Modified Monte Carlo simulations of dynamic magnetic properties

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Standard Monte Carlo (MC) approach is often first method of choice for testing the static properties of a system. However, there are a lot of simulations where detailed dynamic information is required. The distribution of states obtained on a short-time scale usually has different configuration than the stationary ones. Here, we show that simple modification of MC algorithm, named step Monte Carlo (sMC), allows to simulate processes far from equilibrium and/or obtain information about dynamic properties of the system under investigation. The details of sMC approach are explained for the case of simple spin model. The comparison of its results with the ones obtained within the frame of stochastic Landau-Lifshitz-Gilbert (Langevin dynamics) indicates the correctness of sMC. In our opinion, the proposed here method can be applied to simulate other processes, for example dynamics of classical atoms and complex fluids, diffusion, nucleation, surface adsorption and crystal growth processes.

I. INTRODUCTION

The Monte Carlo (MC) method has proved to be a valuable simulation tool in many branches of science such as physics, chemistry [1], biology [1], computer science [1], economics, finance [2, 3] and engineering [4]. In the field of condensed matter physics and materials science MC can be used to study, among many others, classical spin systems, nucleation and crystal growth processes, polymer solutions, percolation and fractals problems. MC algorithm is natural choice for studying the static properties of a system, where dynamical effects are not required. Then, the advantages of Monte Carlo are relative ease of implementation and rapid convergence to steady state. In general, the theory of equilibrium properties is well developed for wide variety of models and materials. Here, however, we shall consider behaviors far from equilibrium. For example, the MBE growth of thin films proceed by both deposition and diffusion processes. The probability of an atom to hop to a nearest empty site, does not depend only on the relative energies of the configuration before and after hopping event, but rather on the barrier height. Kinetic Monte Carlo (KMC) method [5, 6] (though the early papers typically don’t use this term) was developed for evolving systems dynamically from state to state. KMC simulates how the occupation of the sites changes over time in a system with a known transition rates (these rates are inputs to the KMC algorithm).

In modified MC approach proposed here (similarly to KMC approach) the probability of accepting the final state depends on activation energy, not on the relative energy between final and initial state. However, the barrier height is calculated on an ongoing basis, by generating intermediate states with a predefined step ∆. Therefore, we name this method step Monte Carlo (sMC). The details of sMC algorithm are explained for the case of magnetization process. To test the correctness of sMC, we compare its results with those obtained by stochastic Landau-Lifshitz-Gilbert (sLLG) approach. It should be noted, that the sMC approach presented here for spin systems can be generalized in a straightforward way to simulate other processes, for example diffusion, nucleation, surface adsorption and crystal growth processes.

II. STEP MONTE-CARLO METHOD

Here we outline the details of step Monte Carlo method, that allows us to simulate processes far from equilibrium and/or obtain information about dynamic properties of the system under investigation. The differences between sMC and standard MC are shown schematically in Fig. 1 for the case of magnetization process. In sMC, the probability of accepting the final magnetic direction $\mathbf{m}_{\text{final}}$...
depends on activation energy (barrier height) $E_A$, not on the relative energy between final and initial state $E_{final} - E_{init}$. To calculate the barrier height, we probe the energies $E_k = f(m_k)$ of intermediate magnetic states $m_1$, $m_2$, $m_3$, ..., $m_{N-1}$. These intermediate states are generated on the arc connecting the initial $m_{init} = m_1$ and the final $m_{final} = m_N$ magnetization direction. This means that $m_{k+1}$ is obtained using a predefined step $\Delta$ in such a way that $|m_{k+1} - m_k| \propto \Delta$. Details of the generation of intermediate states are shown in Fig. 2. Finally, the barrier height is obtained from

$$E_A = max\{E_2, E_3, ..., E_N = E_{final}\} - E_{init} \quad (1)$$

Finally, we proceed in a similar way to the Monte Carlo Metropolis algorithm for a classical spin system. The complete procedure is shown below:

