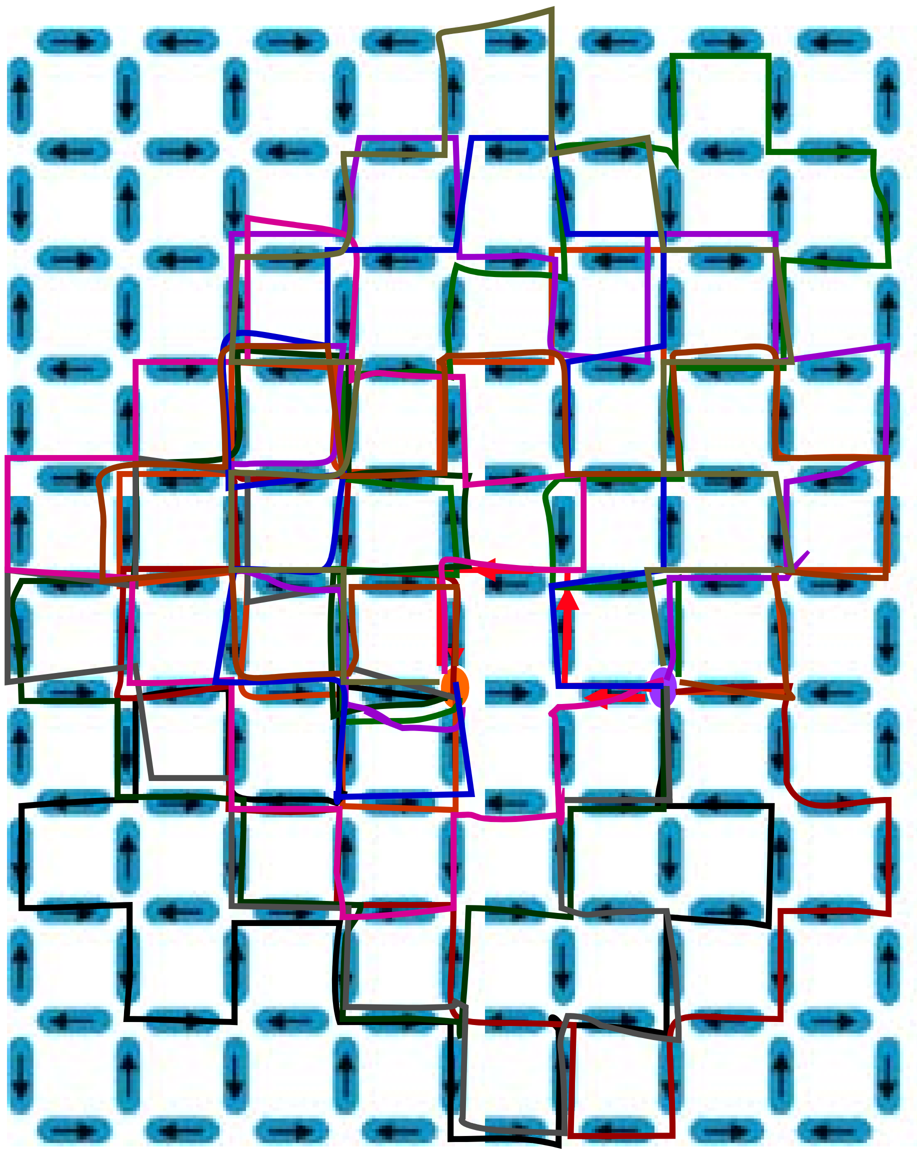


In principle, for the thermodynamics, the following arguments should be valid. There are many possible ways of connecting two monopole defects with a string. Below we show some of them for a string length equal to $X=24a$, $R=2a$.



Indeed, for X sufficiently large ($X>>R$), the number of configurations would be well approximated by the random walk result $p^{X/a}$ (for a 2d square lattice, $p = 3$).

Then, using a very simple estimate, the string configurational entropy (k_B *ln p* $^{X/a}$) is proportional to *X*, and the string free energy can be approximated by



$$F = [b - (\ln 3) k_B T/a] X$$

So we have an effective tension b_{eff}

$$[b - (\ln 3) k_B T/a]$$

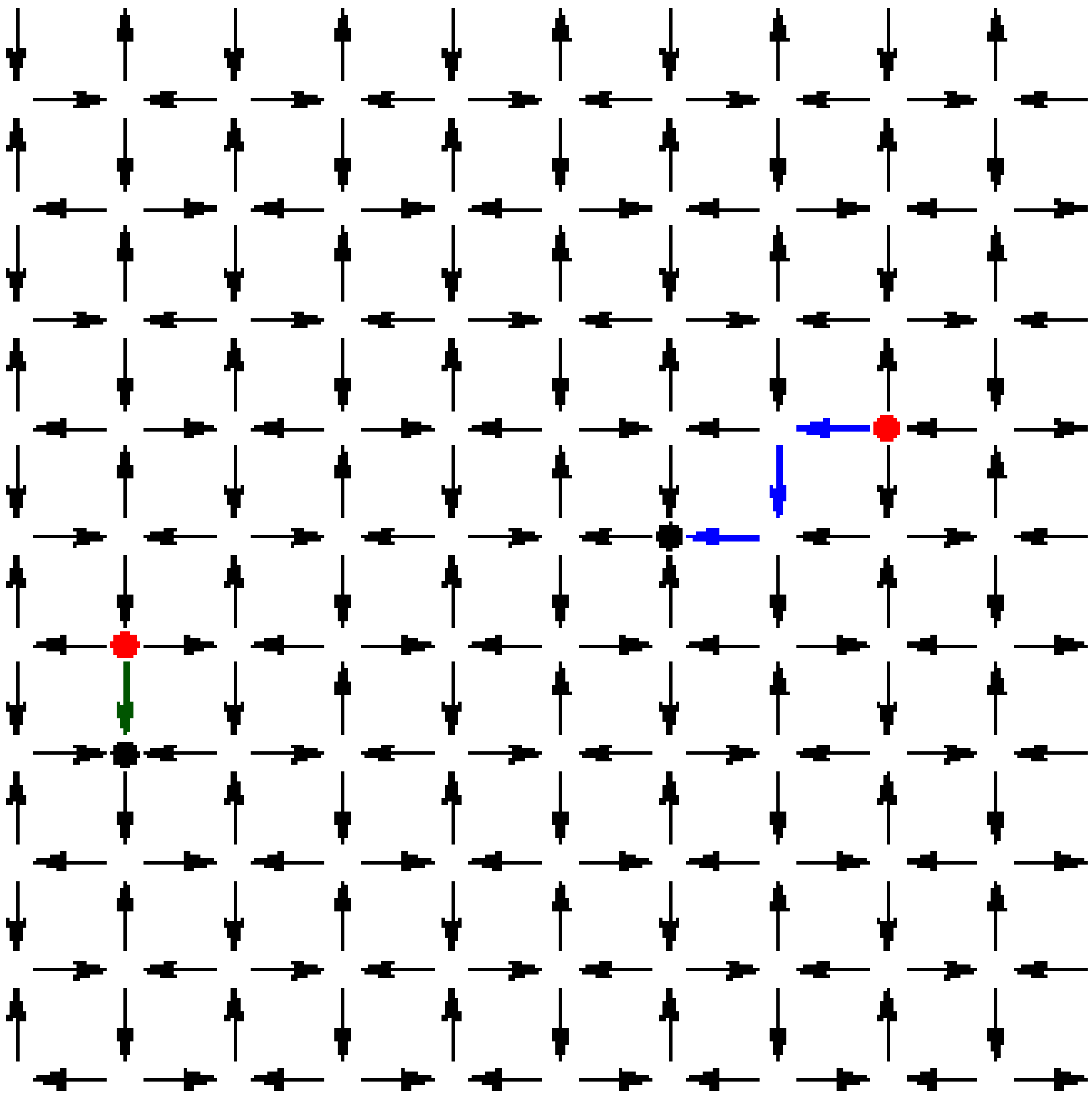
which vanishes for

$k_B T_c \approx ba/\ln(3)$.

$k_B T_c \approx 9.1$ D .

Could the string loose the monopoles at a temperature near 9.1D?

By using Monte Carlo techniques we calculate the specific heat, the density of monopoles and also their average separation as functions of temperature.



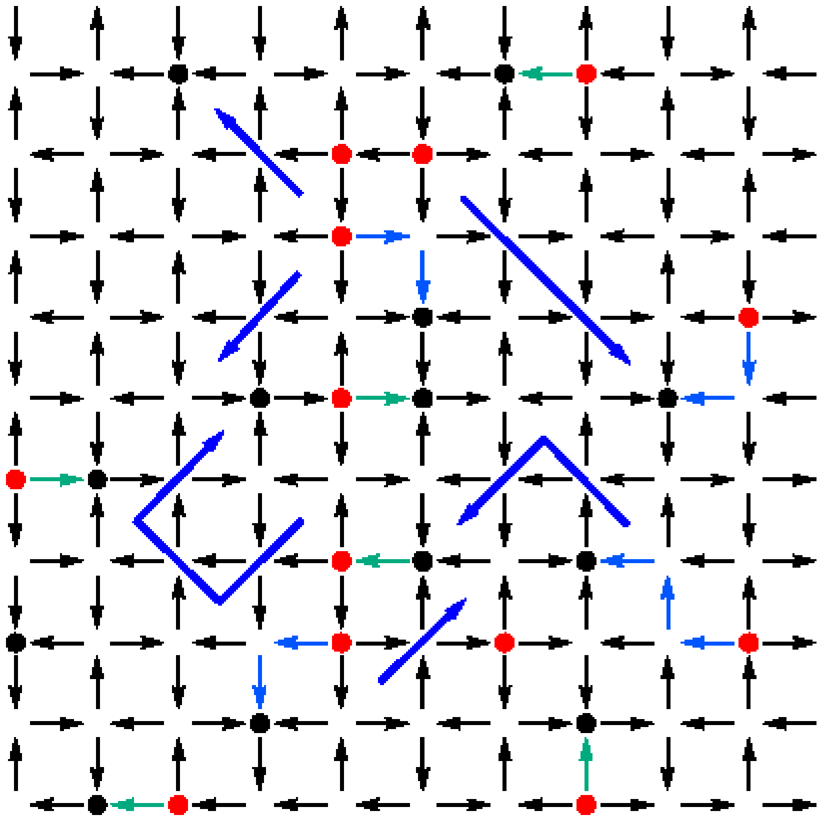
Here, the magnetic moments of the islands are replaced by point-like dipoles (spins). Then, we describe the system by the following Hamiltonian:

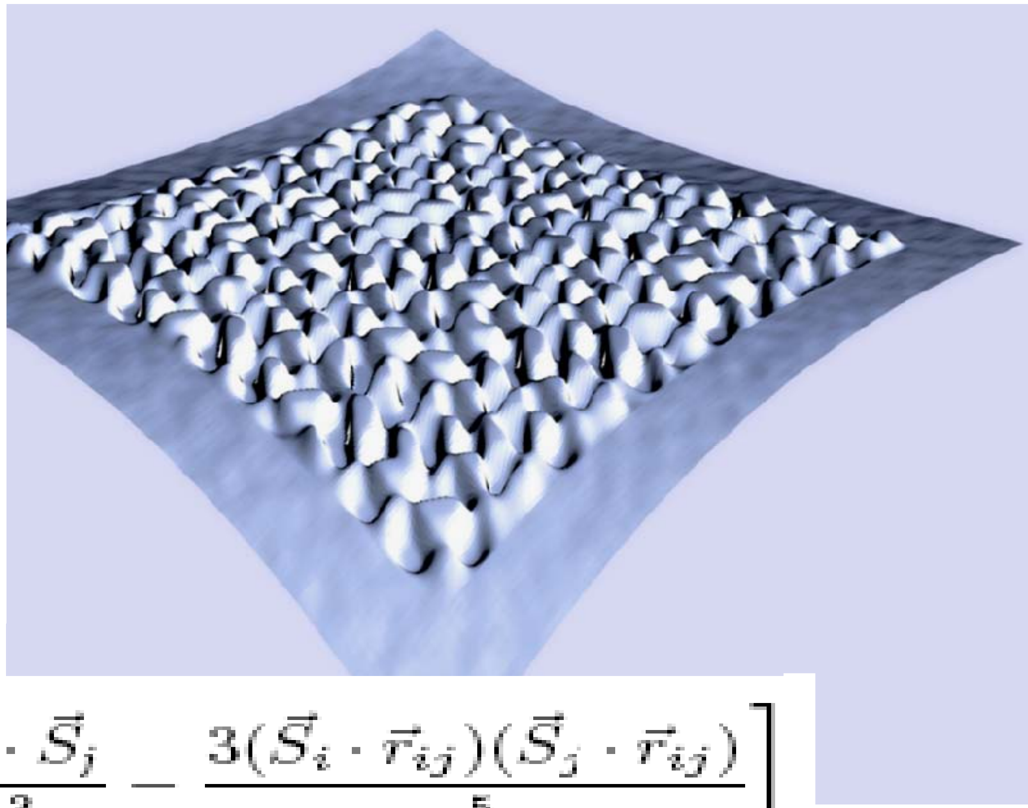
$$H_{SI} = Da^3 \sum_{i \neq j} \left[\frac{\vec{S}_i \cdot \vec{S}_j}{r_{ij}^3} - \frac{3(\vec{S}_i \cdot \vec{r}_{ij})(\vec{S}_j \cdot \vec{r}_{ij})}{r_{ij}^5} \right]$$

where $D = \mu_0 \mu^2 / 4\pi a^3$ is the coupling constant of the dipolar interaction, (from experimental data, $D \approx 2 \times 10^{-19}\, J$,), a is the lattice constant and $\boldsymbol{S}_i$ represents the spins, which can assume only the values: $\boldsymbol{S}_{hi} = (S_x = \pm 1, S_y = 0, S_z = 0)$ or $\boldsymbol{S}_{vi} = (S_x = 0, S_y = \pm 1, S_z = 0)$.

