Introducing the step Monte Carlo method for simulating dynamic properties

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D. Sztenkiel, "Introducing the step monte carlo method for simulating dynamic properties," arXiv:2209.08961, 2022.

Motivation:

The Monte Carlo (MC) applications: physics, finance-economics, biology, engineering, etc.

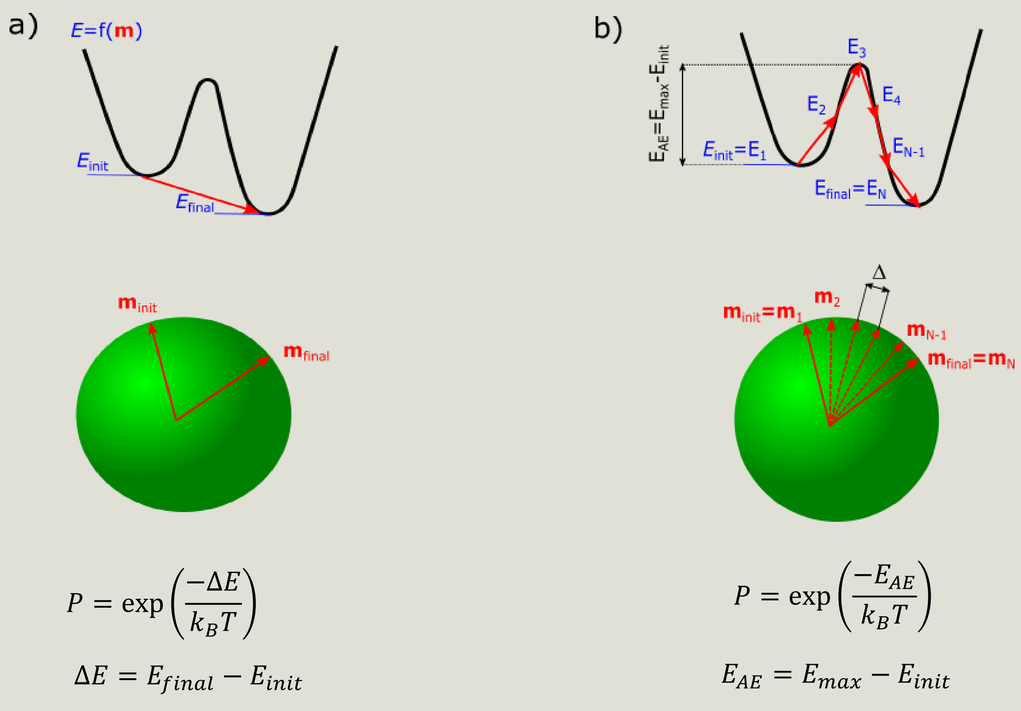
Condensed matter physics and materials science : system of classical particles, classical spin systems, percolation and fractals problems.

Disadvantage : MC is usually optimal approach for determining the equilibrium properties, where dynamics are not required.

Step Monte Carlo (sMC) algorithm:

Standard MC

Step MC (sMC)



$$P = \exp\left(\frac{-\Delta E}{k_B T}\right)$$

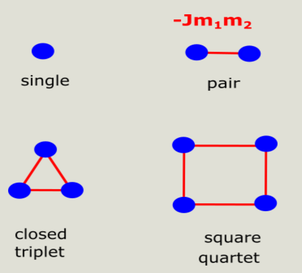
$$\Delta E = E_{final} - E_{init}$$

$$P = \exp\left(\frac{-E_{AE}}{k_B T}\right)$$

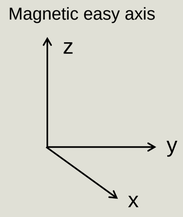
$$E_{AE} = E_{max} - E_{init}$$

In the modified MC approach proposed here (similarly to the kinetic MC approach) the probability of accepting the final state depends on the activation energy, not on the relative energy between the final and initial state. However, the barrier height is calculated on an ongoing basis, by generating intermediate states with a predefined step Δ. Therefore, we name this method step Monte Carlo (sMC)

System under consideration



We analyze a simple model consisting of few interacting magnetic atoms possessing the uniaxial anisotropy along the **z** axis. The atoms are coupled by ferromagnetic exchange interaction.



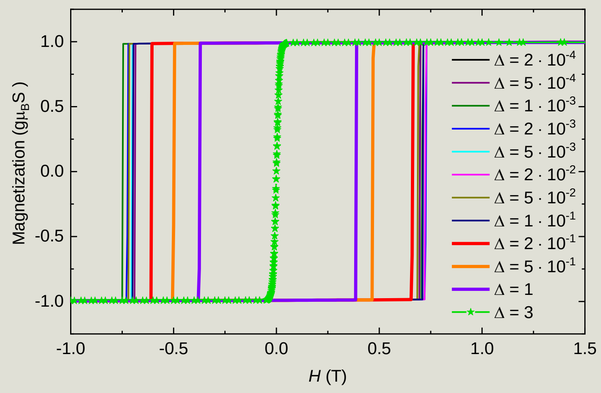
k_Z = 0.4 meV
J = 2 meV

$$\mathscr{H} = -k_z \sum_i m_{iz}^2 - \mu_S \mathbf{H} \sum_i \mathbf{m}_i - J \sum_{i>j} \mathbf{m}_i \mathbf{m}_j$$