1. Select a random atom $j$ with initial magnetic moment direction $m_{j,init}$.
2. Choose randomly a new trial direction $m_{j,final}$.
3. Generate intermediate magnetic states $m_{j,2}, m_{j,3}, ..., m_{j,N-1}$ with a predefined step $\Delta$ on the arc connecting the initial $m_{init} = m_1$ and the final $m_{final} = m_N$ magnetization direction (see Fig. 2).
4. Calculate energies $E_{j,k} = f(m_{j,k})$ and the activation energy $E_A = max\{E_{j,2}, ..., E_{j,N} = E_{j,final}\} - E_{j,init}$.
5. The new trial direction $m_{j,final}$ is accepted with probability $P = \exp(-\frac{E_A}{k_B T})$, that is:
   a. Draw a random number $r$ uniformly distributed between 0 and 1.
   b. If $r \leq \exp(-\frac{E_A}{k_B T})$, accept new state, otherwise reject it.
6. Repeat the procedure.
One complete iteration of sMC consists of \( N_c \) such trial moves (one move corresponds to whole procedure 1-5 presented above), where \( N_c \) is the number of atoms in the system. In sMC approach we use \( 4 \cdot 10^7 \) equilibration and averaging iterations. Here for generation of the trial direction \( \mathbf{m}_{j,\text{final}} \) we choose a mixture of two different trial moves: Gaussian and random (c.f. Fig. 3.b-c and 4.b in Ref. 7). The Gaussian trial move creates \( \mathbf{m}_{j,\text{final}} \) by shifting the initial direction \( \mathbf{m}_{j,\text{init}} \) on the unit sphere according to the formula:

\[
\mathbf{m}_{j,\text{final}} = \frac{\mathbf{m}_{j,\text{init}} + \sigma_g \Gamma}{|\mathbf{m}_{j,\text{init}} + \sigma_g \Gamma|},
\]

where \( \Gamma \) is a 3D random vector characterized by the Gaussian distribution with a mean of zero and a standard deviation of 1. The width of the cone \( \sigma_g \) takes the following form

\[
\sigma_g = \frac{2}{5} \left( \frac{k_B T}{\mu_B} \right)^{1/5},
\]

what results in a move acceptance rate of around 50\%.

We can see, that implementation of sMC algorithm is a little more difficult than standard MC one. Also execution time for one sMC iteration is longer than in MC case, especially for small values of \( \Delta \). Another difference between standard MC and sMC is that MC provides proper Boltzman distribution of states in relation to the global energy minimum, whereas sMC provides Boltzman distribution of states relative to the local energy minimum. This guarantees proper dynamics of sMC, as energy barriers higher than \( k_B T \) prevent from too fast global thermalisation of spins.

One should note, that the sMC approach presented here for spin systems can be generalized in a straightforward way to simulate other processes, for example diffusion, nucleation, surface adsorption, crystal growth processes and dynamics of classical atoms. Then we just generate intermediate states on the line connecting the initial and final (trial) states.

To test the correctness of sMC, we compare its results with those obtained by stochastic Landau-Lifshitz-Gilbert (sLLG) equation [7–9]. Using the sLLG approach, it was possible to simulate the dynamic properties of magnetic materials [8] including ferromagnetic hysteresis loops [7], time evolution of a system of spins [7], spin waves [10], domain wall motion [11, 12] and magnetization switching processes [13, 14]. The sLLG equation, applied at the atomistic level, reads

\[
\frac{\partial \mathbf{m}_i}{\partial t} = -\frac{\gamma}{1 + \alpha_G} \left[ \mathbf{m}_i \times \mathbf{H}_{eff}^i + \alpha_G \mathbf{m}_i \times (\mathbf{m}_i \times \mathbf{H}_{eff}^i) \right],
\]

Here \( \gamma \) is the gyromagnetic ratio, \( \alpha_G \) is the damping parameter. The symbol \( \mathbf{m}_i \) describes normalized (\(|\mathbf{m}_i| = 1\)) direction of the local magnetic moment of atom \( i \) and \( \mathbf{H}_{eff}^i \) corresponds to effective magnetic field acting on this spin. \( \mathbf{H}_{eff}^i \) is calculated from the first derivative of the total spin Hamiltonian \( \mathcal{H} \) and incorporates also the instantaneous thermal magnetic field \( \mathbf{H}_{Th}^i \), according to the following formula

\[
\mathbf{H}_{eff}^i = -\frac{1}{\mu_s} \frac{\partial \mathcal{H}}{\partial \mathbf{m}_i} + \mathbf{H}_{Th}^i
\]

with

Figure 3. Investigated magnetic clusters composed of up to four magnetic ions (blue circles) coupled by a ferromagnetic exchange interaction (red lines).
\[ H_{Th}^t = \Gamma(t) \sqrt{\frac{2\alpha Gk_B T}{\gamma \mu S \Delta t}} \]  

(5)

\( \Gamma(t) \) is a Gaussian distribution in 3D space with a mean of zero and a standard deviation of 1. \( \mu_S = g \mu_B S \) is an actual value of atomic moment with spin \( S = 2 \), electron g-factor \( g = 2 \) and \( \Delta t = 5 \times 10^{-5} \) ns is the time step of simulation. Additionally, in sLLG method we use \( \alpha_G = 1 \) and \( 2 \times 10^{10} \) equilibration and averaging iterations.