Periodic boundary conditions were implemented by means of the Ewald Summation.

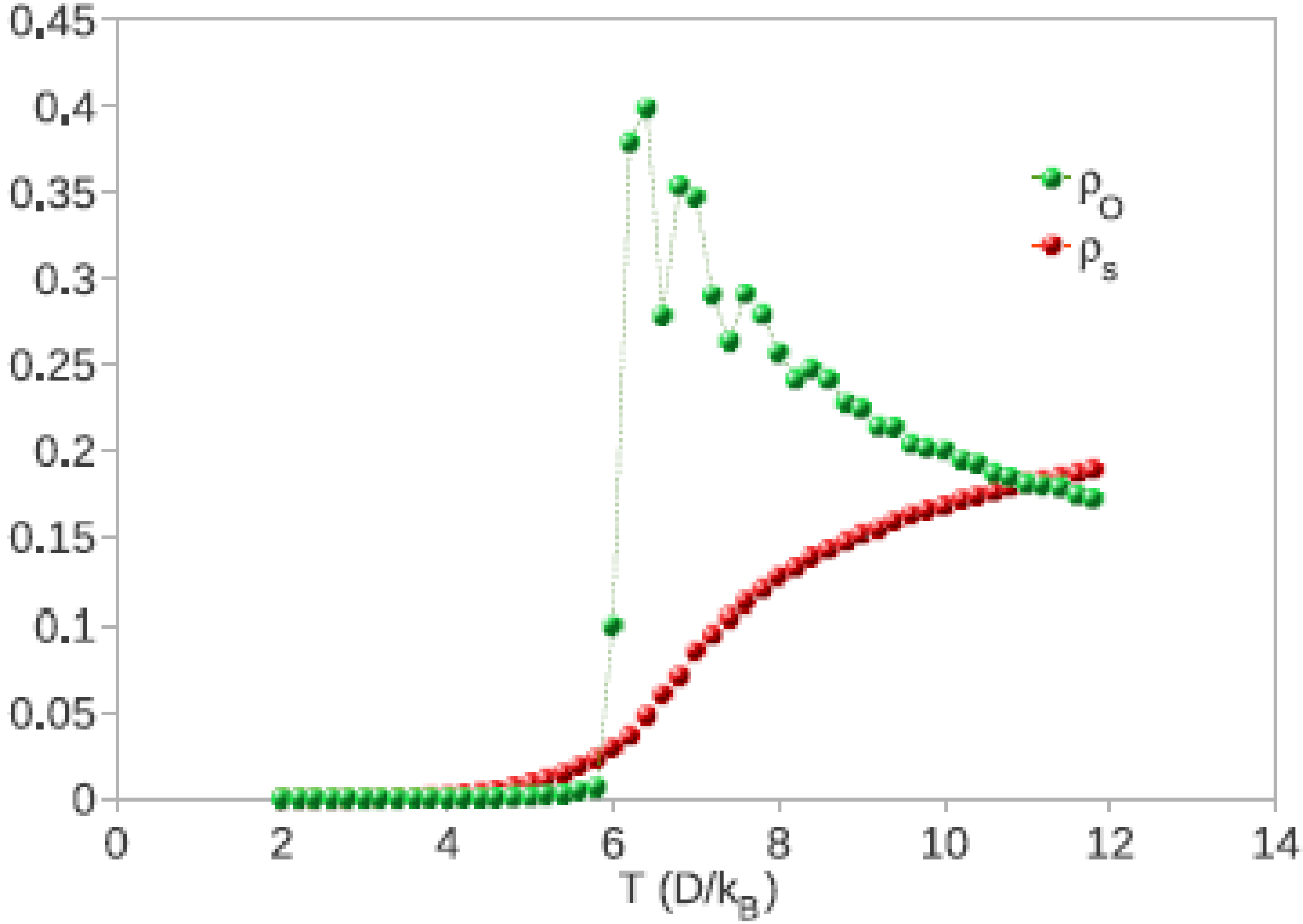
We have studied lattices with several different sizes (L from 10a to 80a). Now we discuss the MC results.



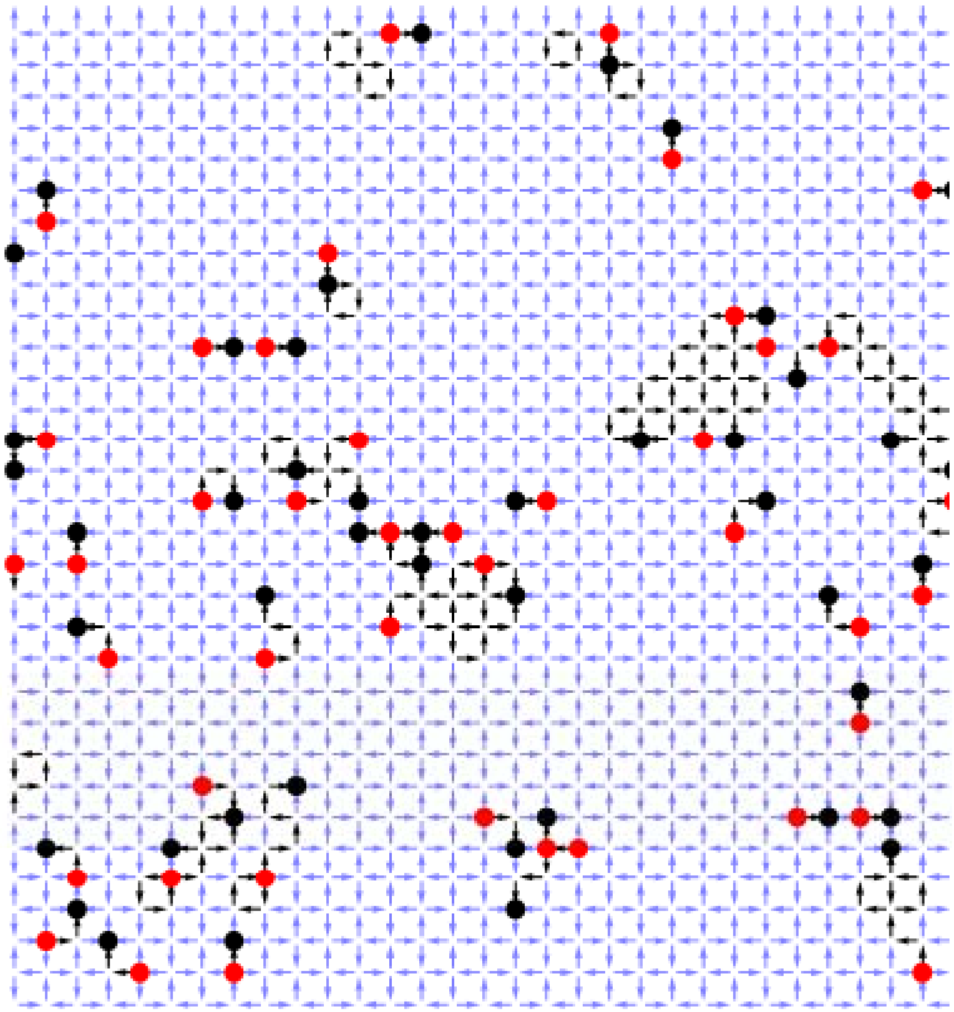


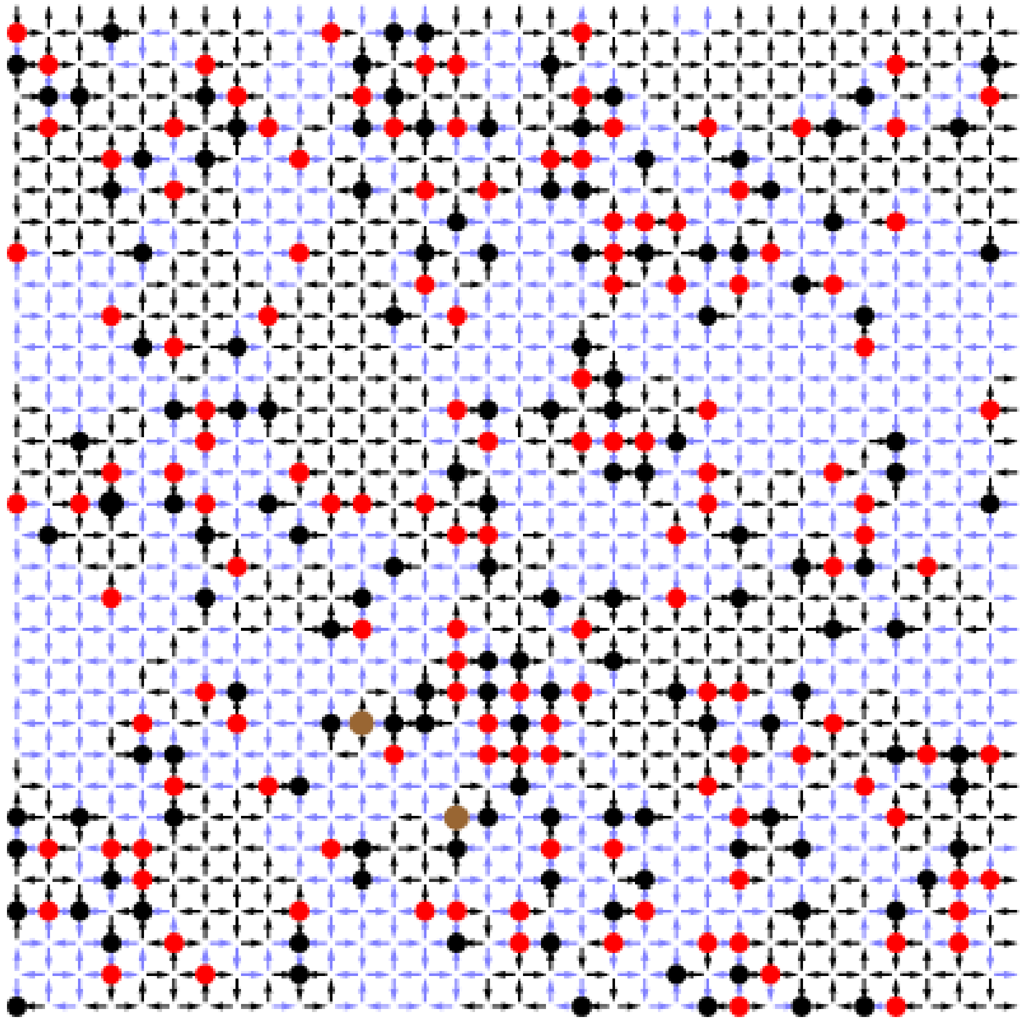
$$H_{SI} = Da^3 \sum_{i \neq j} \left[\frac{\vec{S}_i \cdot \vec{S}_j}{r_{ij}^3} - \frac{3(\vec{S}_i \cdot \vec{r}_{ij})(\vec{S}_j \cdot \vec{r}_{ij})}{r_{ij}^5} \right]$$

1. Density of monopoles and density of string loops (4O).
The last presents a maximum at a temperature around $k_B T = 7.2D$.

