

Thinning algorithms for the Monte Carlo simulation of kinetic Ising models

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The thinning method for numerically generating the arrival times of nonhomogeneous Poisson processes (NHPPs) has been adapted to accelerate Monte Carlo simulations of kinetic Ising models (KIMs) with Glauber spin-flip dynamics. The performance of the proposed algorithms is illustrated through simulations of the decay of metastable states in stationary KIMs and of the hysteresis of KIMs in a periodic external field. The thinning is implemented using piecewise-constant majorizing functions that bound from above or are equal to the NHPP rate. In favorable cases, this approach enables the simulations of hysteresis at frequencies in the tens of nanohertz and the decay of metastable states with lifetimes many orders magnitude longer than those accessible in previous simulations. The simulated results show good agreement with low-temperature analytical theories. Although algorithmic acceleration becomes more pronounced at lower temperatures, hysteresis has been simulated at moderately low temperatures of practical relevance, ranging from below room temperature up to values used in hyperthermia applications.

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I. INTRODUCTION

The kinetic Ising models (KIMs) have been widely used in modeling diverse systems in many fields [1]. Besides traditional use in studies of uniaxial magnets, lattice gases, and alloy kinetics [2], the KIM framework has been also adapted to study protein folding [3], optimization of neural networks [4,5], and many other topics [1].

A major reason for KIMs widespread use is their suitability for simulation with the kinetic Monte Carlo (KMC) method [6,7], which provides reliable quantitative insight into model behavior. However, in many cases the computer time required for such simulations becomes prohibitively long, thus severely minimizing the practicality of the KMC method. This problem is typically exacerbated at low temperatures, where long-lived metastable states tend to occur [8] and the performance of the conventional Metropolis algorithm (MA) decreases due to low acceptance rates [6,9,10]. Furthermore, in studying kinetics one cannot resort to the approach widely used in equilibrium studies when the microscopic dynamics is artificially modified to accelerate the equilibration [6,10,11]. For example, in such simulations the MA can be accelerated by updating spins sequentially in a convenient order [6,9]. In simulation of real physical evolution, however, spins should be chosen randomly in accordance with the microscopic stochastic dynamics.

To address this problem, KMC algorithms have been developed that enable considerable acceleration of simulations for KIMs with stationary Hamiltonians [7,10–15]. However, certain important phenomena can be studied only with Hamiltonians that explicitly depend on time. A well-known example is the hysteresis in oscillating magnetic field, a phenomenon which is of both considerable scientific interest and important technical and biomedical relevance [16–18].

In the absence of more efficient techniques, hysteresis in KIMs has been studied using the MA [19,20]. Because of its limitations, simulations were performed either at high temperatures to increase the acceptance rate or at relatively large frequencies, where more cycles of the external field can be simulated within available computer time.

In biomedical applications, however, the temperature corresponding to 80% of the Curie temperature used in the KMC simulations of Ref. [19] is unrealistically high for iron and magnetite nanoparticles (materials often used in hyperthermia studies [18]) because their Curie temperatures are on the order of 10^3 K. The simulations at lower temperatures in Ref. [20], on the other hand, did not cover the frequency range of interest in biomedical studies [18].

A detailed discussion of physical behaviors encountered in KIM simulations can be found in Refs. [11,19–23]. In the present study, however, the main focus is on KMC performance. Our aim is to propose accelerated algorithms that enable KMC simulations of magnetic nanoparticles within temperature and frequency ranges of practical interest. This will be achieved by adapting to the nonstationary case the Bortz-Kalos-Lebowitz algorithm (BKLA), which enhances the KMC performance at low temperatures [10] and the

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Monte Carlo (MC) algorithm with absorbing Markov chains (MCAMC) or the Novotny algorithm (NA) [11], which has proven effective for simulating the decay of metastable states [11,24].

Formally, the difference between KMC simulation of stationary and nonstationary processes lies in the fact that in the latter the transition rates of the stochastic matrix are time dependent. Consequently, one is faced with the necessity of simulating a nonstationary or nonhomogeneous Poisson process (NHPP). This problem has been extensively addressed in the literature (see, e.g., Refs. [25–29]) and the general conclusion is that, with some exceptions, the fastest algorithms to generate an NHPP are based on the thinning approach [30], typically using a piecewise-constant majorizing function. Here a majorizing function is defined as one that is greater than or equal to the rate it bounds. We adopt this terminology from Ref. [26], although in the mathematical literature the term majorization is often used with different meaning [31].

