The mechanisms of thermally activated magnetization switching in small ferromagnetic particles driven by an external magnetic field are investigated. For low uniaxial anisotropy the spins rotate coherently while for sufficiently large uniaxial anisotropy they behave Ising-like, i.e., the switching then is due to nucleation. The crossover from coherent rotation to nucleation is studied for the classical three-dimensional Heisenberg model with uniaxial anisotropy by Monte Carlo simulations. From the temperature dependence of the metastable lifetime the energy barrier of a switching process can be determined. For the case of infinite anisotropy we compare numerical results from simulations of the Ising model with theoretical results for energy barriers for both, single-droplet and multi-droplet nucleation. The simulated barriers are in agreement with the theoretical predictions.

With decreasing size ferromagnetic particles become single-domain which improves their quality for magnetic recording. On the other hand, when the particles are too small they become superparamagnetic and then due to thermal fluctuations no magnetic information can be stored (see e.g. [1] for a review). Hence, much effort has been devoted to an understanding of the behavior of small magnetic particles experimentally [2–4], analytically [5], and in computer simulations. In the latter case, mainly magnetization switching by nucleation [6–8] has been studied using Ising models of finite size, but also other reversal mechanisms in models with continuous degrees of freedom like coherent rotation, single-droplet nucleation, and multi-droplet nucleation have been discussed [9,8].

In this paper we focus on different thermally activated reversal mechanisms occurring in ferromagnetic particles. We will consider a finite, spherical, three-dimensional system of magnetic moments. These magnetic moments may represent atomic spins or also block spins following from a coarse graining of the physical lattice. Our system is defined by a classical Heisenberg Hamiltonian,

\[ H = -J \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j - d \sum_i (S_z^i)^2 - B \cdot \sum_i \mathbf{S}_i, \]

where the \( \mathbf{S}_i \) are three dimensional vectors of unit length. The first sum which represents the exchange of the spins is over nearest neighbors with the exchange coupling constant \( J \). The second sum represents an uniaxial anisotropy which favors the \( z \)-axis as easy axis (anisotropy constant \( d > 0 \)). The last sum is the coupling of the spins to an applied magnetic field, where \( B \) is the strength of the field times the absolute value of the magnetic moment of the spin. We neglect the dipolar interaction. Therefore, the validity of our results is restricted to particles which are small enough to be single-domain in the remanent state [1].

In the following we will investigate the thermally activated reversal of the magnetization of a particle which is destabilized by a magnetic field pointing into the direction antiparallel to the initial magnetization which is parallel to the easy axis of the system initially. In this case after some time the particle will reverse its magnetization.

Due to the many degrees of freedom of a spin system numerical methods have to be used for a detailed microscopic description. Since we are especially interested in the thermal properties we use Monte Carlo (MC) methods for the simulation. Although a direct mapping of the time scale of a MC simulation on experimental time scales is not possible this method provides information on the dynamical behavior since it solves the master equation for the irreversible behavior of the system.

We consider spins on a simple cubic lattice of size \( L \times L \times L \) and simulate spherical particles with radius \( R = L/2 \) and open boundary conditions on this lattice using the MC algorithm described in [3]. We start our
simulations with an initial spin configuration where all spins are pointing up (\(S_i = (0,0,1)\)). The magnetic field \(\mathbf{B} = (0,0,-B)\) destabilizes the system and after some time the magnetization will reverse. The metastable lifetime \(\tau\) is defined by the condition \(M_z(\tau) = 0\) where \(M_z\) is the \(z\)-component of the magnetization \(\mathbf{M} = (1/N) \sum_i S_i\).

For sufficient low anisotropy the spins can be expected to rotate coherently. Such a reversal process is shown in Fig.1 where a spin configuration of a simulated system of size \(R = 6\) spins during the reversal process is represented. The spins are nearly parallel, except of thermal fluctuations. Following the theory of Néel \([12]\) and Brown \([13]\) the energy barrier which has to be overcome during the reversal is only due to the anisotropy of the system,

\[
\Delta E_{cr} = \frac{4\pi R^3 d}{3} - \frac{4\pi R^3 B M}{3} + \frac{\pi R^3 B^2 M^2}{3d}, \tag{2}
\]

where \(M\) is the saturation magnetization of the system.

For particles larger than \(R_c\) reversal by nucleation has the lower energy barrier while the opposite is true for particles smaller than \(R_c\).

Another possibility of a reversal process driven by nucleation is the growth of several droplets at the same time (multi-droplet nucleation). This reversal process occurs when the probability for the growth of large droplets is high enough and when the critical droplet size is smaller than the system size so that many droplets may occur in the system at the same time. This is the case for higher fields or larger temperatures \([15,16]\). The lifetime for the multi-droplet nucleation in \(D\)-dimensions is \([14]\)

\[
\tau \sim \exp \left( \frac{\Delta E_n}{T} \right)^{(D+1)T}. \tag{6}
\]

Hence, the exponent of the exponential function changes by a factor of \(1/(D+1)\) which is 1/4 in our case. In order to quantify the crossover from single droplet to multi-droplet nucleation we consider the case of infinite anisotropy in which case we can directly simulate an Ising system. We performed a standard MC simulation of the Ising Hamiltonian

\[
\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - B \sum_i S_i \tag{7}
\]

with \(S_i = \pm 1\).

Fig.3 shows a corresponding spin configuration during the reversal. The Ising spins are represented as light (spin up) and dark (spin down) grey boxes. The reversal process is initiated by many droplets at the boundary of the system. Later all these droplets join each other so that the outer shell of the particle is reversed while the inner parts have still the initial magnetization direction.
and the predictions obtained from both single- and multi-

the energy barriers obtained from the numerical data

6.

ted since we do not know the prefactors in Eqs. 4 and

simulated data. Note that the position of all lines are fit-

from theory showing again very good agreement with the

here (\(R\) lines shown are the energy barriers \(\Delta\)
factor of (4). The slopes of the straight lines shown are the energy barriers \(\Delta\)
theoretical prediction, Eqs. (3, 4). The slopes of

occurs and we can compare the corresponding data with

for multi-droplet nucleation in which case
find a crossover to multi-droplet nucleation in which case

theoretical predictions. For higher temperatures we

theoretical prediction, Eqs. (3, 4). The slopes of

metastable lifetime following from simulations for two

fields. Each data point is an average over 100

different fields. For low temperatures single-droplet nucleation

occurs and we can compare the corresponding data with

the theoretical prediction, Eqs. (3, 4). The slopes of

the straight lines shown are the energy barriers \(\Delta E_n\) obtained from Eq. 6 which have the theoretical values 40.4 \(J\)

\(B = 0.5J\) and \(T = 2.8J\).

To conclude we found very good agreement between

the energy barriers obtained from the numerical data and the predictions obtained from both single- and multi-

Fig. 4. Metastable lifetime \(\tau\) vs. \(1/T\) for two different magnetic fields. System size \(R = 4\) spins.

Fig. 3. Snap-shot of a simulated spin system at the lifetime \(\tau\) for multi-droplet nucleation. Shown is an Ising system of

size \(R = 8\) spins. In order to show the interior of the system

we have cut the sphere and show only one half of the system.

\(B = 0.5 J\) and \(T = 2.8 J\).

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Acknowledgments: We thank M. Acharyya and K. D. Usadel for helpful discussions. The work was supported by the Deutsche Forschungsgemeinschaft through Sonderforschungsbereich 166 and through the Graduiertenkolleg ”Struktur und Dynamik heterogener Systeme”. 

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