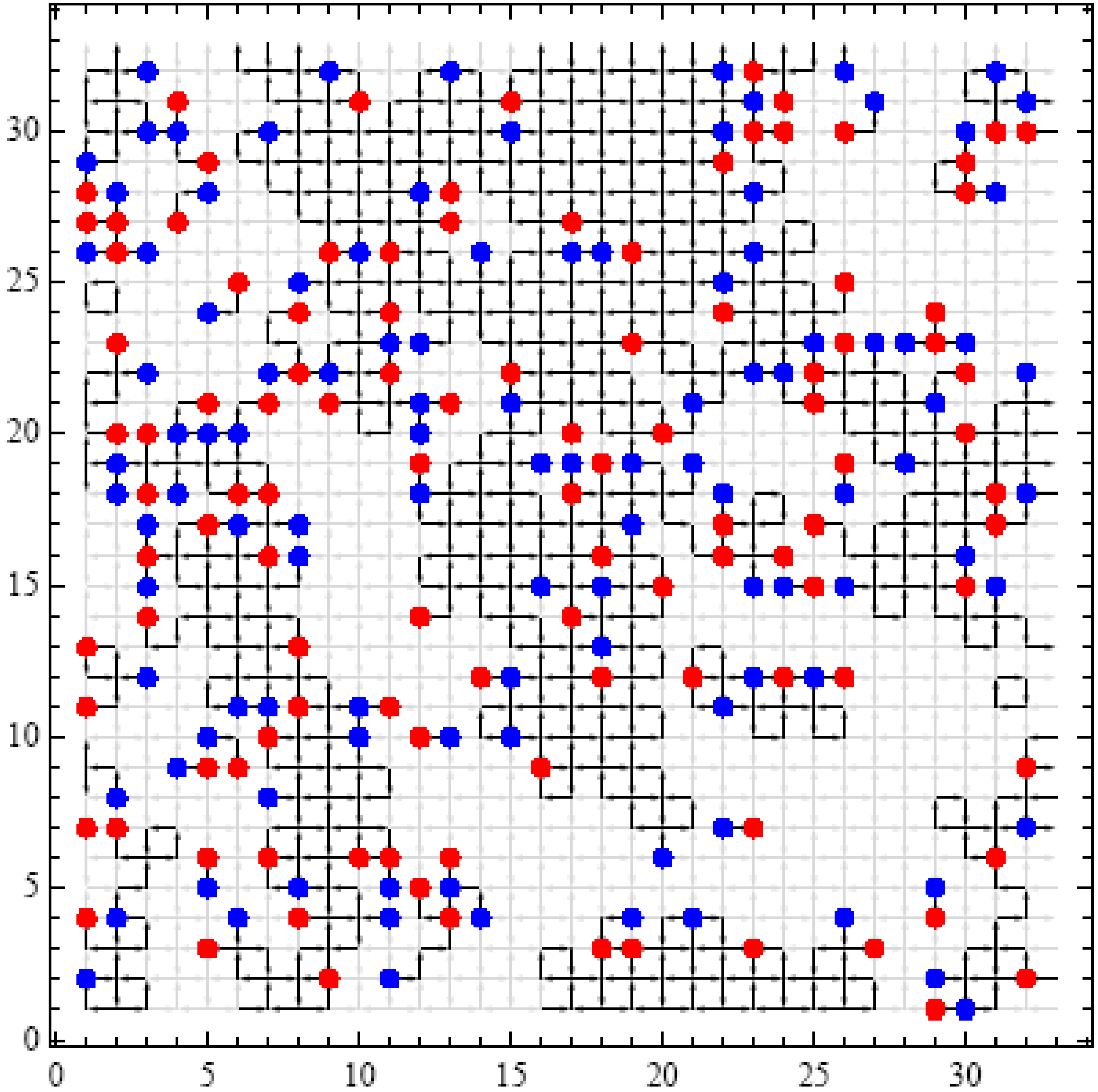


The figures show typical distributions of magnetic charges and string loops without charges (4O) for temperatures below $k_B T=7.2D$ (left for 6D) and above $k_B T=7.2D$ (right for 8D).

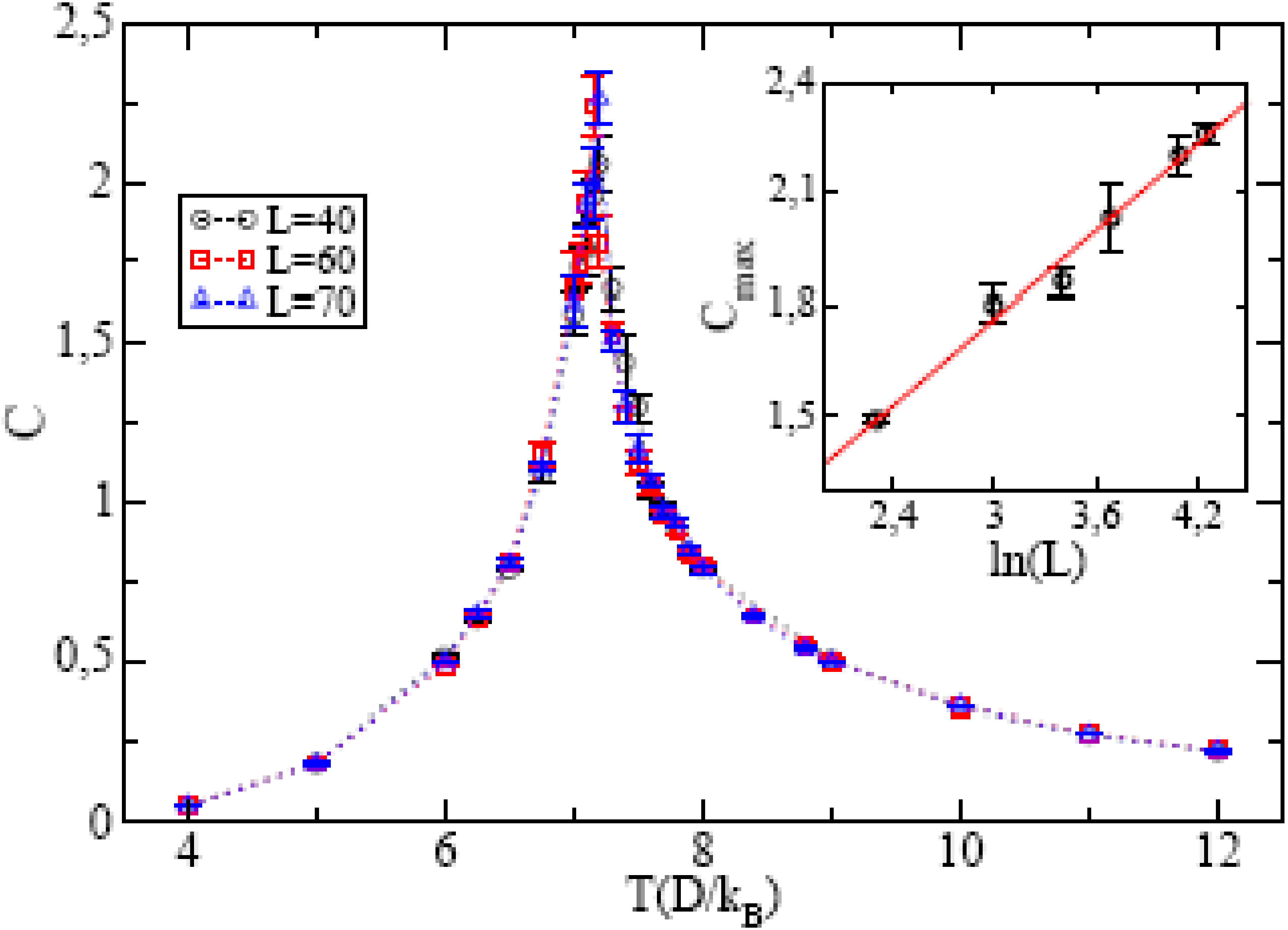




4O excitations may form clusters at low temperature that percolate the array at the critical temperature, justifying thus the increasing number of these excitations at $k_B T=7.2D$.

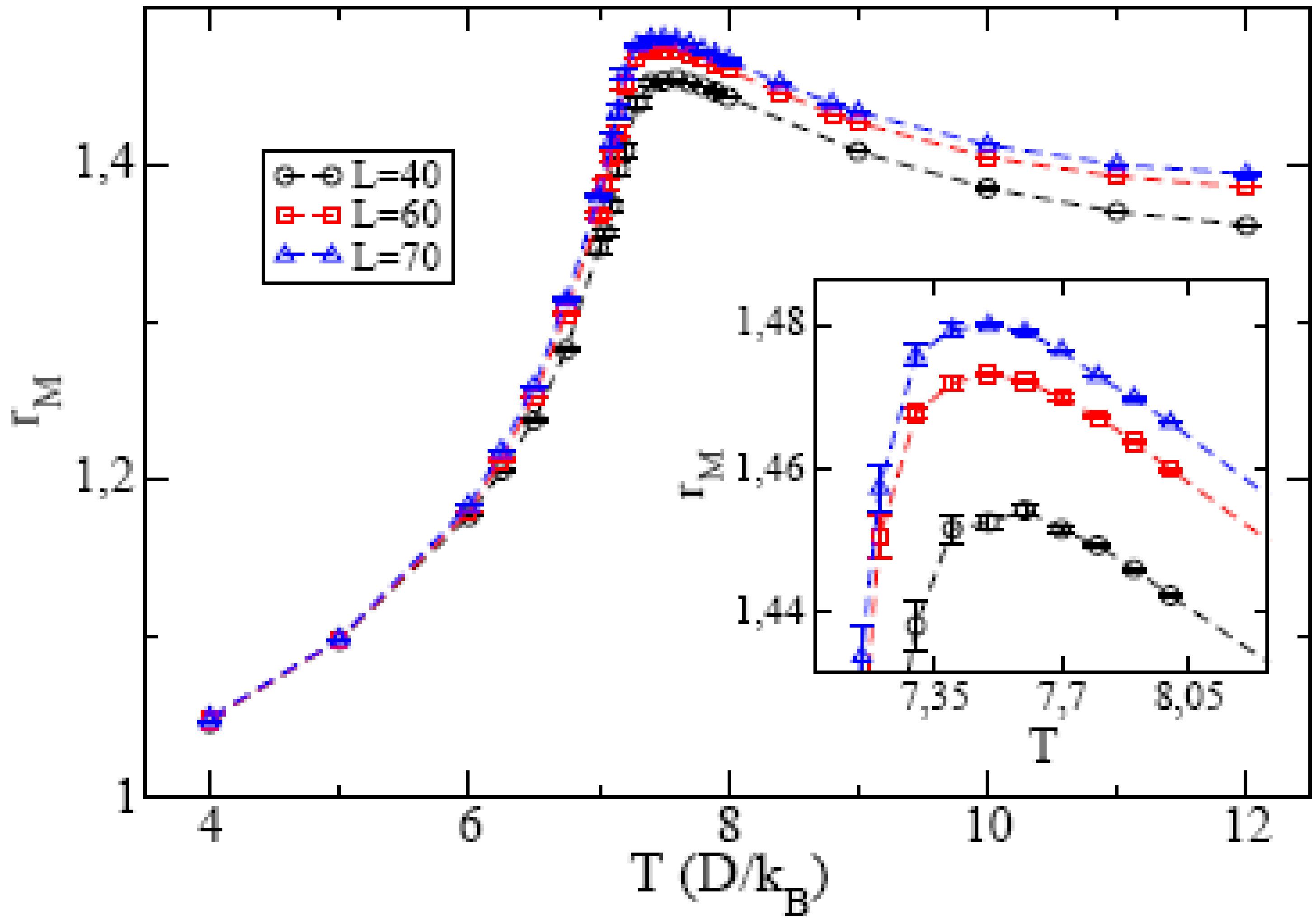


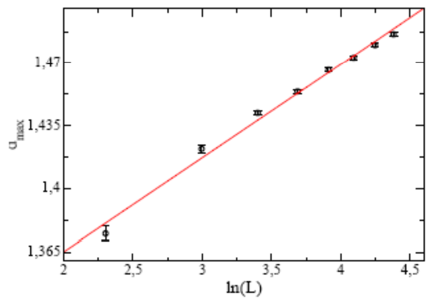
2. Specific heat. It presents a sharp peak around $k_BT=7.2D$. The peak increases logarithmically with the system size.