In this study we apply thinning algorithms to simulations of a ferromagnetic KIM in an oscillating magnetic field at temperatures and frequencies of practical relevance, as well as to the decay of metastable states in the stationary KIM. We will prefix the letter T to their abbreviations, i.e., TBKLA and TNA, to distinguish our algorithms from their stationary counterparts. It should be emphasized, however, that the thinning approach offers considerable flexibility through the choice of majorizing function and thus can be implemented in various ways. In what follows, we develop two algorithms, the thinned BKLA (TBKLA) and thinned NA (TNA), based on a constant majorization function and an additional variant of the TNA employing a piecewise-constant majorizing rate. Finally, to enable quantitative comparison with simulations based on the MA [19,20] we show that the conventional MA is formally equivalent to a thinning algorithm, implying that that the physical time simulated by the MA is identical to that in our methods.

The paper is organized as follows. In the next section we specify our KIM. In Sec. III thinning with a constant majorization is applied to the BKLA and the resulting TBKLA is used to illustrate its advantage over the MA at low temperatures in a high-frequency hysteresis simulation. In Sec. IV the NA is accelerated using thinning and in Sec. V the efficiency of the TNA is illustrated through simulations of decay of metastable states. In Sec. VI the TNA is further extended by introducing a piecewise-constant majorization function to simulate the KIM in a periodic external field. In Sec. VII the low-frequency behavior of hysteresis loop areas is simulated at two temperatures; at the lower temperature, good agreement with adiabatic theory at low frequencies is demonstrated. In Sec. VIII we provide a brief summary and possible directions for further improvement of the proposed algorithms.

II. MODEL

To simplify simulations and to facilitate comparison with the theoretical predictions of Refs. [21,32–34] and with previous KMC simulations [11,19,23], we consider ferromagnetic KIMs with nearest-neighbor (NN) spin interactions. The spins occupy N sites of a toroidal hypercubic lattice with L lattice

sites in each of D directions ($D = 2, 3$) so that $N = L^D$. In this geometry all spins are equivalent, which greatly simplifies combinatorics. In real nanostructures the boundary spins would differ from those in the bulk, but generalization to this more realistic case should be straightforward, albeit more computationally demanding.

We consider the Ising Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - H(t) \sum_i s_i, \quad (1)$$

where $J > 0$ is the pair spin interaction and $s_i = \pm 1$ are the Ising spins. The first summation on the right-hand side (RHS) is over all NN spin pairs and the second one is over N lattice sites. The external magnetic field $H(t)$ is of the oscillating form

$$H(t) = -H_0 \cos(\omega t), \quad (2)$$

where $H_0 > 0$ is the field amplitude and $\omega = 2\pi\nu$, with ν the oscillation frequency. The stationary case is recovered at $\omega = 0$. More general periodic fields, such as those studied in Ref. [35], can be treated similarly.

In the Glauber dynamics the spin-reversal (or spin-flip) rate is given by [36]

$$r_i(t) = \frac{v_0}{1 + \exp(\beta \Delta_i \mathcal{H})}, \quad (3)$$

where v_0 is a characteristic frequency in the range 10^9 – 10^{12} Hz [19] and $\beta = 1/T$, where temperature T is in energy units (achieved by setting the Boltzmann constant to unity [20,23,37]). The change of the Hamiltonian under spin i reversal $s_i \rightarrow -s_i$ in an NN KIM is

$$\Delta_i \mathcal{H} = -2J s_i \sum_{\text{NN}} s_{i_{\text{NN}}} + 2H_0 s_i \cos(\omega t), \quad (4)$$

where s_i is the spin value after the flip and $s_{i_{\text{NN}}}$ are its nearest neighbors. The total spin-flip rate in the system is

$$\lambda(t) = \sum_i r_i(t), \quad (5)$$

which serves as the NHPP rate to be simulated.