### III. COMPARISON WITH STOCHASTIC LLG APPROACH

Having outlined the details of modified MC (sMC) method we now proceed to comparative study of magnetization dynamics obtained within the frame of sMC and standard sLLG approach. We analyze simple model consisting of few interacting magnetic atoms possessing uniaxial anisotropy along the \( z \) axis. The investigated small magnetic clusters are shown in Fig. 3. The Hamiltonian of the system reads

\[ H = -\sum_i k_z m_i z^2 - \mu_S H \sum_i m_i - J \sum_{i>j} m_i m_j \]  

(6)

with appropriate terms relating to uniaxial anisotropy energy, Zeeman energy and the exchange coupling between atoms. Here \( k_z = 0.4 \) meV is the anisotropy constant, \( J = 2 \) meV describes the exchange parameter. The symbol \( H \) corresponds to the external magnetic field.

In Fig. 4 we present the magnetization \( M \) of single ion, computed as a function of the external magnetic field \( H \) applied along the magnetic easy axis, namely \( H \parallel z \). The simulations are obtained using sMC method with different steps \( \Delta \). The standard MC approach is represented by \( \Delta = 3 \).

![Figure 4](image1.png)  
Figure 4. The magnetization \( M \) of single ion, computed as a function of the external magnetic field \( H \) applied along the magnetic easy axis at \( T = 0.04 \) K. The simulations are performed using the sMC method with different steps \( \Delta \). The standard MC approach is represented by \( \Delta = 3 \).

In Fig. 5 we present the magnetization \( M \) of single ion with the magnetic field \( H \) applied at different angles \( \theta \) from the easy axis \( z \) at temperature \( T = 0.04 \) K. The simulations are obtained using sMC method with different steps \( \Delta \). The standard MC approach is represented by \( \Delta = 3 \).

![Figure 5](image2.png)  
Figure 5. The comparison of numerical results between sMC (\( \Delta = 10^{-3} \)) and sLLG methods. a) Magnetization \( M \) of single ion with the magnetic field \( H \) applied at different angles \( \theta \) from the easy axis \( z \) at temperature \( T = 0.04 \) K. b) Magnetization \( M \) of single ion at different temperatures \( T \) with the magnetic field \( H \) applied along the easy axis \( H \parallel z \).
we observe saturation of $H_C$ and clear presence of thermal fluctuations.

![Diagram](image)

Figure 6. The comparison of numerical results between sMC ($\Delta = 10^{-3}$) and sLLG methods for different clusters with size $N_c$. Magnetization $M$ of pair (a), closed triplet (b) and square quartet (c) at temperature $T = 0.04$ K. The magnetic field $H$ is applied at two different angles $\theta$ from the easy axis $z$, namely $\theta = 0$ and $\theta = 45^\circ$.

In Fig. 5 the comparison of numerical results obtained using sMC ($\Delta = 10^{-3}$) and sLLG method is displayed. First, in Fig. 5 a. we plot magnetization $M$ of single ion with the magnetic field $H$ applied at different angles from the easy axis $z$ at temperature $T = 0.04$ K. As we see both approaches give very similar quantitative results. Small discrepancies are due to the presence of thermal fluctuations. These discrepancies decrease with lowering the temperature as shown in Fig. 5 b. Additional source of the observed discrepancy between the results of sLLG and sMC is the fact, that sLLG equation consists of two processes: precessional motion of magnetization along the effective magnetic field and damping term parametrized by $\alpha_G$. In MC method only the last term, related to the relaxation of the system to equilibrium, is present.

Finally, the magnetizations for larger clusters are presented in Fig. 6. At finite temperature, the coercive field increases slightly with the size of the cluster $N_c$, as expected. Again, the consistency between the sLLG and sMC results is very well, indicating a correct assumptions and implementation of the sMC algorithm.

Interestingly, the coercive field obtained from sLLG is slightly smaller than the one obtained from sMC approach. This is especially noticeable for magnetic filed applied along the easy axis $H||z$ ($\theta = 0$). In our opinion, it is connected with the fact that in sMC algorithm the Landau-Lifshitz (LL) term is absent. This LL term producing precessional motion of magnetization along the effective magnetic field seems to be important in switching processes.