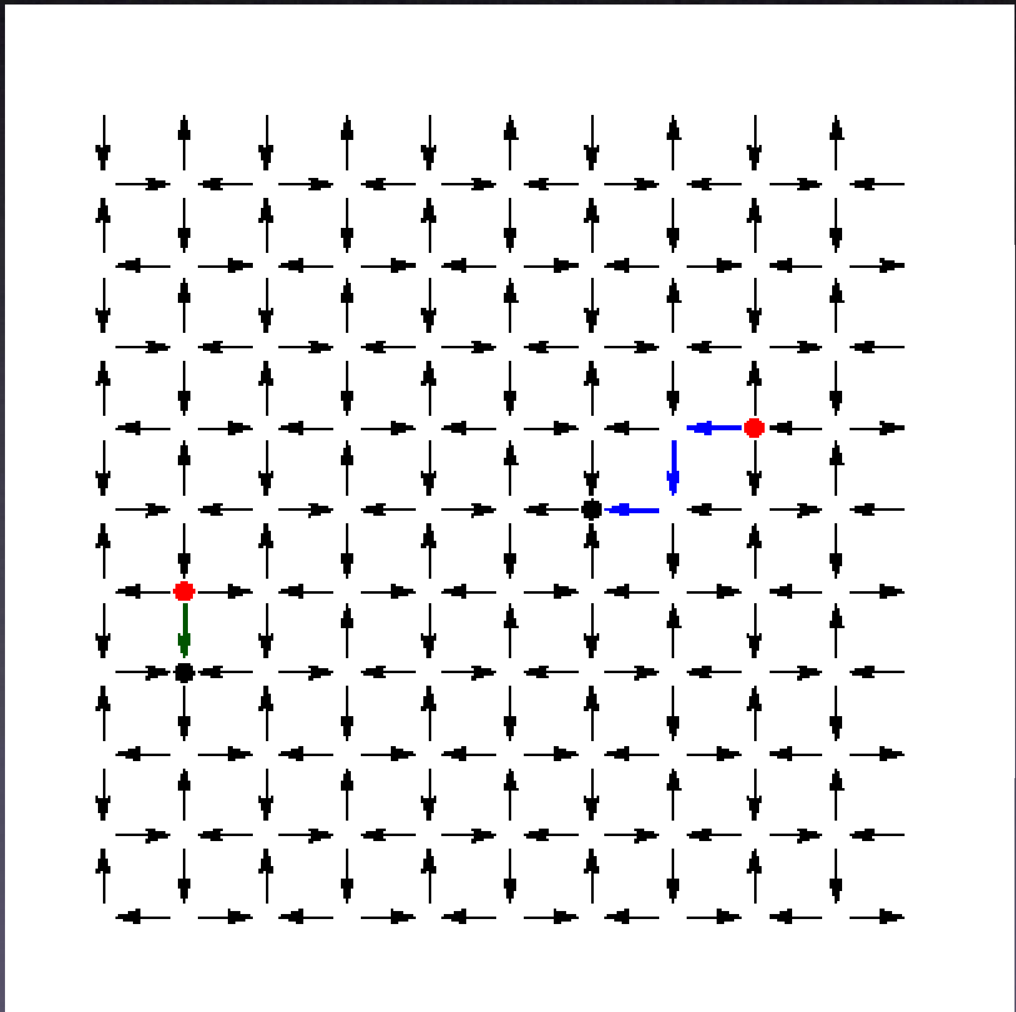
Average distance between monopoles and antimonopoles.

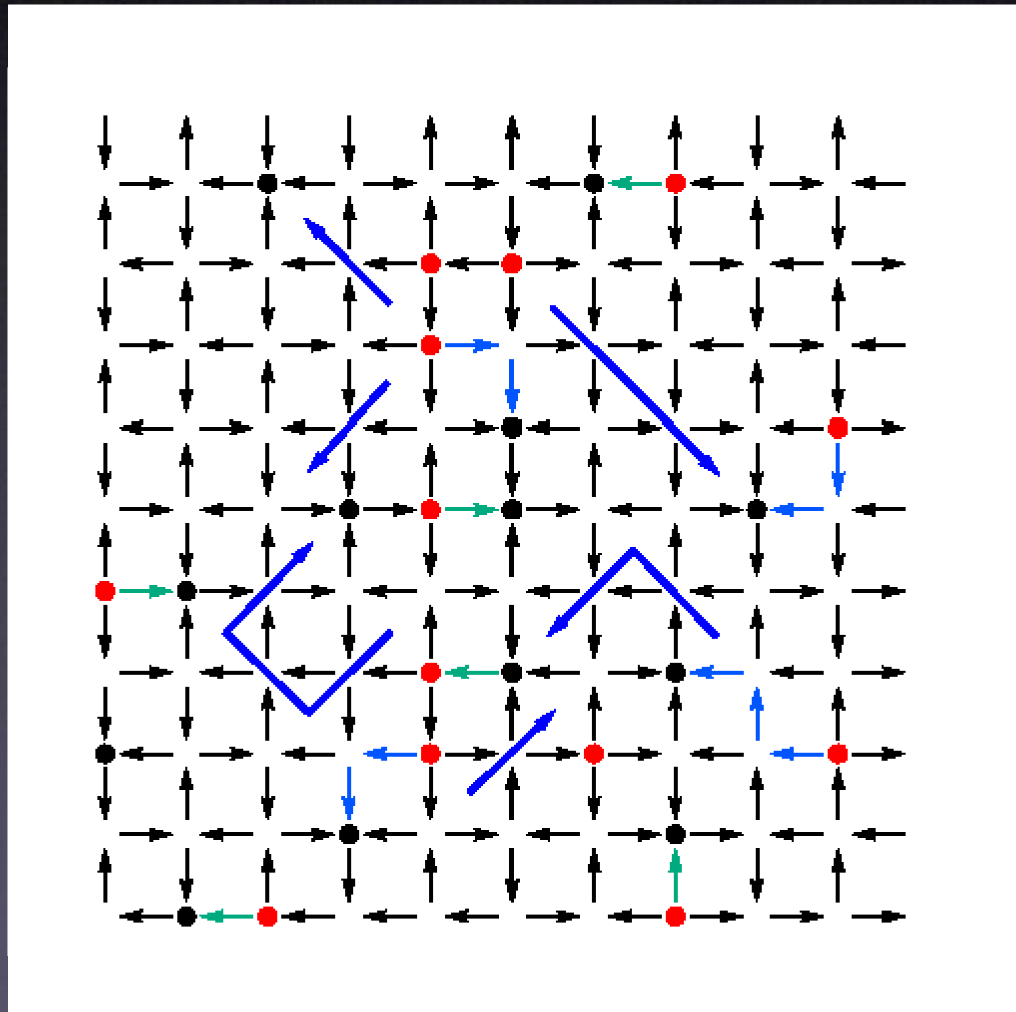
It presents a maximum at a temperature around *$k_BT=7.2D$* (i.e., at the same temperature in which the specific heat exhibits a peak). In addition, the height of the maximum also increases **logarithmically with *L***.





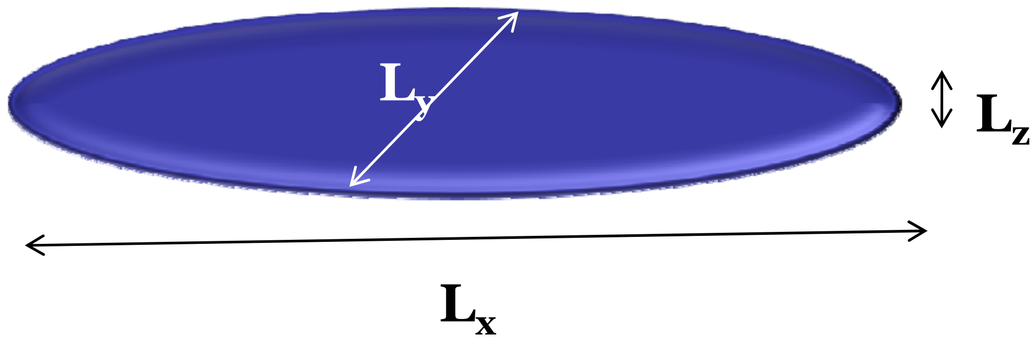
Typical configurations of charges for temperatures below (left) and above (right) $k_B T=7.2D$. Since the average distance between opposite charges diverges in the thermodynamic limit, we expect completely isolated charges for infinite systems. For viable compounds at temperatures above $k_B T=7.2D$ we observe some charges without strings and pieces of strings without charges disperse around the array.

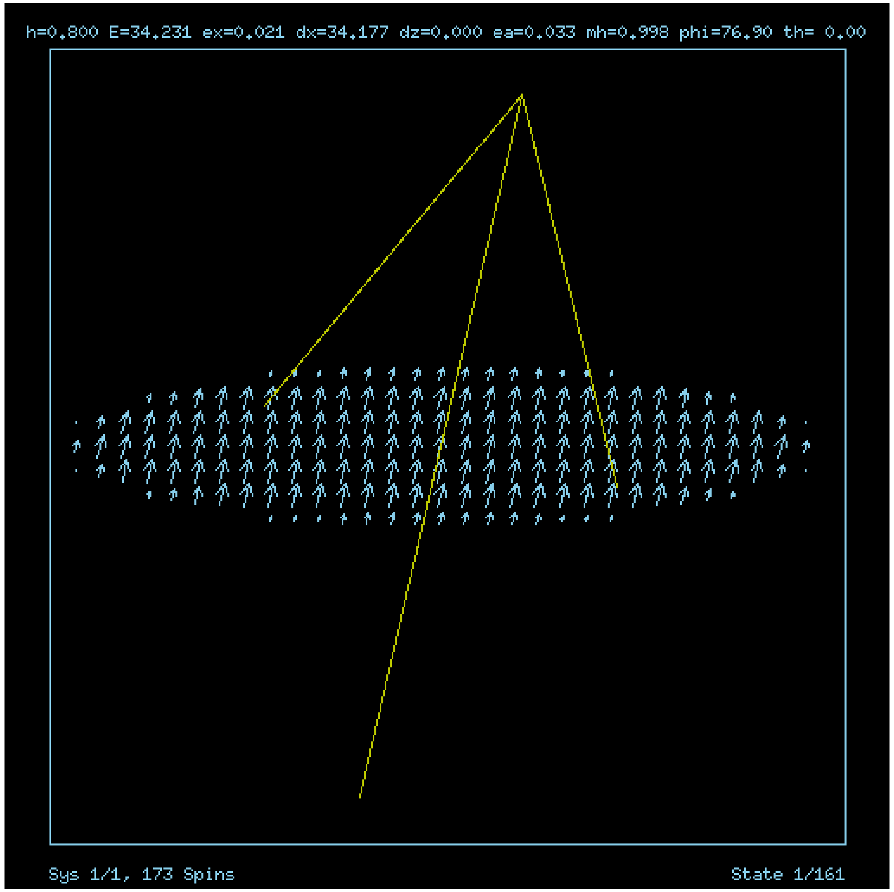




The point-like dipoles used for studying the thermodynamics is only an approximation. We are now considering the internal structure of the islands.

The typical islands have Lz much less than Lx or Ly.





1. The idea of an Ising spin for a particle is replaced by a 3d magnetic moment , moving in some anisotropic potential, but free to point in any direction, if enough energy becomes available to it .

2. This type of potential is continuous, in contrast to the two-state Ising particle, having a well-defined energy barrier .

3. We find that for high aspect ratio (Lx >> Ly) ellipses, an uniform rotation model is very useful.

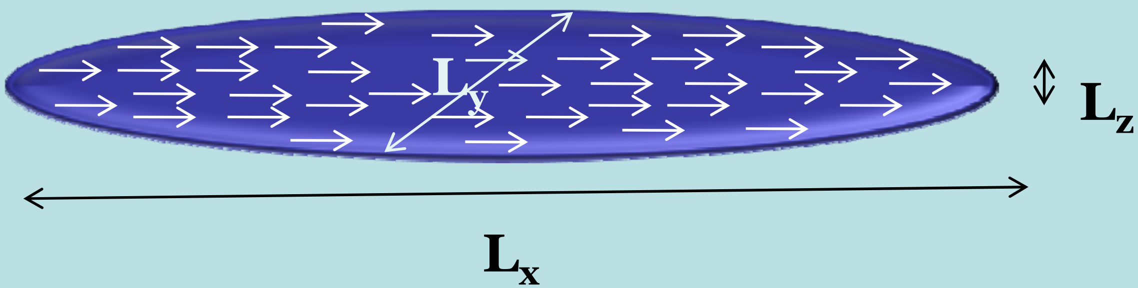
For a particle whose hard axis is along z and easy axis along x, an effective potential that approximately represents the energies is shown to be

$$E = E_0 + K_1\left[1 - (\hat{\mu}\cdot\hat{x})^2\right] + K_3(\hat{\mu}\cdot\hat{z})^2$$

where **μ** is the unit vector pointing in the direction of the particle's net magnetic moment.

1. **We considered thin elliptical particles with thicknesses g3 = Lx/Lz = 20, and aspect ratios g1 = Lx/Ly = 3, 5 and 8.**

2. **The lengths ranged from 120 nm to 480 nm.**



Magnetic anisotropy of elongated thin nano-islands

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(Dated: December 2, 2011)

The energetics of thin elongated ferromagnetic nano-islands is considered for some different shapes, aspect ratios, and applied magnetic field directions. These nano-island particles are important for artificial spin-ice materials. For low temperature, the magnetic internal energy of an individual particle is evaluated numerically as a function of the direction of a particle's net magnetization. This leads to estimations of effective anisotropy constants for (1) the easy axis along the particle's long direction, and (2) the hard axis along the particle's thin direction. A spin relaxation algorithm together with fast Fourier transform for the demagnetization field is used to solve the micromagnetics problem for a thin system. The magnetic hysteresis is also found. The results indicate some possibilities for controlling the equilibrium and dynamics in spin-ice materials by using different island geometries.