Formally, the problem is as follows. Given the previous arrival time t_0 , by using Eqs. (A2) and (A3) in Appendix A it is easy to show that the next arrival t can be found as the solution of equation

$$\int_{t_0}^t \lambda(t') dt' = -\ln u, \quad (6)$$

where u is a random variate uniformly distributed within the range $0 < u < 1$; in addition, we have used the fact that $1 - u$ and u are distributed identically. Here a remark on terminology is in order. Throughout the paper we use term “arrival time” or simply “arrival” for the value of the evolution parameter as generated by a Poisson process (PP) that is either homogeneous or nonhomogeneous [25]. In our opinion, the alternative term “event” [26] can be misleading in the thinning approach that we use because nothing happens if the generated time is rejected. However, each arrival generated with the exact equation (6) does lead to an event, that is, to a spin flip in the case of the Glauber dynamics.

From Eq. (5) it is seen that in general a numerical solution of Eq. (6) can be computationally costly because in iterative solution methods the quadrature will have to be computed numerically many times.

However, in some cases the problem simplifies. For example, if λ does not depend on time, the solution is easily found as [6]

$$t = t_0 - \ln u/\lambda. \quad (7)$$

A somewhat more complex but still computationally easy case provides a piecewise-constant rate when $\lambda(t)$ remains constant on consecutive time intervals with the time dependence restricted to discontinuities at the interval boundaries [25–28]. These particular cases in conjunction with the thinning technique allow for a fast generation of the NHPP with the rates as complex as $\lambda(t)$ [Eq. (5)].

III. THINNING ALGORITHM

The KMC simulation of an NHPP with the use of thinning algorithms is based on the theorem of Ref. [30], which states that any NHPP with a rate function $\lambda(t)$ can be generated through thinning of arrival times generated with the use of a majorizing rate function $\bar{\lambda}(t) \geq \lambda(t)$ as follows (see, e.g., Ref. [25]). First one generates an increasing sequence of arrival times $\{t_i\}$, $i = 1, 2, \dots$, within the interval $t_0 < t_i \leq t_{\max}$ ($t_{\max}$ is an arbitrarily chosen maximum time), using Eq. (6) with $\bar{\lambda}(t)$ instead of $\lambda(t)$ as

$$\int_{t_{i-1}}^{t_i} \bar{\lambda}(t) dt = -\ln u'_i, \quad (8)$$

where u'_i are independent uniform random variates. Next a new sequence of the variates $\{u_i\}$ is generated and for each t_i the acceptance criterion

$$\bar{\lambda}(t_i)u_i \leq \lambda(t_i) \quad (9)$$

is tested. If the arrival time t_i does not satisfy the criterion it is discarded while the remaining “thinned” set $\{t_i\}^{\text{th}}$ gives the statistically same sequence of arrival times as if generated with the use of Eq. (6) [30]. By using a time-independent (constant) majorizing function, the sequence $\{t_i\}$ can be easily generated with the use of Eq. (7), and because the acceptance criterion Eq. (9) does not include quadratures, the generation of $\{t_i\}^{\text{th}}$ that we are interested in becomes faster than with the use of Eq. (6) with nontrivial $\lambda(t)$.

To proceed further, we first note the difference between simulation setups usually discussed in mathematical literature on the NHPP [25–28,30] and the KIM simulations. In the former case one considers the rate $\lambda(t)$ as an immutable function and therefore the batch simulation of arrivals is warranted. However, in KIMs the rate is known only for an actual spin configuration e acquired by the system at an earlier arrival t_e which should be updated at every configuration change. In fact, in the case of KIMs the rate should be more comprehensively written as $\lambda(t, e, t_e)$, but because this is always the case, we will omit two last arguments for brevity. Thus, only the nearest arrival time is reasonable to generate to avoid superfluous computations.

Therefore, to use the thinning method we test the acceptance criterion at every arrival according to the following

general thinning algorithm (GTA) that is used throughout the paper. For definiteness, the simulation time span is chosen to be from $t = 0$ to $t_{\max}$. The initial configuration e at $t_e = 0$ can in principle be arbitrary, but in our low-temperature simulations we find convenient to choose it as e_0 , the fully ordered state with negative magnetization. Explicit forms of the corresponding $\bar{\lambda}(t)$ and $\lambda(t)$ at $t = t_e = 0$ should be obtained with the use of appropriate definitions, such as Eq. (5). Then the following three steps are repeated until termination.