### CONCLUSIONS

Here, we present a simple modification of MC algorithm, named step Monte Carlo (sMC), that allows to simulate dynamic properties of various classical systems. In modified sMC approach the probability of accepting the final state depends on activation energy (barrier height), not on the relative energy between the final and initial state. This barrier height is probed by generating intermediate states with a predefined step $\Delta$. To test the correctness of sMC, we simulate dynamic magnetic properties for interacting spin system and compare its results with those obtained by stochastic Landau-Lifshitz-Gilbert (sLLG) approach. The obtained excellent correspondence of both methods indicates the correctness of the proposed approach. In our opinion, sMC method can be applied to simulate other processes, for example dynamics of classical atoms and complex fluids, diffusion, and crystal growth processes.
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[1] J. S. Liu. Monte Carlo Strategies in Scientific Computing. Springer Series in Statistics. Springer-Verlag, NY, 2004. doi:https://doi.org/10.1007/978-0-387-76371-2
[2] P. Glasserman. Monte Carlo Methods in Financial Engineering. Stochastic Modelling and Applied Probability. Springer Science+Business Media, NY, 2003.
[3] T. Gerstner and P. Kloeden. Recent developments in computational finance : foundation, algorithms and applications. Interdisciplinary Mathematical Sciences. Singapore World Scientific, 2013.
[4] G. S. Fishman. Monte Carlo : Concepts, Algorithms, and Applications. Springer Series in Operations Research and Financial Engineering. Springer New York, NY, 2003. doi:https://doi.org/10.1007/978-0-387-98433-4
[5] W. M. Young and E. W. Elcock. Monte carlo studies of vacancy migration in binary ordered alloys: I. Proc. Phys. Soc., 89(3):735–746, 1966. doi:10.1088/0370-1328/89/3/329
[6] A.B. Bortz, M.H. Kalos, and J.L. Lebowitz. A new algorithm for monte carlo simulation of ising spin systems. J. Comp. Phys., 17(1):10–18, 1975. ISSN 0021-9991. doi:https://doi.org/10.1016/0021-9991(75)90060-1
[7] R. F. L. Evans, W. J. Fan, P. Chureemart, T. A. Ostler, M. O. A. Ellis, and R. W. Chantrell. Atomistic spin model simulations of magnetic nanomaterials. J. Phys.: Condens. Matter, 26:103202, 2014. doi:http://dx.doi.org/10.1088/0953-8984/26/10/103202
[8] R. F. L. Evans, U. Atxitia, and R. W. Chantrell. Quantitative simulation of temperature-dependent magnetization dynamics and equilibrium properties of elemental ferromagnets. Phys. Rev. B, 91:144425, 2015. doi:http://dx.doi.org/10.1103/PhysRevB.91.144425
[9] K. Edathumkandy and D. Sztenkiel. Comparative study of magnetic properties of Mn^{3+} magnetic clusters in GaN using classical and quantum mechanical approach. J. Magn. Magn. Mater., 562:169738, 2022. doi:https://doi.org/10.1016/j.jmmm.2022.169738
[10] Scott A. Bender, Hans Skarsvåg, Arne Brataas, and Rembert A. Duine. Enhanced spin conductance of a thin-film insulating antiferromagnet. Phys. Rev. Lett., 119:056804, 2017. doi:10.1103/PhysRevLett.119.056804
[11] F. Schlickeiser, U. Ritzmann, D. Hinzke, and U. Nowak. Role of entropy in domain wall motion in thermal gradients. Phys. Rev. Lett., 113:097201, 2014. doi:10.1103/PhysRevLett.113.097201
[12] D. Hinzke and U. Nowak. Domain wall motion by the magnonic spin seebeck effect. Phys. Rev. Lett., 107:027205, Jul 2011. doi:10.1103/PhysRevLett.107.027205
[13] M. O. A. Ellis and R. W. Chantrell. Switching times of nanoscale fept: Finite size effects on the linear reversal mechanism. Appl. Phys. Lett., 106(16):162407, 2015. doi:10.1063/1.4919051
[14] W. Scholz, T. Schrefl, and J. Fidler. Micromagnetic simulation of thermally activated switching in fine particles. J. Magn. Magn. Mater., 233(3):296–304, 2001. doi:https://doi.org/10.1016/S0304-8853(01)00032-4