PACS numbers: 75.75.+a, 85.70.Ay, 75.10.Hk, 75.40.Mg
Keywords: magnetic anisotropy, magnetic hysteresis, micromagnetics, spin-ice, effective potential.

I. INTRODUCTION: ELONGATED THIN NANO-ISLANDS

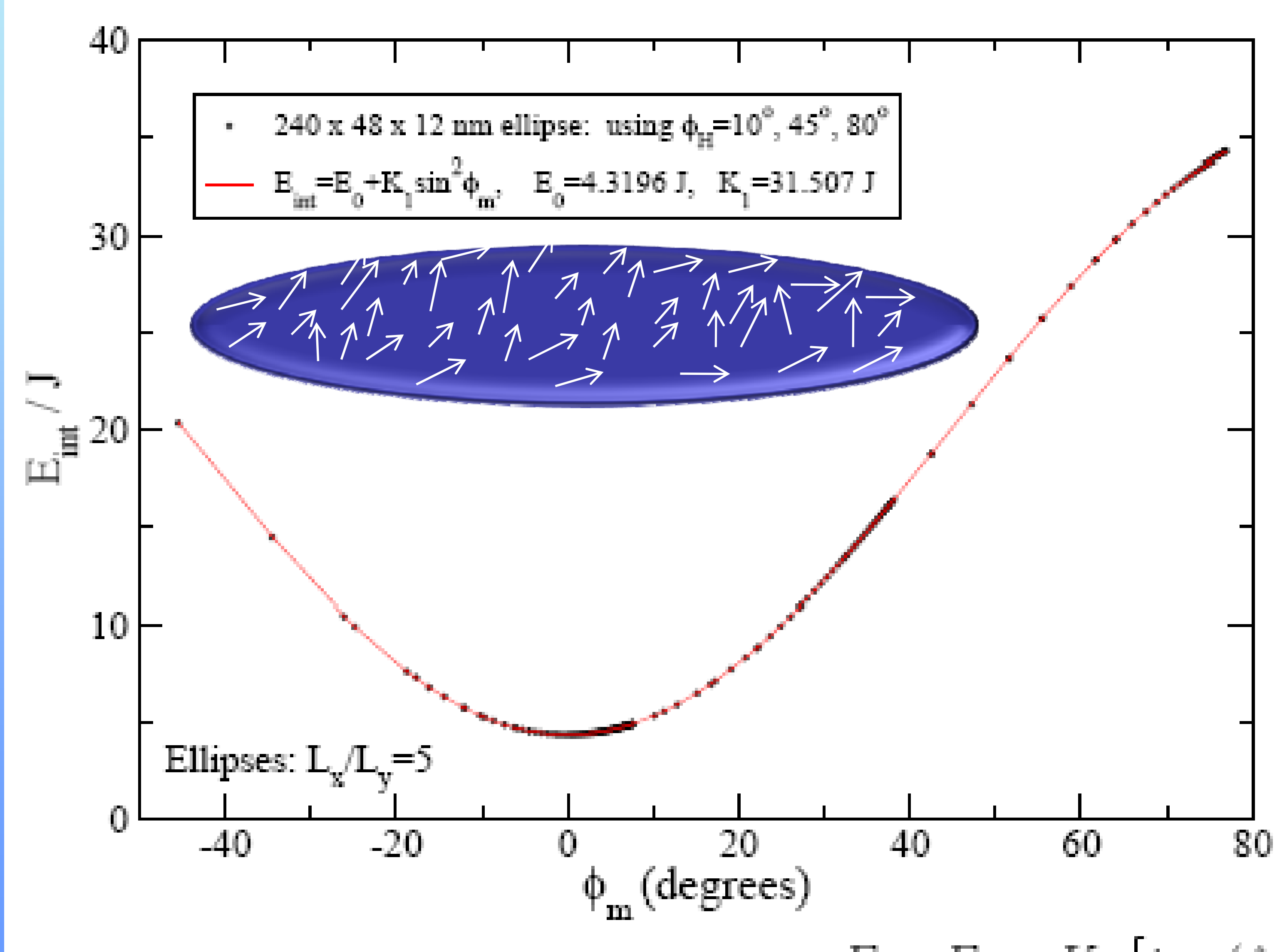
Disordered and frustrated magnetic states such as those present in artificial spin ices[1,2] continue to draw interest, due to their competing ground states, magnetic monopole excitations[3], string excitations[4–7] and the difficulty to achieve thermal equilibrium. Those systems are composed from elongated magnetic islands or particles of some length L_x (several hundred nanometers) and width L_y grown or etched lithographically to a small height L_z on a substrate, whose geometric demagnetization effects (effectively, internal dipolar interactions) lead to a strong magnetic anisotropy. The typical islands have L_z much less than L_x or L_y. Obviously any very thin magnet acquires an effective easy-plane anisotropy[8], and if the particle is narrow as well, the long direction becomes an easy axis. The demagnetization field within an individual particle is responsible for this, making the plane of the island (xy-plane) an easy plane, and the x-axis an easy axis. Then net magnetic moment $\vec{\mu}$ acts somewhat like an Ising variable with a defined easy axis $\hat{x}$. These islands are arranged into ordered arrays to produce, for example, square lattice or kagome lattice artificial spin-ices. The analysis of spin ice models assumes that such particles have only the two states with $\vec{\mu}$ either aligned or anti-aligned to the particle's easy axis. The dipolar interaction between different particles on one of the spin-ice lattices leads to the ice-rules, such as the "two in / two out" rule for the square lattice and pyrochlore spin ices[3]. Such ice rules are only energetic *preferences*, however, and only indicate the preferred states of the magnetic moments. They are not absolute rigid statements about the allowed states. Thus, the intention here is to investigate the energetics of the fluctuations away from this Ising aligned state, in the individual elliptical islands that are used to compose a spin-ice system.

At some level, there must be transitions between these Ising-like states. An individual particle may contain thousands of atomic spins, leading to a substantial energy barrier that must be surpassed to flip the Ising state of a particle. Hence, the dynamics is greatly constrained by such energy barriers. It is our interest here to discuss how this barrier depends on the particular geometry of the islands, and make some evaluations of the dependence of the effective potential on the island shape and height. The types of shapes we consider are ellipses. Thin single domain ellipses were studied by Wei *et al.*[9], who found that the reversal process involves close to a uniform Stoner-Wohlfarth rotation, but with reduced energy barriers due to some non-uniformity of the magnetization. However, we find here that for high-aspect ratio ellipses, this non-uniformity is minimal and a uniform rotation model could be very useful.

Although the theory for spin ice has been developed for Ising-like magnetic moments, their dynamics requires a different model. In reality, the underlying magnetic moment must be evolving from much more complex dynamics. The reversal of an individual island, in the dipolar fields of its surrounding islands, must be a complex process, and could involve the motion of domain walls and vortices within the individual particles, or an impeded rotation of the local magnetization mostly in unison. But in the assumption of strong ferromagnetic exchange inside a particular particle, and a uniform externally applied field, one can investigate the reversal process using different approaches to the micromagnetics[10], and see whether vortices or domain walls play any significant role. Especially, one can investigate whether there are intermediate metastable vortex or domain-wall states as steps of the reversal. To a great extent for the thin elliptical particles considered here, the reversal proceeds mostly as a nearly

Some typical results for the internal energy curves are shown below for the in-plane potential of an elliptical particle with g1 = Lx/Lz= 5, with major axis 240 nm, minor axis 48 nm and thickness 12 nm. The potentials for in-plane motion of μ fit very well to the functional form,

$$E_{\text{int}}(\phi_m) = E_0 + K_1 \sin^2 \phi_m.$$



The angle ϕ_m is the direction of the net particle moment $\boldsymbol{\mu}$ in the easy plane.

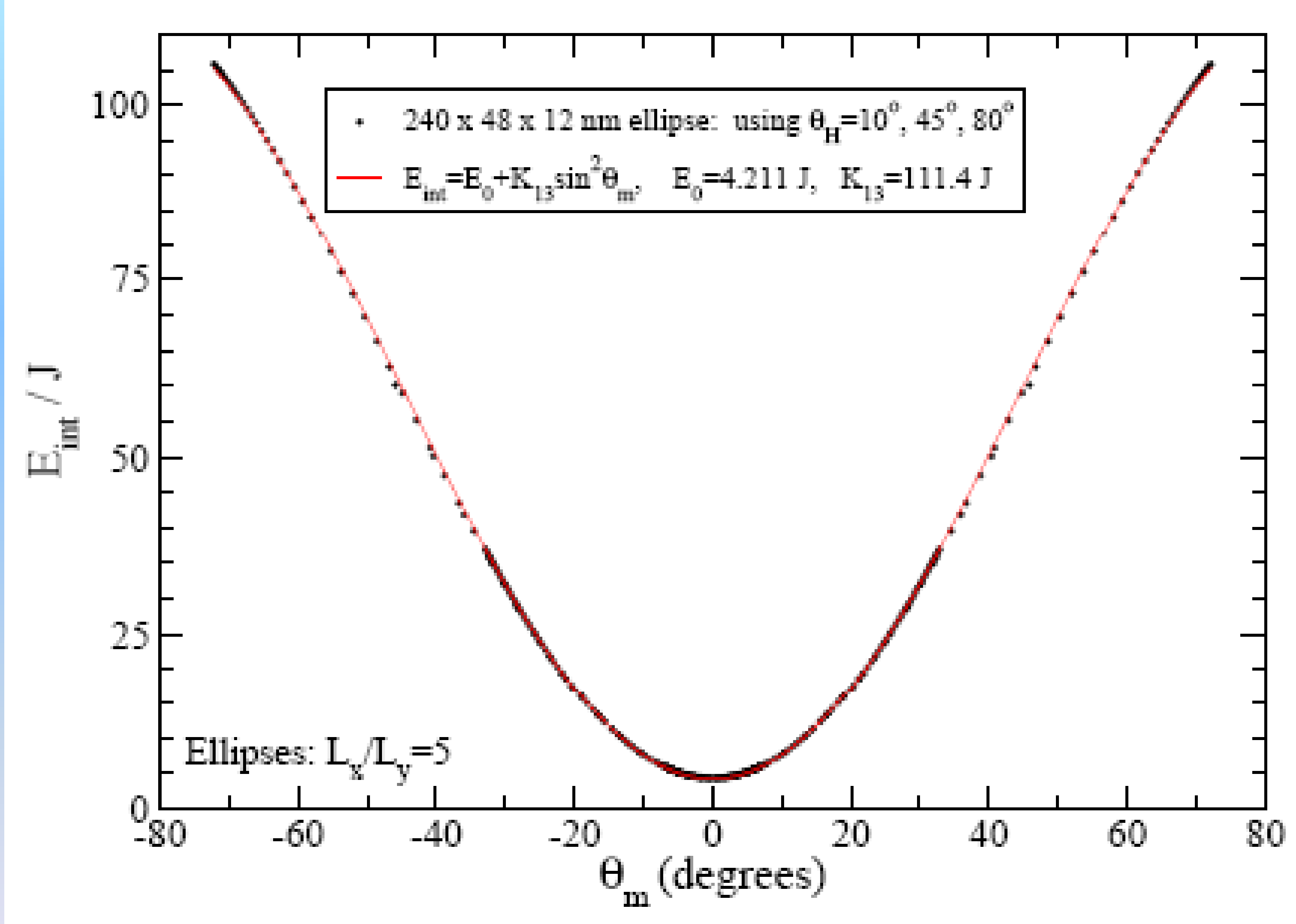
The points come from the simulations at the different angles ϕ_H of the applied field from the long axis; all fall onto the same curve.

The fit gives a reliable estimate of anisotropy constant K_1

$$-K_1(\hat{\mu}\cdot\hat{x})^2$$

$$E = E_0 + K_1\left[1-(\hat{\mu}\cdot\hat{x})^2\right] + K_3(\hat{\mu}\cdot\hat{z})^2$$

The out-of-plane potential for the same elliptical particle (g1 = Lx/Lz= 5, with major axis 240 nm, minor axis 48 nm and thickness 12 nm). The points from simulations at different angles θ_H of the applied field are combined into one curve.



The angle θ_m is the tilting of the net particle moment $\boldsymbol{\mu}$ out of the easy plane.