Step 1. Set $t_0 = t$, generate a uniform random variate $u \in (0, 1)$, and solve Eq. (8) for the arrival time t by setting t as the upper integration limit, t_0 as the lower one, and u as the logarithm argument; if $t > t_{\max}$ terminate.

Step 2. Calculate $\lambda(t)$ and generate a random variate $u \in (0, 1)$; if $u\bar{\lambda}(t) > \lambda(t)$ return to step 1.

Step 3. For $u\bar{\lambda}(t) \leq \lambda(t)$ set $t_e = t$ and determine a new configuration e as stipulated by the KIM dynamics; define $\bar{\lambda}(t)$ and $\lambda(t)$ corresponding to e and t_e ; return to step 1.

We note that there would be no need to differentiate between t_0 and t_e if the exact equation (6) were used in the simulation because in this case all arrivals would cause the configuration change. However, the distinction is important in the presence of rejected arrivals because they do not change the system and so cannot influence the NHPP rates which may depend on t_e .

A. Equivalence of the MA to a thinning algorithm

Arguably, the MA is the most widely known MC algorithm. In view of differing definitions, we will understand by the MA the one called in Ref. [10] the standard MC algorithm. Although originally developed for the stationary case [9], the MA has been widely used in the hysteresis simulations (see, e.g., Refs. [19,20]). Our aim here is to show that the MA is equivalent to a thinning algorithm for the KIM considered in this work. Consequently, the physical results obtained with the MA should be identical to those produced by our simulations.

Let us consider a constant majorizing rate

$$\bar{\lambda}^{\text{MA}} = N\nu_0, \quad (10)$$

which exceeds $\lambda(t)$ in Eq. (5) for any values of the parameters, as can be seen from Eq. (3).

Assume the current time is t_0 . Using the constant majorizing function $\bar{\lambda}^{\text{MA}}$ [Eq. (10)] as $\bar{\lambda}(t)$, we generate the next arrival time t using Eq. (7). In our GTA we now have to calculate $\lambda(t)$ using Eq. (5) and to test the acceptance criterion by generating a uniform random variate u . This is visualized in Fig. 1(a), where the test reduces to the question about whether $u\lambda = uN\nu_0$ falls into the empty region of the rectangle or in the shaded one.

An advantage of the MA is that there is no need to calculate $\lambda(t)$ in Eq. (5) by accounting for all r_i in Eq. (3), which may be computationally costly, for example, in the case of long-range interactions. Instead, one first randomly chooses one of the spins, say, i , and then compares $u\nu_0$ with only $r_i(t)$. In Fig. 1(b) the acceptance or rejection would correspond to whether $u\nu_0$ falls into the shaded or open region within cell i .

The statistical equivalence of this procedure to the GTA is a consequence of the uniform distribution property that the probability of $uN\nu_0$ falling into, say, the shaded region is the

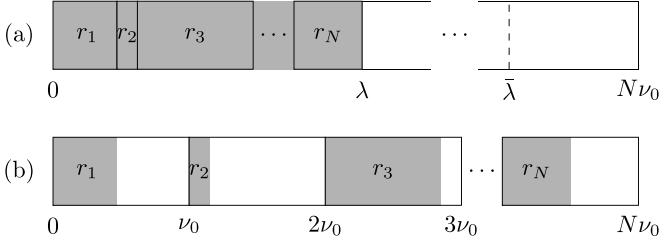


FIG. 1. Visualization of the interrelation between the BKLA with rate λ [10], the conventional MA with total rate $N\nu_0$, the improved MA with $\bar{\lambda} = N\bar{\nu}$ [Eq. (13)], and the thinning. Shaded areas correspond to accepted arrivals and empty space to rejected ones; for a detailed explanation see the text.

same in both rectangles in Fig. 1. The subscript i value of the spin s_i that need to be tested can be found as $i = [uN] + 1$, where $[\dots]$ means the integer part, and acceptance or rejection is decided from the fulfillment or violation of inequality $uN - [uN] = \{uN\} \leq r_i(t)$ ($\{\dots\}$ denotes the fractional part).