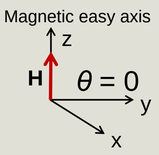
Conclusions

- We presented a modification of MC algorithm, named step Monte Carlo (sMC), that allows to simulate dynamic properties of spin systems
- sMC approach fulfills two general conditions for validity of Monte Carlo algorithms : ergodicity and the condition of detailed balance.
- Excellent agreement between sMC and sLLG results.
- In our opinion, the sMC approach can be applied to simulate other processes, for example diffusion, nucleation, surface adsorption, crystal growth processes and dynamics of classical atoms.

Validity testing of sMC



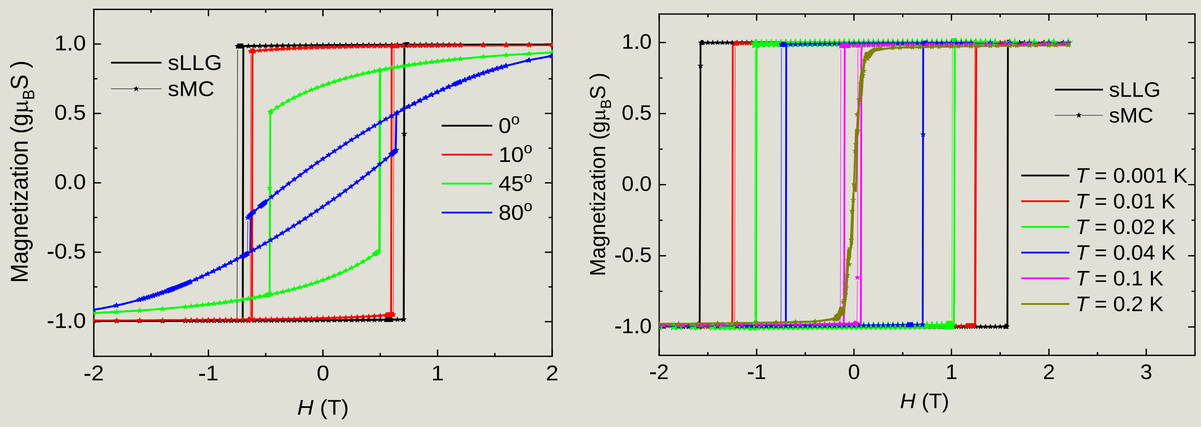
Single ion, T=0.04 K,
k_Z=0.4 meV



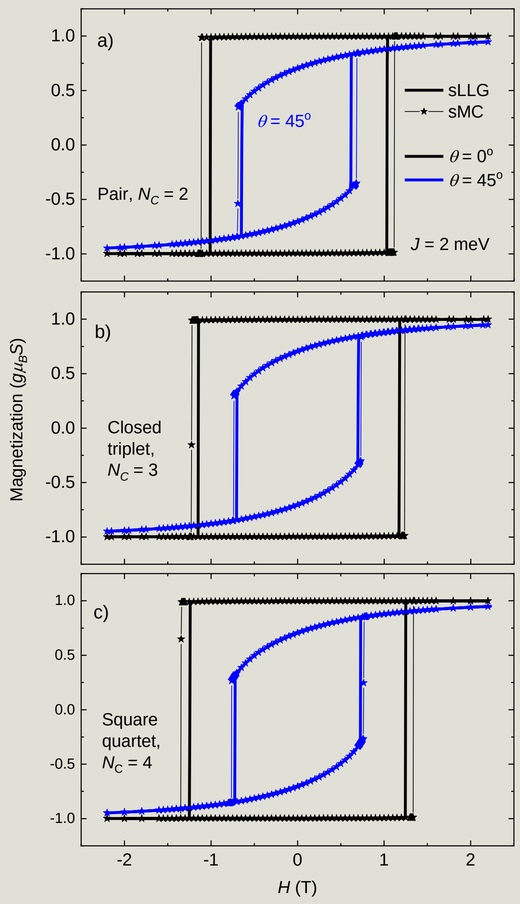
The simulations are performed using the sMC method with different steps Δ. The standard MC approach is represented by Δ = 3.

Comparison : sMC vs sLLG

To test the correctness of sMC, we compare its results with those obtained by stochastic Landau-Lifshitz-Gilbert (sLLG) equation



The comparison of numerical results between sMC (Δ = 10^{-3}) and sLLG methods. a) The magnetization M of a single ion with the magnetic field **H** applied at different angles θ from the easy axis z at temperature T = 0.04 K. b) The magnetization M of a single ion at different temperatures T with the magnetic field **H** applied along the easy axis **H** || **z**.



The comparison of numerical results between sMC (Δ = 10^{-3}) and sLLG methods for different clusters with size NC. The magnetization M of a pair (a), closed triplet (b) and square quartet (c) at the temperature T = 0.04 K. The magnetic field **H** is applied at two different angles θ from the easy axis **z**, namely θ = 0 and θ = 45°.

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