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Liashko, S. Y.; Uzdin, V. M.; Jónsson, H.

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Published in:
Journal of Physics: Conference Series

DOI:
[10.1088/1742-6596/741/1/012182](https://doi.org/10.1088/1742-6596/741/1/012182)

Published: 15/09/2016

Document Version
Publisher's PDF, also known as Version of record

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Please cite the original version:
Liashko, S. Y., Uzdin, V. M., & Jónsson, H. (2016). Rate of thermal transitions in kagome spin ice. *Journal of Physics: Conference Series*, 741(1), 1-5. [012182]. <https://doi.org/10.1088/1742-6596/741/1/012182>

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2016 J. Phys.: Conf. Ser. 741 012182

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Rate of thermal transitions in kagome spin ice

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Abstract. The rate of thermal transitions in a kagome spin ice element is calculated using harmonic transition state theory for magnetic systems. Each element consists of six prolate magnetic islands. Minimum energy paths on the multidimensional energy surface are found to estimate activation energy. Vibrational frequencies are also calculated to estimate the rate of the various transitions. An overall transition rate between equivalent ground states is calculated by using the stationary state approximation including all possible transition paths. The resulting transition rate is in a good agreement with experimentally measured lifetime.

1. Introduction

Artificial spin ice is a frustrated system of magnets with ground state entropy. Such systems are made to study various new physical effects such as magnetic monopoles [1], temperature induced disordering (melting) [2] and new kinds of thermodynamic phase transitions [3]. In particular, experimental measurements of temperature induced magnetic switching [4] with timescale ranging from days to seconds depending on temperatures have been made for kagome spin ice. This research is dedicated to theoretical study of such transitions.

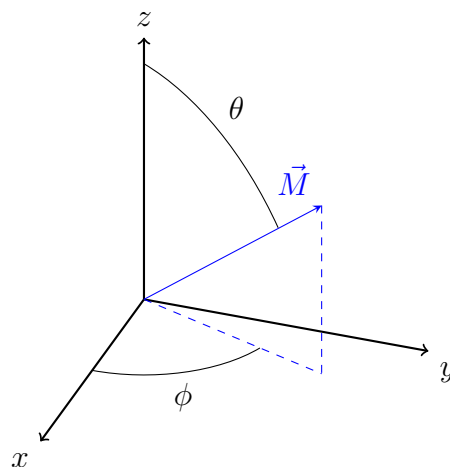


Figure 1. Schematic representation of the magnetic island in 3 dimensions, where \vec{M} is a magnetic moment of the island with respected angles ϕ and θ . Axis OZ is aligned with easy anisotropy direction \vec{K} .

We focus here on a single kagome ring formed by six islands and study how the interaction between them affects the activation energy and mechanism of the transitions.

A single prolate magnetic island is described as a single-domain ferromagnetic particle with uniaxial anisotropy (Figure 1). Such approach assumes that the re-magnetization process involves simultaneous rotation e.g. at any moment of time all magnetic moments of the island are parallel. In such cases, the total energy of the islands includes an anisotropy term of the form:

$$E_{islad} = -(\vec{M}\vec{K})^2 \quad (1)$$

In order to form the kagome spin ice element we combine six islands and include the interaction between them as described by equation (2). Since the size of a typical island in spin ice is a few nanometers, the interaction between islands is dominated by the dipole-dipole interaction. Therefore, the energy of the system becomes

$$E = \sum_i^N (\vec{M}_i \vec{K}_{out})^2 - \sum_i^N (\vec{M}_i \vec{K}_{in})^2 - \frac{1}{2} \sum_{i \neq j}^N \left(\frac{(\vec{M}_i \vec{M}_j)}{|\vec{r}_{ij}|^3} - \frac{3(\vec{M}_i \vec{r}_{ij})(\vec{M}_j \vec{r}_{ij})}{|\vec{r}_{ij}|^5} \right) \quad (2)$$

Where \vec{K}_{out} and \vec{K}_{in} are respectively the in-plane shape anisotropy and out-of-plane shape anisotropy. The vector \vec{r}_{ij} is the distance vector between centres of i -th and j -th islands. The summation limit N is the number of islands.