Thus, the MA simulates the same KMC process as the GTA, though there is a small difference. In practice, usually in the MA a constant time increment is used [9],

$$\Delta t^{\text{MA}} = (\bar{\lambda}^{\text{MA}})^{-1} = (N\nu_0)^{-1}, \quad (11)$$

instead of the stochastic value from Eq. (7) [12]. Although the latter approach is more rigorous, if one is interested only in an average evolution obtained in as many simulation runs as possible, the use of a constant increment can be fully justified for stationary Hamiltonians. The random variates used in the increment simulation and those in determining the spin flips are statistically independent, so the time increment can be averaged analytically, which amounts to $\langle \Delta t \rangle = \Delta t^{\text{MA}}$. However, in a nonstationary case the spin-flip rate will depend on time and thus correlate with the increment. However, for the time variation in Eqs. (1) and (2) on a much larger scale than Δt^{MA} the constant increment approximation should be quite accurate. The condition $\omega \Delta t^{\text{MA}} \ll 1$ can be rewritten as

$$\nu \ll N\nu_0, \quad (12)$$

so with ν_0 in the range 10^9 – 10^{12} Hz [19] the condition in practical applications may be violated only in extreme cases [12].

The advantages of the MA are that there is no need to calculate $r_i(t)$ for all i and $\bar{\lambda}$ at each KMC step; the only needed quantity is $\bar{r} = \nu_0$, known beforehand. Moreover, to accelerate the MA it can be lowered by using instead

$$\bar{r} = \max_{e,i,t} r_i(t), \quad (13)$$

which is always smaller than ν_0 , as can be seen from Eq. (3). The average time step in this case is $\langle \Delta t \rangle = 1/N\bar{r}$. This can be especially useful at high temperatures where $\bar{r}$ approaches $\nu_0/2$ [10,12], thus making the use of the MA at such temperatures more efficient.

However, among all configurations e in Eq. (13) there always exist configurations with spin i being in an energetically unfavorable state, which at low temperatures would lead to $\bar{r} \approx \nu_0$. However, in a fully ordered state the spin-reversal rates at low temperatures are very small for all i , which under

the MA would cause many rejections, resulting in a slow evolution [10].

In contrast, the sum of all rates r_i in Eq. (5) in the ordered state will be much smaller than $N\nu_0$, so with the use of an appropriate $\bar{\lambda}$ the simulation might proceed faster despite the extra computations needed. This can be achieved with the use of the BKLA technique [10], where the computation of $\lambda(t)$ in Eq. (5) is greatly facilitated in the NN KIMs.

B. Simulation of high-frequency hysteresis using the TBKLA

When temperature lowers, the spin flips become less frequent. However, the time step in the MA Δt^{MA} [Eq. (11)] remains the same, which means that the rejection rate grows. Below some temperature there are so many rejections that the calculation of the rejected individual spin rates r_i will eventually exceed the computational cost of updating the total rate given by Eq. (5) at each KMC step. This happens especially fast in the case of NN spin interactions when only a small number of rates have to be updated [10]. For example, in the case of a hypercubic lattice each spin has only $2D$ nearest neighbors. In the stationary case $2(2D + 1)$ different spin-flip rates should be calculated and stored only once. Although updating the transition rates at each MC step requires additional computations, the absence of rejections in the BKLA makes it more efficient than the MA already at moderately low temperatures [10].

To generalize the BKLA to the nonstationary case by means of thinning, it is possible in principle to make the rejection rate in the TBKLA arbitrarily small by using a sufficiently tight majorization function. However, to reduce the computational overhead, a compromise should be sought between the admissible rejection rate and the complexity of $\bar{\lambda}$. In addition, the simplicity of implementation would facilitate the adaptation of the TBKLA to possible model modifications.