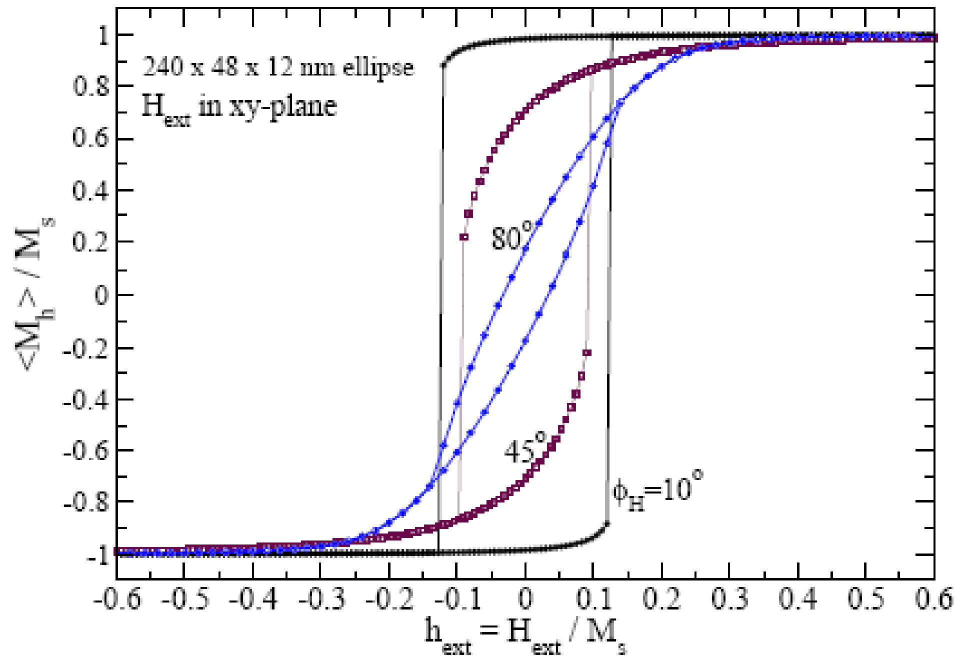
The fit gives a reliable estimate of anisotropy constant for the hard axis K_3

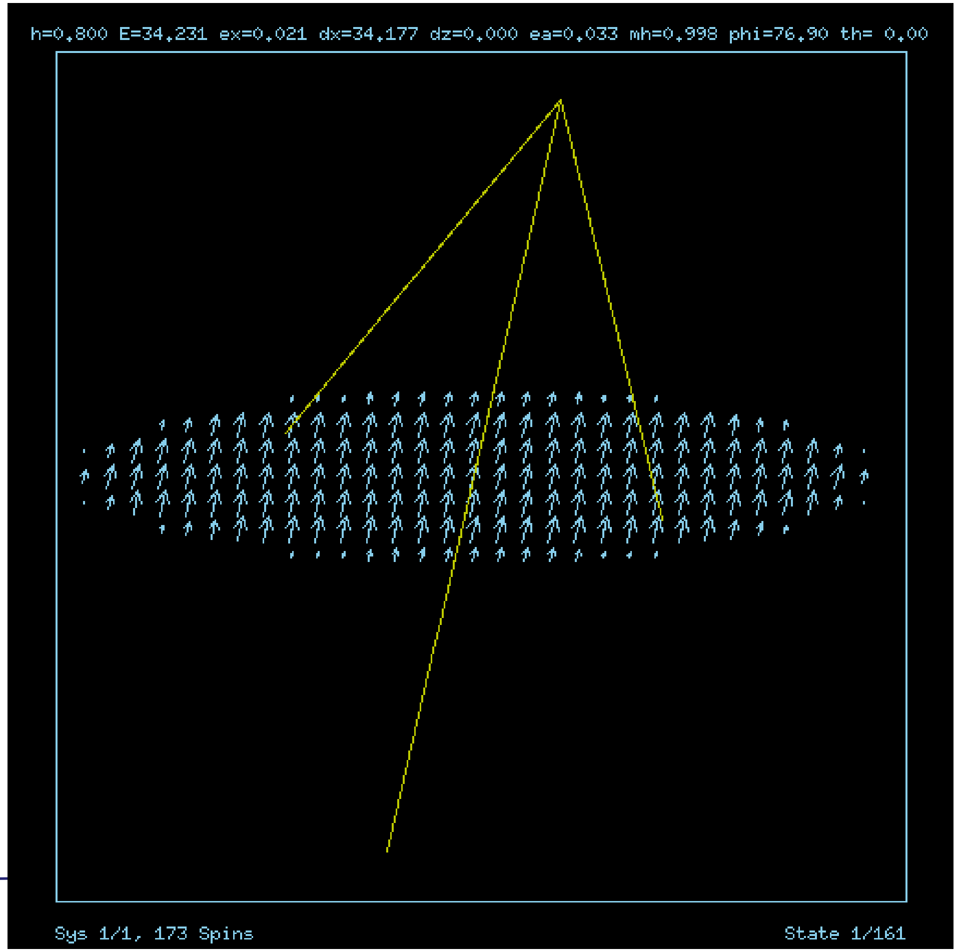
$$K_3(\hat{\mu} \cdot \hat{z})^2$$

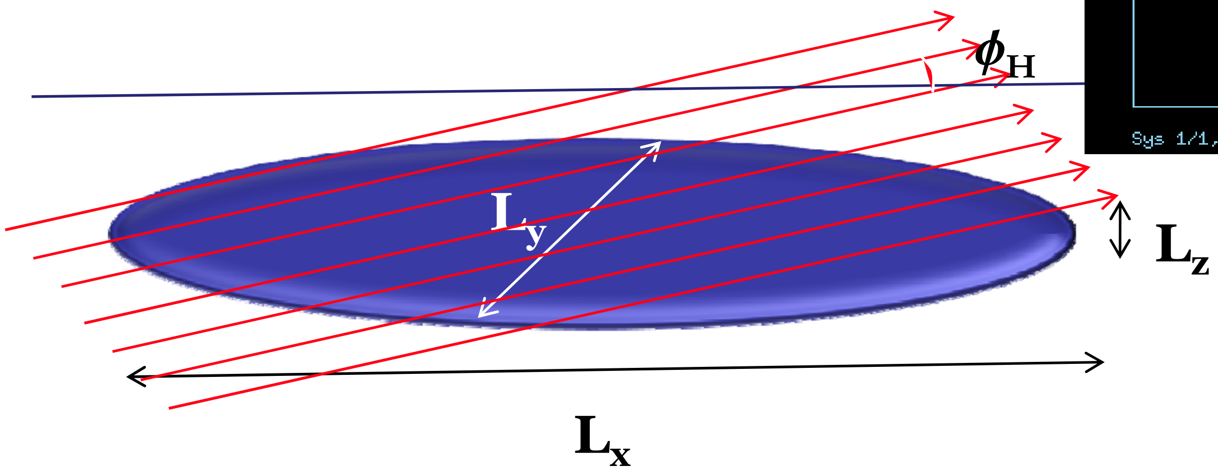
$$E = E_0 + K_1 \left[1 - (\hat{\mu} \cdot \hat{x})^2\right] + K_3(\hat{\mu} \cdot \hat{z})^2$$

$$E_{\text{int}}(\theta_m) = E_0 + (K_1 + K_3)\sin^2\theta_m .$$

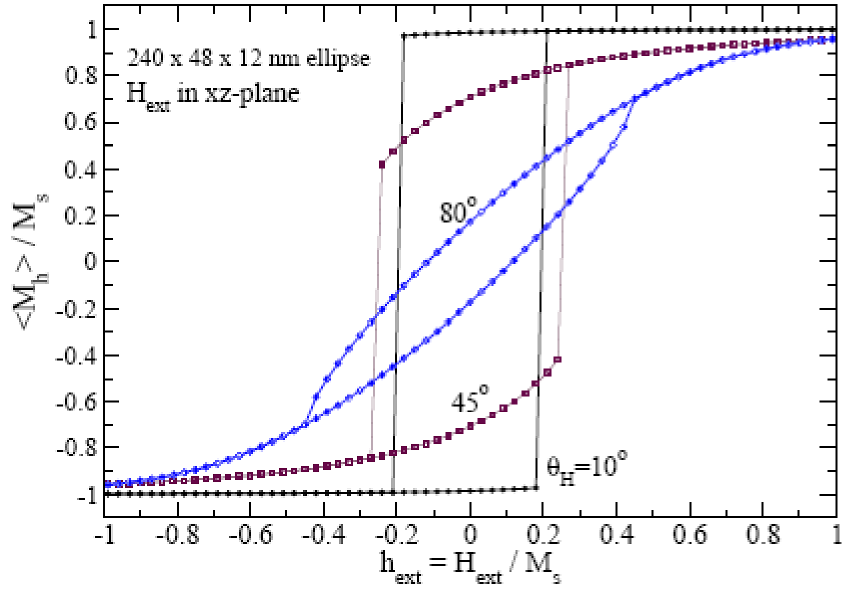
Hysteresis loops for an elliptical particle with an in-plane applied field at the indicated angles ϕ_H to the long axis of the particle.

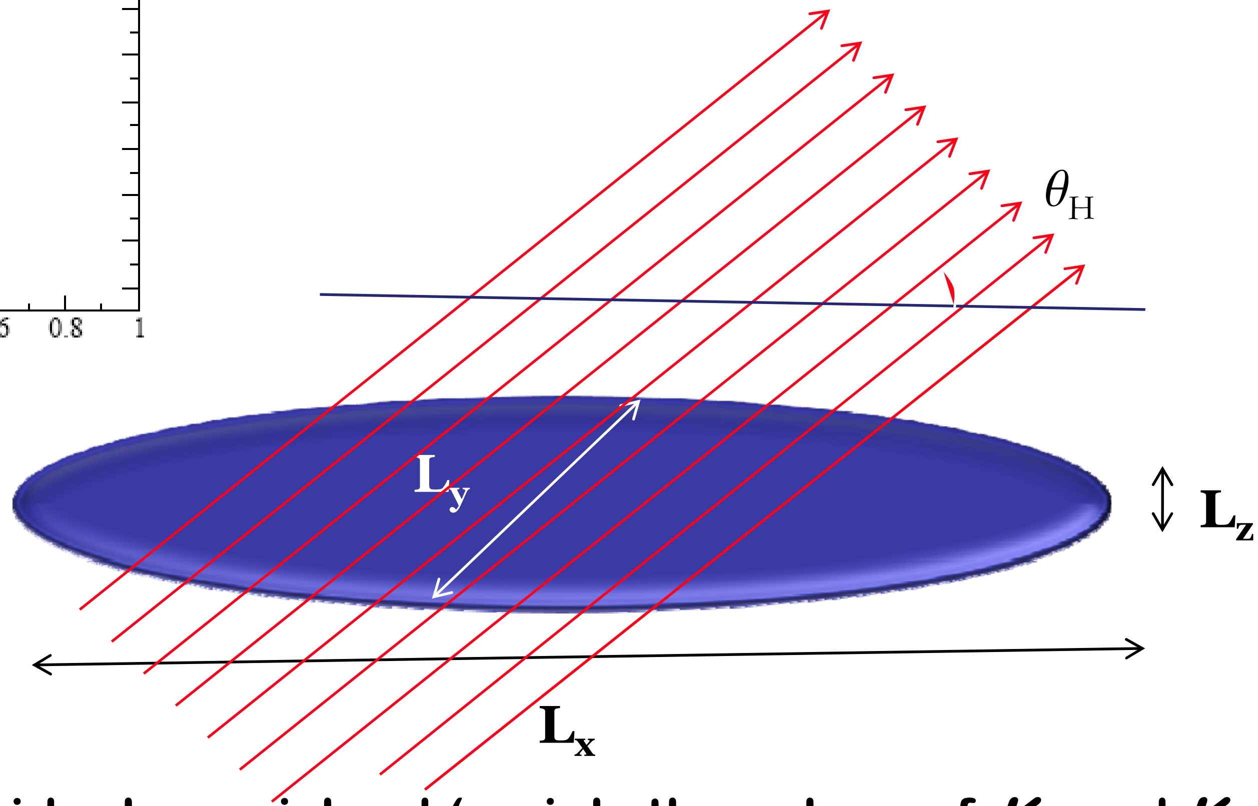






Hysteresis loops for an elliptical particle with the applied field tilted out of the xy-plane at the indicated angles θ_H from the long axis of the particle.