2. Simulations

The kagome spin ice element consists of 6 islands ($N = 6$) placed on the kagome lattice. Given the geometry, the distance vectors \vec{r}_{ij} can easily be found. The calculations are based mainly on experimentally determined values of the parameters e.g. the volume of an island and saturation magnetization of an island ($V = 470 \times 170 \times 3 \text{ nm}^3$, $M_s = 166 \times 10^3 \text{ A/m}$). The in-plane shape anisotropy parameter K_{in} and out of plane shape anisotropy parameter K_{out} were calculated by using micro-magnetic simulation from the volume and saturation magnetization. This is in an effort to simulate as closely as possible the experiment and to avoid any fitting parameters. The ratio between out-of-plane and in-plane anisotropy is about a factor of 4 ($K_{in} = 4550 \text{ erg/cm}^3$ and $K_{out} = 17991 \text{ erg/cm}^3$), so only rotation in plane is possible and this approximation implied in equation (2) is fully valid for the simulations.

The nudged elastic method (NEB) [5] was applied to find minimum energy paths (MEPs) on the energy surface determined by our model. The MEP represents the most probable, from a statistical point of view, path for the remagnetization process between the two ground states. Such paths show the mechanism of the transition and identify intermediate states. Maxima along the MEP give estimates of the activation energy for each of the elementary steps in the transition. There are, in fact, multiple different minimum energy paths and they have all been calculated (an example of such a path is shown in Figure 2). The two ground states of the kagome spin ice element correspond to clockwise and anticlockwise orientation of the magnetic moments of the islands (number I and VII in Figure 2).

3. Rate calculation

The transition rates are calculated using harmonic transition state theory (HTST) for magnetic systems [6]. This gives an Arrhenius law for the transition rate of each elementary step:

$$k = A \exp\left(-\frac{E_a}{k_b T}\right) \quad (3)$$

Here, E_a is the activation energy which in HTST is given by the difference in energy between the maximum along the MEP and the initial state, k_b is the Boltzmann constant and T is temperature. The pre-factor A is in many cases taken from the literature or is considered to be a fitting parameter. but we have applied the HTST to calculate the pre-exponent factor for our

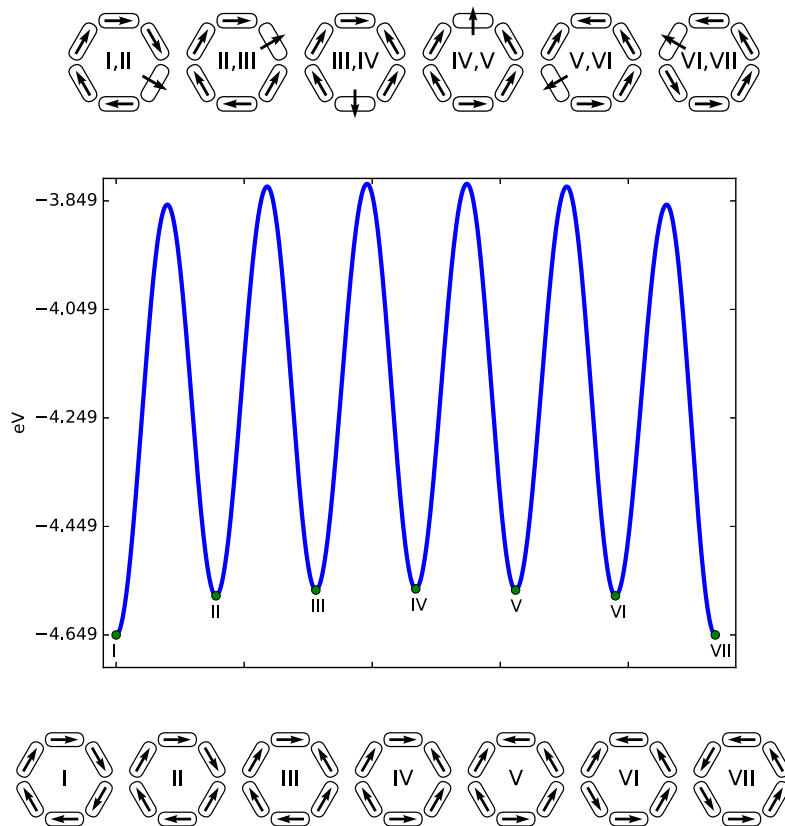


Figure 2. Minimal energy path(MEP) between ground states with respected configurations in the minima and maxima.

