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Energy surface and transition rates in a hexagonal element of spin ice

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Abstract. The energy surface of a hexagonal element of Kagome spin ice consisting of six prolate magnetic islands is investigated as a function of applied magnetic field. Minimum energy paths for magnetic reversals are determined to estimate energy barriers and the transition rates estimated using harmonic transition state theory for magnetic systems. The overall transition rate between equivalent ground states is calculated using the stationary state approximation including all possible transition paths. The calculated transition rates are in close agreement with reported experimental measurements taken in the absence of an applied field. Predictions are made for the change in the energy landscape and transition rates as a magnetic field is applied.

1. Introduction

Artificial spin ice systems make it possible to study new magnetic phenomena at various spatial and time scales ranging from atomic to micromagnetic dimensions. Temperature induced magnetic switching of magnetization has been observed experimentally with typical lifetime ranging from seconds to days as temperature changes from 300 K to 400 K [1]. Here, we present results of calculations of the rate of magnetisation reversals using rate theory and analysis of the multidimensional energy surface. We study a hexamer of islands arranged as a unit of a Kagome lattice. 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. The total energy of the hexamer is written as

\[
E = \sum_6 V(\vec{M}_i \vec{R}_{\text{out}}) + \sum_6 V(\vec{M}_i \vec{R}_{\text{in}}) - \frac{1}{2} \sum_{i<j} \left( \frac{\nu^2(\vec{M}_i \vec{M}_j)}{|\vec{r}_{ij}|^2} - \frac{3\nu^2(\vec{M}_i \vec{r}_{ij})(\vec{M}_j \vec{r}_{ij})}{|\vec{r}_{ij}|^4} \right) - \sum_6 V(\vec{M}_i \vec{H}) \tag{1}
\]

where $\vec{R}_{\text{out}}$ and $\vec{R}_{\text{in}}$ are respectively the in-plane and out-of-plane shape anisotropy. The dimensions of an island are chosen in such a way that the volume is $V = 470 \times 170 \times 3$ nm$^3$, the saturation magnetization $M_s = 166 \times 10^3$ A/m and the anisotropy $K_m = 4550$ erg/cm$^3$ $K_{\text{out}} = 17991$ erg/cm$^3$ to mimic an experimentally measured system [1]. The values of $K_m$ and $K_{\text{out}}$ are obtained from micromagnetic simulations given the volume and saturation magnetization. $H$ is the external magnetic field applied in plane, perpendicular to the long side of the top and bottom islands. The applied magnetic field strongly changes the energy surface both the location of energy minima and the height of energy barriers between states. The geodesic nudged elastic band (GNEB) method [2] is used to find minimum energy paths (MEPs) for various values of $H$. 

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2. Lifetime calculation
By identifying all the possible paths, the reversal of the total magnetization of the hexamer and the transition rate for each of the elementary steps, the lifetime of the system in a particular ground state can be estimated. The rate is estimated using harmonic transition state theory (HTST) for magnetic systems [3]. The rate constant of an elementary transition, k, is given by the Arrhenius law:

\[ k = A \exp \left( -\frac{E_a}{k_BT} \right) \]  

The steady state approximation is applied to determine the lifetime of the ground state as a function of external field strength. The set of master equations, i.e. differential equations for the variation of occupation probabilities of the various states (see figure 1) as a function of time, is

\[
\begin{align*}
\frac{dn_1}{dt} &= -6W_{1,2}n_0 + 6W_{2,1}n_2 \\
\frac{dn_2}{dt} &= -(2W_{2,3} + W_{2,1})n_2 + W_{2,1}n_1 + 2W_{2,3}n_3 \\
\frac{dn_3}{dt} &= -(2W_{i,i+1} + 2W_{i,i-1})n_i + 2W_{i,i-1}n_{i-1} + 2W_{i,i+1}n_{i+1} \\
\ldots \\
\frac{dn_6}{dt} &= -W_{6,7}n_6 - 2W_{6,5}n_6 + 2W_{5,6}n_5
\end{align*}
\]  

where \( n_i \) is the occupation probability of a particular state. \( W_{i,j} \) is the transition rate between states \( i \) and \( j \). In order to find the overall transition rate between ground states of the hexamer, eqn. (3) is solved in terms of \( n_0 \) to give the equation \( \frac{dn_1}{dt} = -n_1(G) \), where the \( G \) is a combination of the \( W_{i,j} \). Each elementary transition rate, \( W_{i,j} \), is given by eqn. (2) with \( E_a \) obtained from calculated MEPs and \( A \) obtained from HTST [3]. From the temperature dependence of the overall rate, an effective activation energy and pre-exponential factor can be extracted.

3. Results
The applied field strongly affects the energy surface as can be seen in figure 1. The energy of the various local minima and the energy barriers between them change. Some of the intermediate energy minima disappear when an even stronger field is applied.

![Fig. 1. Minimum energy paths between the clockwise and anti-clockwise ground states for various values of the applied magnetic field, H.](image)
By using the methodology described above, we first studied the case where an applied field is not present. The lifetime of a ground state of the kagome ring was estimated to be 12 seconds at 420K but several days at 300K. These values are in close agreement with the experimental measurements [4]. The effective pre-exponential factor turns out to be ca. $10^8$ s$^{-1}$ and the effective activation energy 0.74 eV. These values are, however, quite different from what has been used in previous modeling of the system [1]. When the external field is included, the lifetime of the various intermediate states as well as that of the ground states changes. Some of the states become less stable, as shown in figure 1, and even completely disappear as local minima on the energy surface when the field is strong.

It can be important to take into account the internal magnetic structure of the islands during spin transitions. This is schematically illustrated in figure 2a.

![Figure 2a](image)

**Fig. 2.** A schematic comparison of different magnetization reversal mechanisms: (a) Each island is described as a set of interacting magnetic moments that can rotate in different ways; (b) Each island is described as a macrospin undergoing coherent rotation. The former description is needed for long enough islands.

When an island is long compared with the length scale characterizing the exchange coupling of spins within the island, the macrospin approximation illustrated in figure 2b overestimates the energy barrier for the transition. The magnetization reversal of an island then occurs via a temporary domain wall mechanism, as has recently been illustrated for Fe islands on a substrate [3]. This effect will in future work be included in long time scale simulations of spin ice systems using the AKMC method [5].

**References:**


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