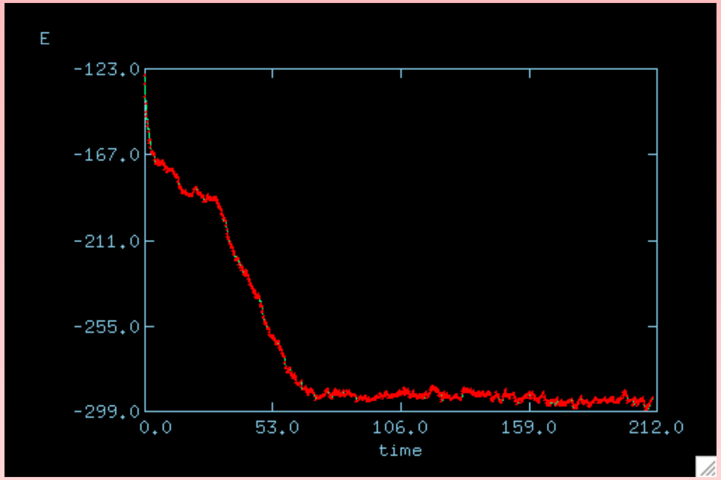


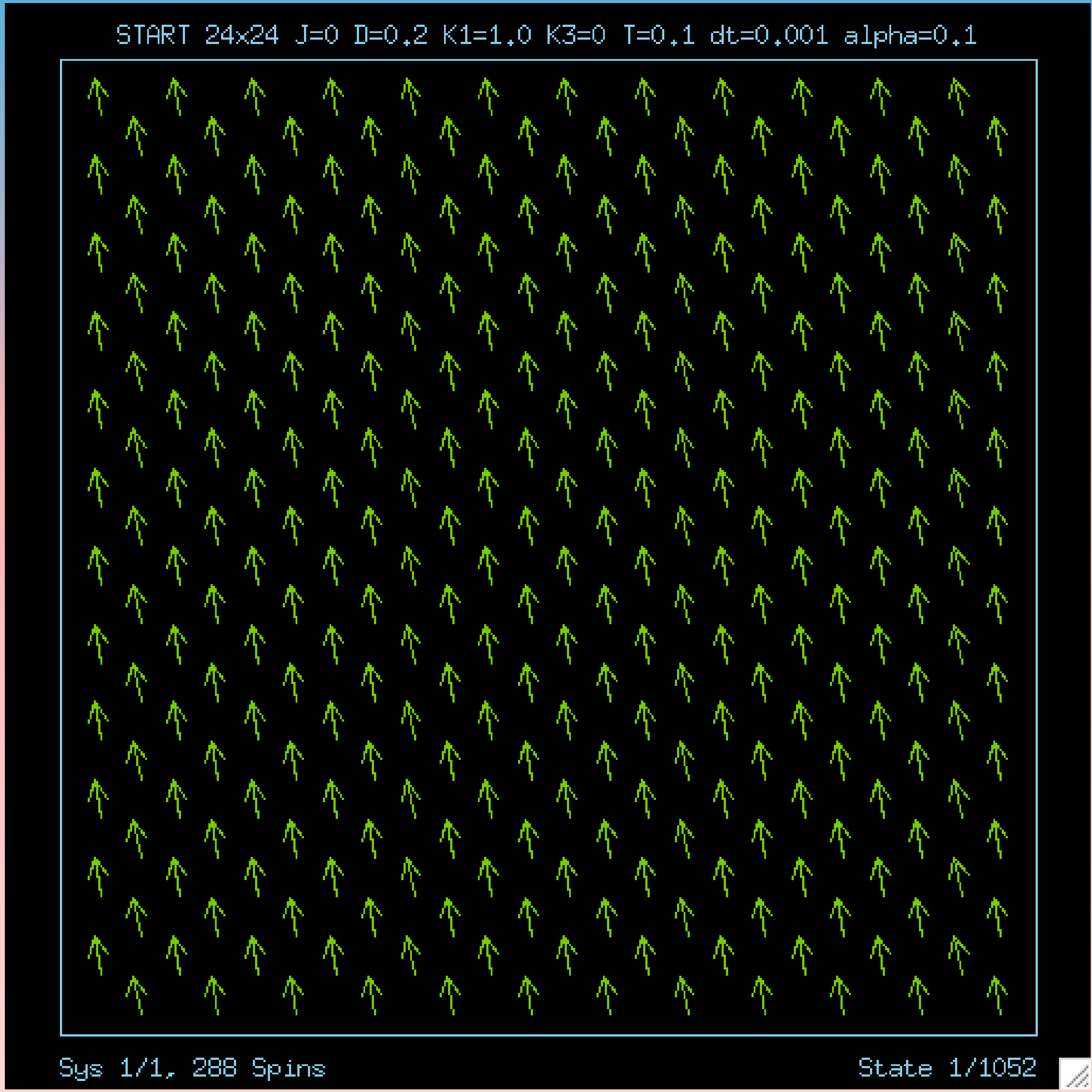
With these results for an individual nanoisland (mainly the values of K_1 and K_3) we study now the dynamics of artificial spin ices (in square and kagome lattices) at finite temperatures. We have only preliminary calculations…

These are only preliminary calculations. All simulations were performed with the following fictitious constants: J=0, K1=1, K3=0, D=0.2.

$k_B T=0.1=D/2$

It starts in an uniform state, relaxing…

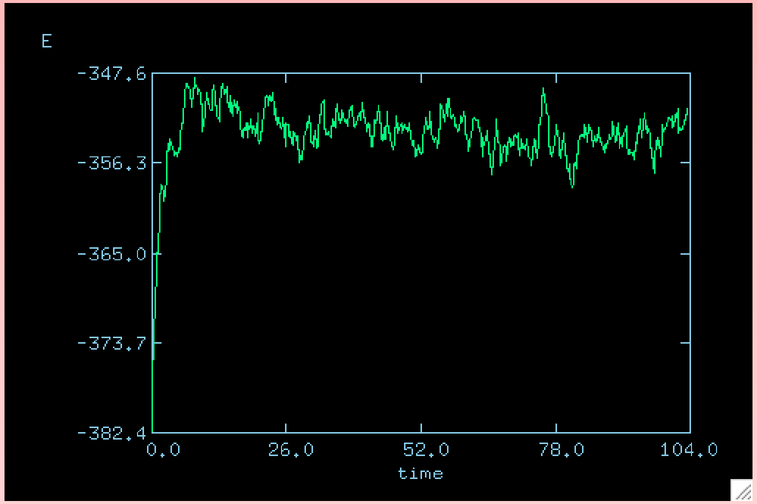


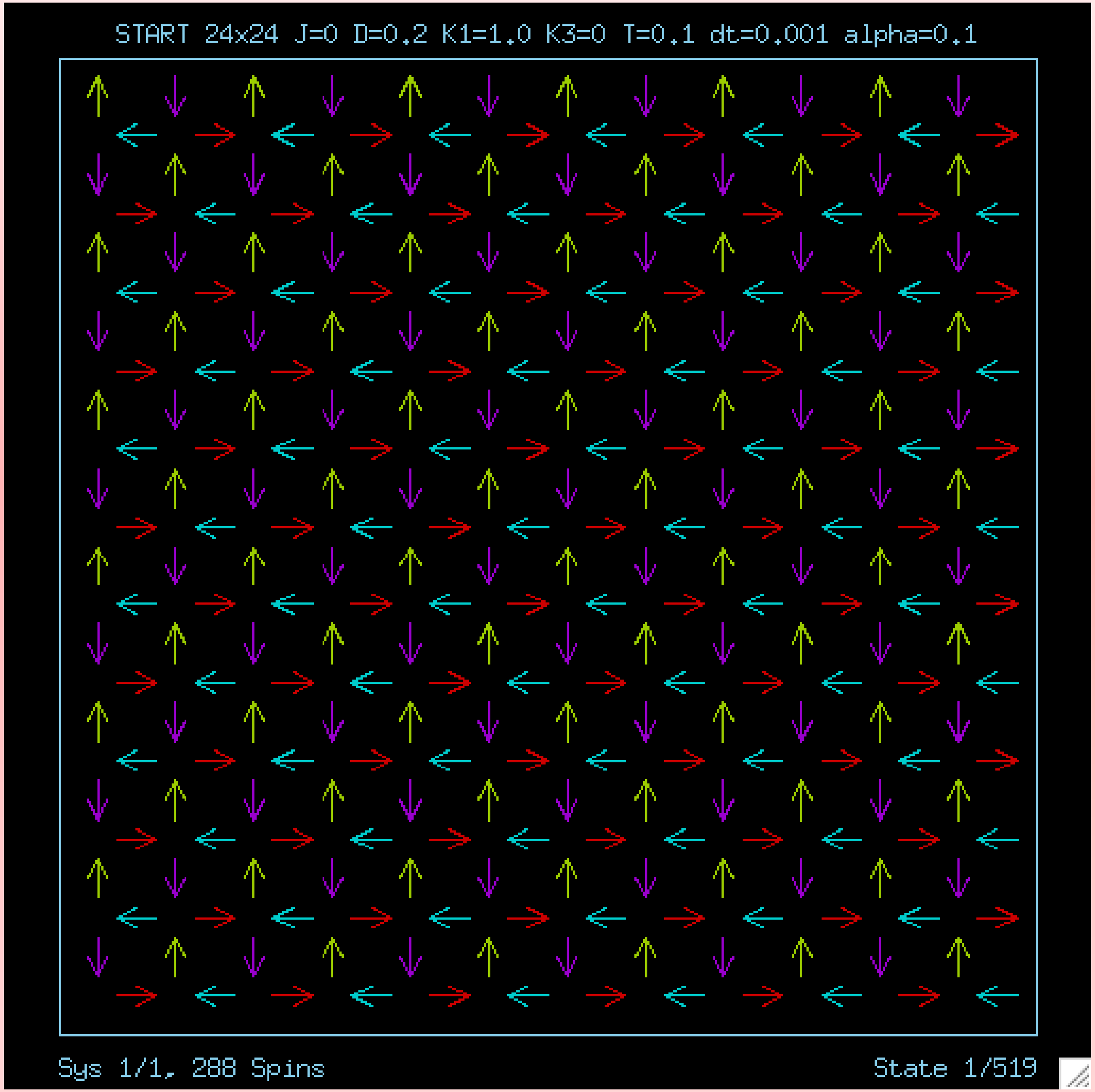


These are only preliminary calculations. All simulations were performed with the following fictitious constants: **J=0, K1=1, K3=0, D=0.2.**

$k_B T = 0.1 = D/2$

It starts in the ground state.





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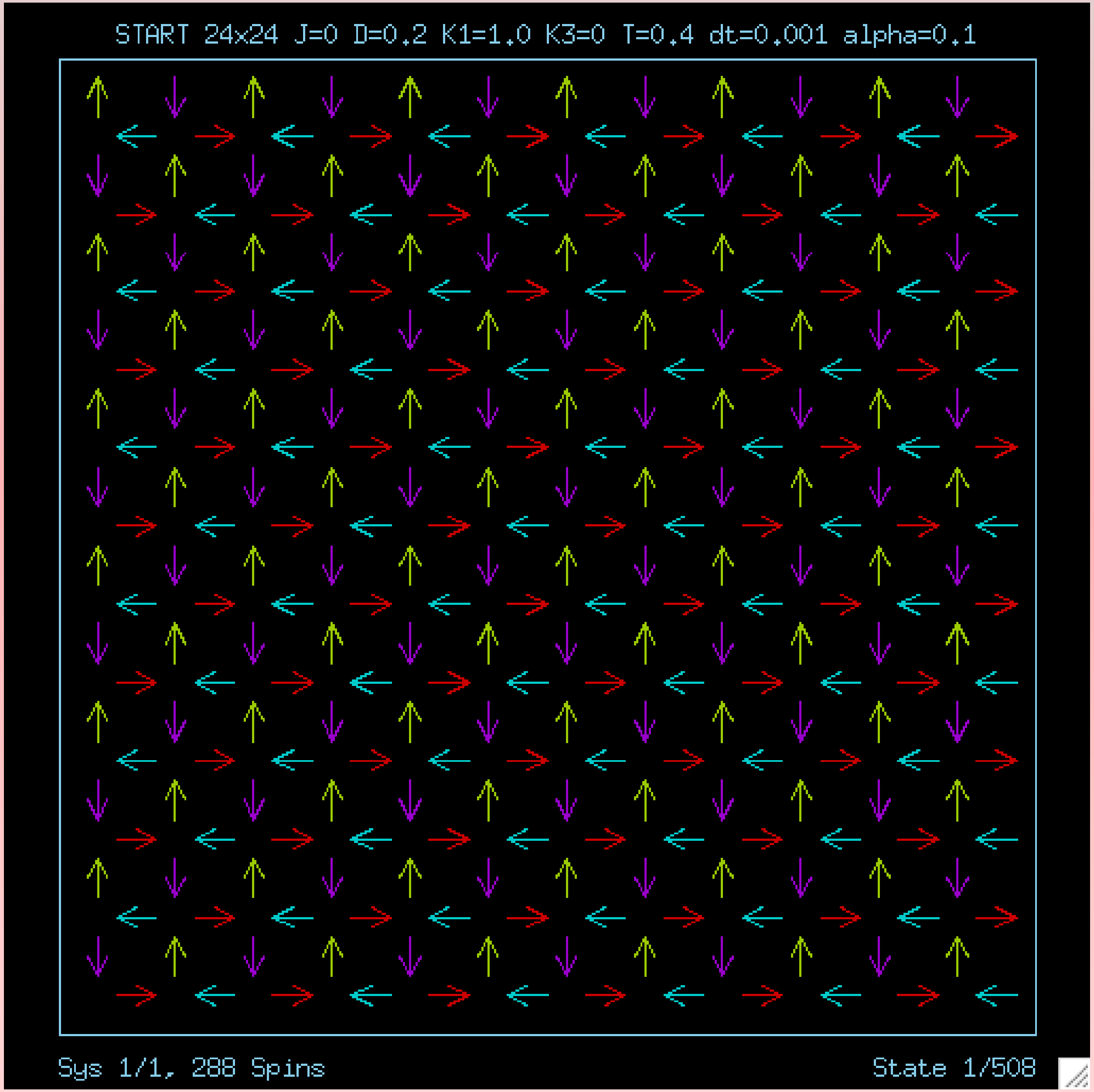
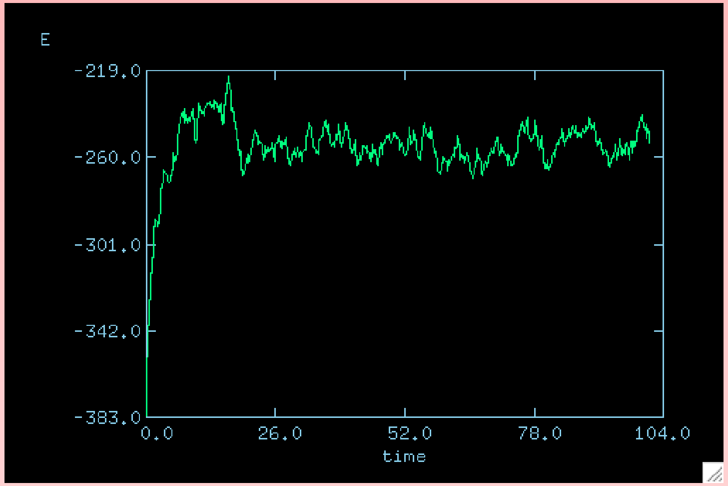