particular system:

$$k_{htst} = \frac{1}{2\pi} \frac{J_s}{J_m} \sqrt{\sum_{j=2} \frac{a_j^2}{\lambda_{s,j}}} \sqrt{\frac{\det H_{min}}{\det^* H_{sad}}} \quad (4)$$

Here, J_s and J_m are Jacobians at the saddle point and at the initial state minimum. H_{min} and H_{sad} are the Hessian matrices at the minimum and at the saddle point. The $\lambda_{s,j}$ are the eigenvalues of the Hessian at the minimum. \det^* is the determinant of the matrix excluding the row with the negative eigenvalue. This expression makes it possible to calculate the transition rate as well as the lifetime of a given state by using only observable parameters of the material as mentioned earlier, without any fitting to the measured rates.

As can be seen from Figure 2, the transition between the two degenerate ground states occurs via a set of intermediate minima. So, there is not just one activation barrier but rather a set of activation barriers. In such a case HTST can be used to find the rate of each elementary step and the overall rate of the sequence of steps estimated using stationary state approximation including all possible transition paths. This is based on a set of master equations, differential equations for the variation over time of the probabilities that the system occupies each of the different possible states

$$\left\{ \begin{array}{l} \frac{dn_0}{dt} = -W_{0,1}n_0 + W_{1,0}n_1 \\ \dots \\ \frac{dn_i}{dt} = -(W_{i,i+1} + W_{i,i-1})n_i + W_{i,i-1}n_{i-1} + W_{i,i+1}n_{i+1} \\ \dots \\ \frac{dn_n}{dt} = -W_{n,n-1}n_n + W_{n,n-1}n_{n-1} \end{array} \right. \quad (5)$$

In our case, n_i is a particular energy state. $W_{i,j}$ is a transition parameter between particular n_j and n_k or in other words a transition rate. The task is to find $\frac{dn_0}{dt}$ in terms of n_0 . In this way all elementary steps between n_0 and n_n can be included to give an overall rate and effective lifetime of one of the ground states. We take n_n to be the final state, i.e. if the system gets into that state it cannot go back until a long time has passed. The stationary state approximation means that we assume $\frac{dn_i}{dt}$ is equal to zero for all the intermediate states.

As we mentioned earlier, there are several equivalent transitions paths. We need to take that into account in the master equations for the system:

$$\left\{ \begin{array}{l} \frac{dn_0}{dt} = -6W_{0,1}n_0 + 6W_{1,0}n_1 \\ \frac{dn_1}{dt} = -(2W_{1,2} + W_{10})n_1 + W_{1,0}n_0 + 2W_{1,2}n_2 \\ \frac{dn_i}{dt} = -(2W_{i,i+1} + 2W_{i,i-1})n_i + 2W_{i,i-1}n_{i-1} + 2W_{i,i+1}n_{i+1} \\ \dots \\ \frac{dn_5}{dt} = -W_{5,6}n_5 - 2W_{5,4}n_5 + 2W_{4,5}n_4 \end{array} \right. \quad (6)$$

When we solve equation (6) to obtain the $\frac{dn_0}{dt} = -n_0(G)$ where the G is a combination of the $W_{i,j}$ and gives the effective transition rate between the two ground states. The resulting rate can be compared with the Arrhenius expression, eq. (3) to extract the effective pre-exponential factor.

4. Results

By using the methodology described above, we have estimated the lifetime of a ground state of the kagome ring at 420K to be around 12 seconds. At 300 K, the lifetime is several days. The effective pre-exponential factor is about 10^8 s^{-1} and the effective activation energy is 0.74 eV. These rates are in excellent agreement with the experiment even though the pre-exponential factor is four orders of magnitude lower than the one assumed in ref. [4] for the interpretation of the experimental data. The next step is to investigate the influence of the internal magnetic structure of an islands during a spin transition. This can be important because the islands are relatively large, so the magnetization reversal process could involve the formation of a temporary domain wall rather than a coherent rotation of all the spins in the island. This would strongly affect the activation energy as well as the pre-exponential factor.

Acknowledgment

This work was financially supported by the Government of Russian Federation, Grant 074-U01, RFBR grant №14-02-00102 and the Icelandic Science Fund.

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