Therefore, similar to the MA, let us consider the simplest case of majorization by a constant rate. This can be achieved by using $\bar{\lambda}$ of the same form as $\lambda(t)$ in Eq. (5) but with all rates $r_i(t)$ replaced by their maximum values

$$\bar{r}_i = \max_t r_i(t) = \frac{\nu_0}{1 + \exp(\beta \bar{\Delta}_i \mathcal{H})}, \quad (14)$$

where

$$\bar{\Delta}_i \mathcal{H} = \min_t \Delta_i \mathcal{H} = -2Js_i \sum_{\text{NN}} s_{i_{\text{NN}}} - 2H_0. \quad (15)$$

Here we employed Eq. (4) and our choice of $H_0 \geq 0$. An advantage of the constant majorization is that the $2(2D + 1)$ different majorizing rates $\bar{r}_i$ can be calculated and stored only once, though the set of independent $r_i(t)$ should be recalculated at each KMC step because of their time dependence. The computational overhead will depend on the rejection rate.

As can be seen from Eqs. (14) and (15), when both β and H_0 are sufficiently large, $\bar{r}_i \simeq \nu_0$ for all spins. In other words, we essentially recover the MA, which is inefficient at low temperatures. Thus, for the constant majorization to be efficient, the external field amplitude should be sufficiently small for the argument of the exponential function in Eq. (14), that is, the RHS of Eq. (15), is positive. This means that the

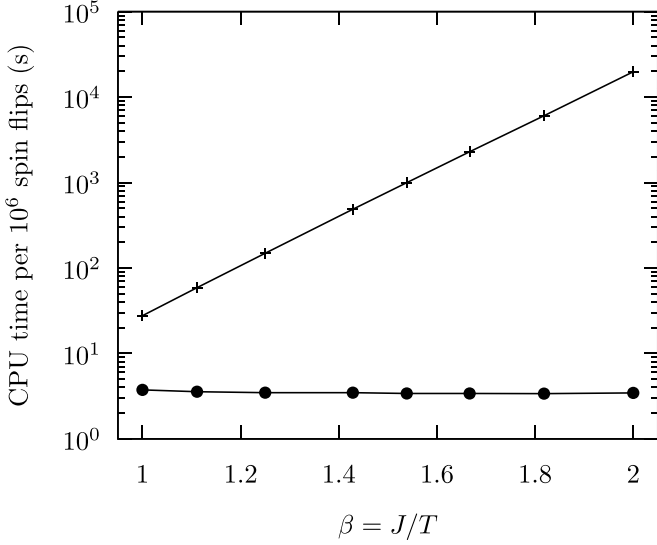


FIG. 2. Temperature dependence of the execution time of the MA (pluses) and the TBKLA (circles) in simulations of 10^6 spin flips in a 2D KIM of size $L = 100$ in oscillating magnetic field of frequency $\omega = \nu_0$ and amplitude $H_0 = J$ (KMC simulated data for all figures can be found in Ref. [38]).

amplitude should satisfy the inequality

$$H_0 < 2DJ = H_{\text{DSP}}(T = 0), \quad (16)$$

where $H_{\text{DSP}}(T)$ is the value of the external field at the dynamic spinodal point [21]. However, even if H_0 satisfies the inequality, the TBKLA performance will worsen when H_0 is too close to $H_{\text{DSP}}(0)$.

1. Asymmetric hysteresis

To illustrate the efficiency of the TBKLA we compare it with simulations by the MA of asymmetric hysteresis in the KIM of Ref. [20]. In our implementation of the MA both the constant and the random time increments are used, but no difference between the results is noticed. The results presented in Fig. 2 show that, as expected, the efficiency of the TBKLA with respect to the MA improves when the temperature is lowered. For example, at $\beta = 2/J$ the BKLA is found to be almost four orders of magnitude (6×10^3 times) faster than the MA. The computer time in the figure corresponds to processor AMD Ryzen 5 4500U in a virtual environment, so we estimate the base frequency to be greater than approximately 2 GHz. This processor is used in all our simulations. Its characteristics can be relevant because, according to Ref. [28], the performance of thinning algorithms may crucially depend on microprocessor architecture. The efficiency of the TBKLA for simulation of the asymmetric high-frequency hysteresis to a large degree is a consequence of the fact that the evolution takes place in the vicinity of stable states which at low temperatures are almost fully ordered (see Fig. 2 in Ref. [20]). Both $\lambda(t)$ and $\bar{\lambda}$ in this case are dominated by the smallest individual spin rates, which makes the time steps in Eq. (7) large.