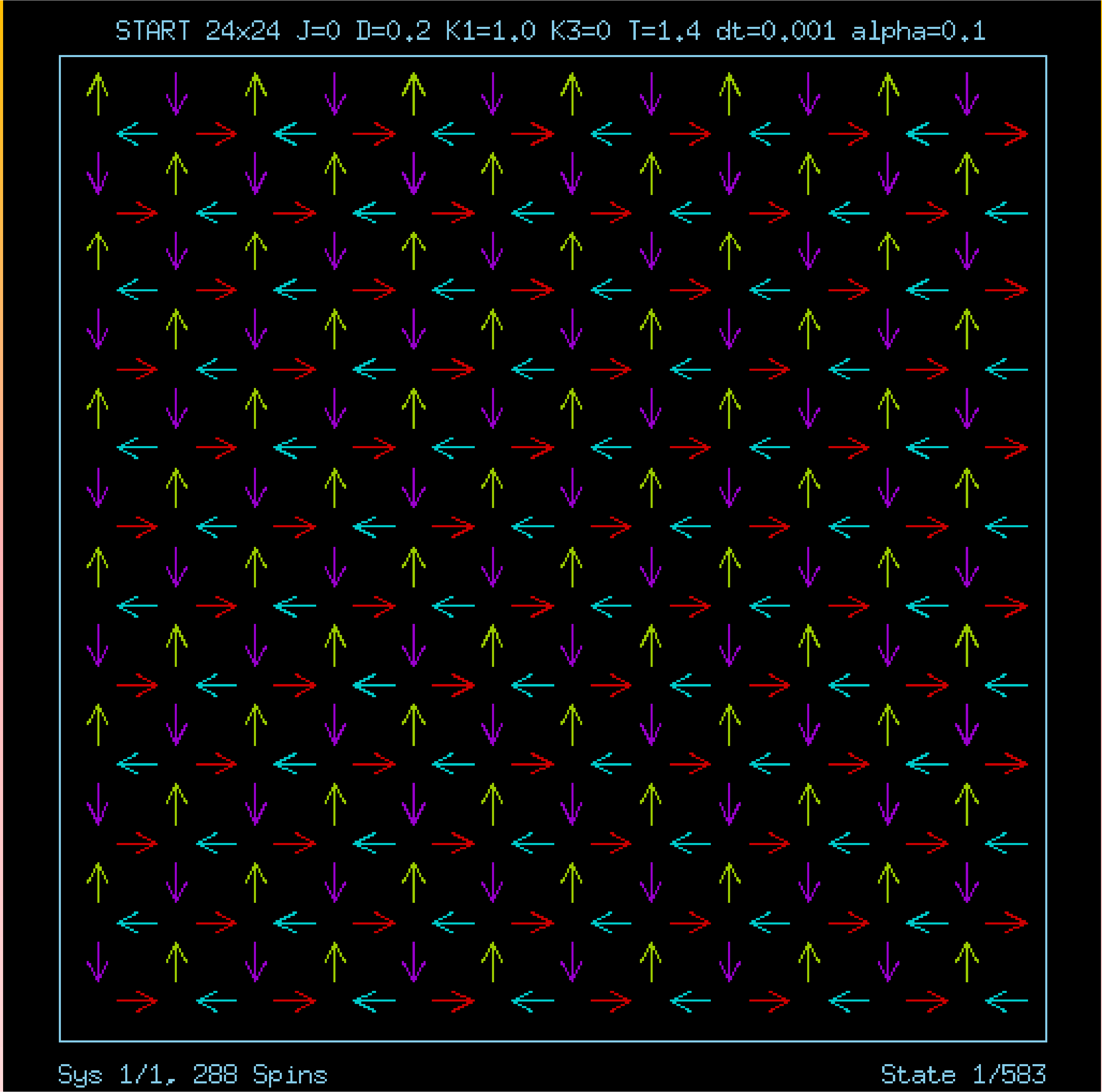
$k_B T$=0.4=2D

It starts in the ground state.



All simulations were performed with the following fictitious constants:

J=0, K1=1, K3=0, D=0.2.

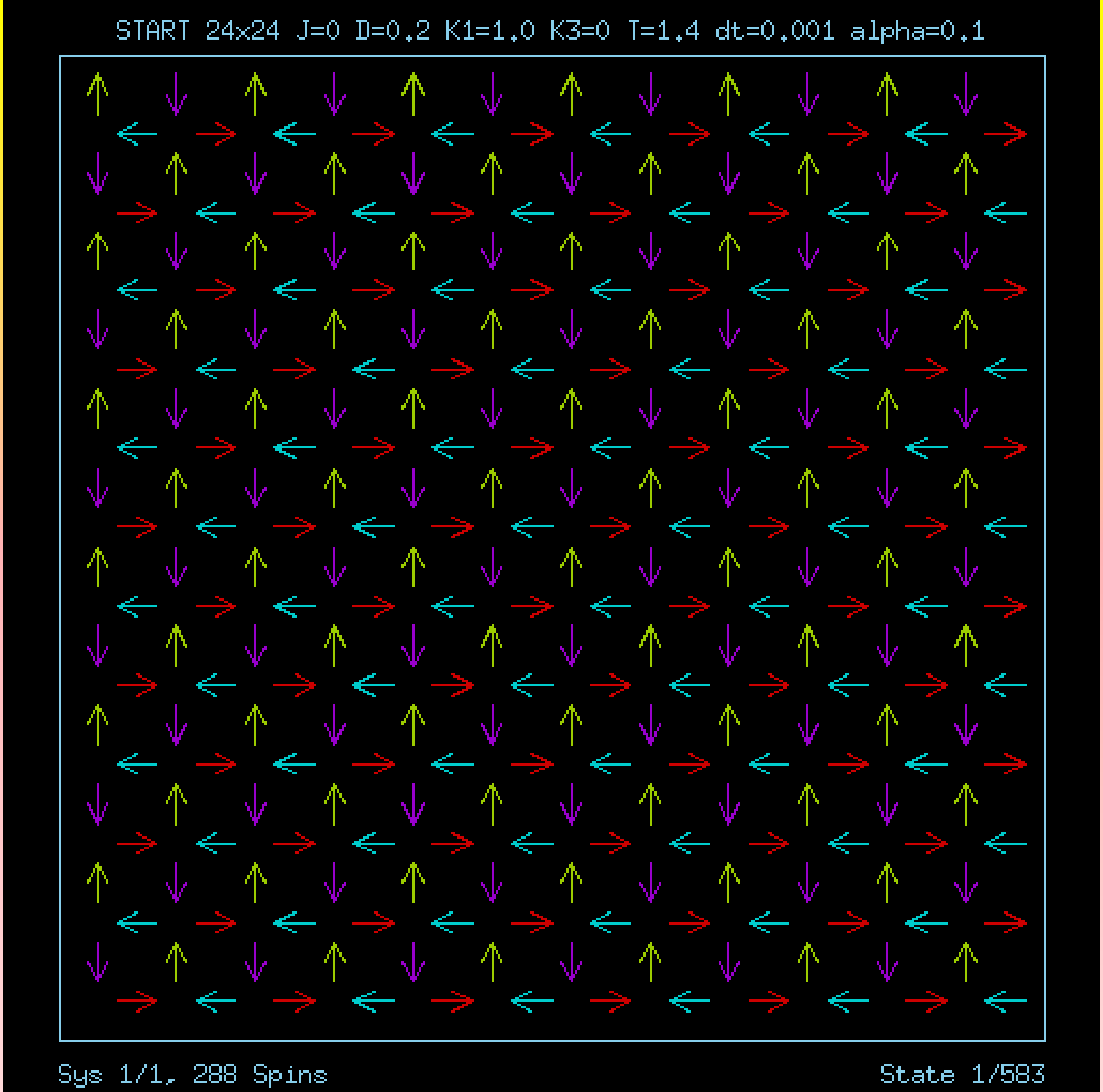


$k_B T = 1.4 = 7D$

It starts in the ground state.

Since the total magnetic moment of the islands has more degrees of freedom, the temperature in which the specific heat exhibits a peak must be much smaller than 7.2D.

It also must depends on the island type: sizes, shapes etc. We are now investigating this possibility.



$k_B T=1.4=7D$

It starts in the ground state.

We would like to thank the Brazilian research agencies.

CNPq
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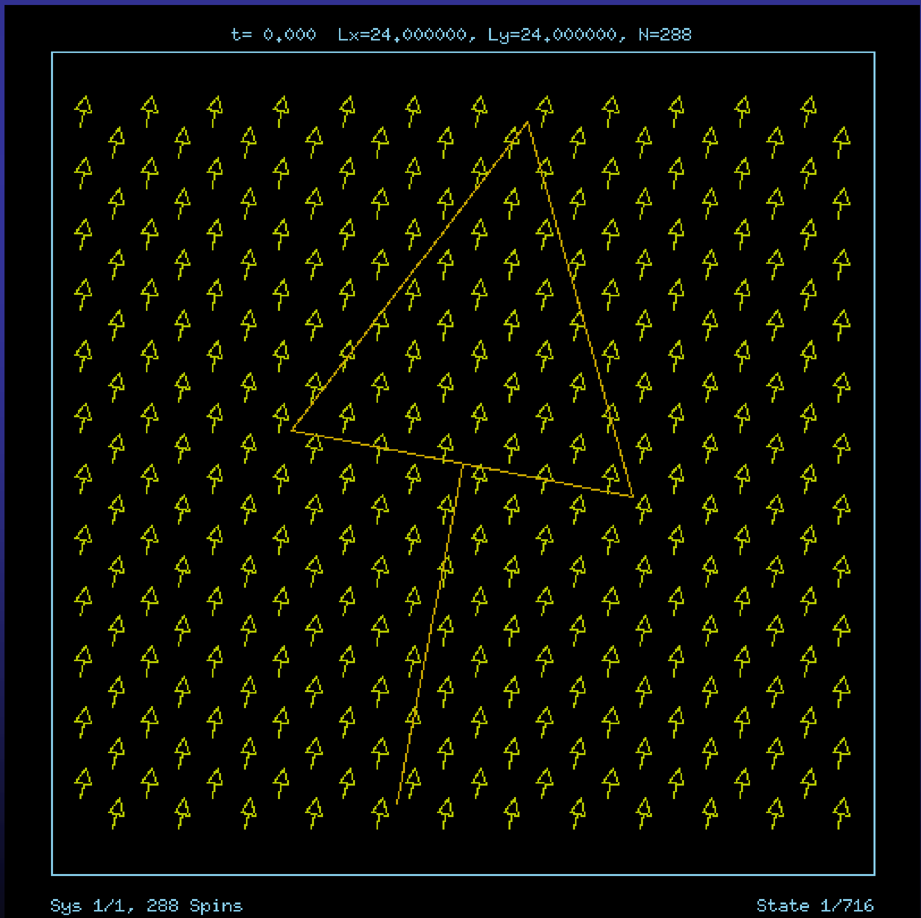

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