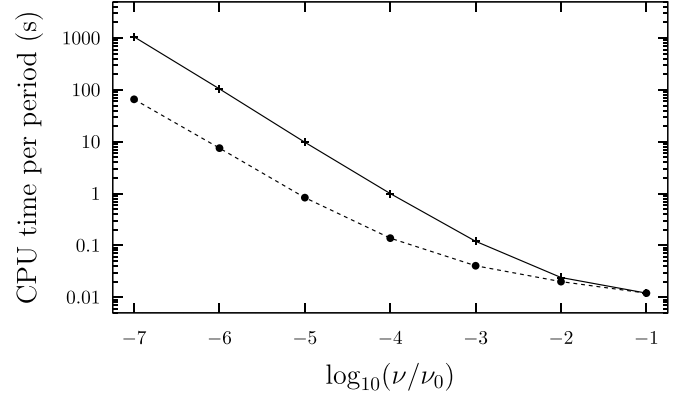


FIG. 3. Dependence of the simulation time on the frequency of oscillations of the external field for a 2D KIM of size $L = 64$ with $H = 3.5J$ at temperature $T = J$. Crosses denote results from the TBKLA and circles the TNA of Secs. VI and VII.

2. Symmetric hysteresis

In practical applications, such as hyperthermia, more interesting is the symmetric hysteresis due to much larger loop areas [18]. The symmetric loops occur at sufficiently low frequencies [39], so we test the TBKLA in this case by simulating a two-dimensional (2D) KIM of size $L = 64$ [19] using two sets of parameters. One set is $T = J$ and $H_0 = 3.5J$ and the other one is $T = 0.5J$ and $H_0 = 1.5J$. Both amplitudes H_0 satisfy Eq. (16), but in the first case, due to closeness to $H_{\text{DSP}}(0)$ and higher temperature, the system is in the deterministic regime. This is established by simulating the average nucleation time $\langle \tau \rangle$ as described in Refs. [21,23]. It is found that it does not depend on system size and is approximately equal to ν_0^{-1} , which means that there is no energy barrier for spin reversals. The average hysteresis curves remain symmetric at all simulated frequencies up to $\nu \leq 100\nu_0$.

The performance of the TBKLA is illustrated by the solid line with pluses in Figs. 3 and 4. As it can be seen from these figures, the algorithm simulates in a short time the hysteresis in the frequency region 10^5 – 10^6 Hz often used in hyperthermia even for ν_0 as large as 10^{12} Hz (using estimates of $\nu_0 \sim 10^9$ – 10^{12} Hz from Ref. [19]). As expected, at lower temperatures and H_0 further from $H_{\text{DSP}}(0)$ the much longer periods at the same computer time could be simulated.

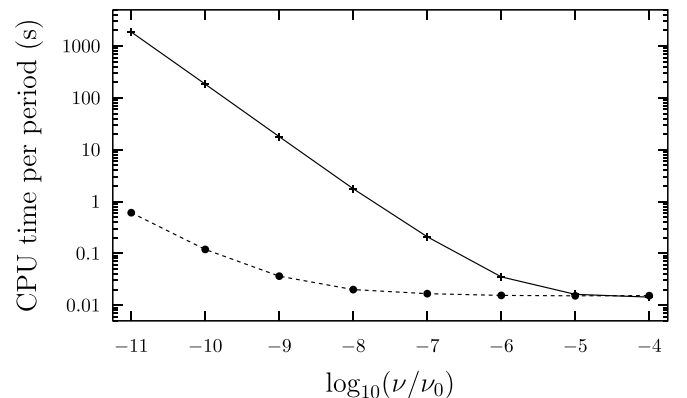


FIG. 4. Same as in Fig. 3 for $H = 1.5J$ and $T = 0.5J$.

However, smaller frequencies can still be of experimental interest [40,41]. In addition, faster simulations allow the possibility of gathering more statistics. Therefore, further acceleration of KMC algorithms at low frequencies is desirable. As it can be seen from Figs. 3 and 4, at low frequencies the simulation time is proportional to the oscillation period $\bar{t} = 1/\nu$, which can be easily understood qualitatively. According to Eqs. (1)–(5), the time variation of $\lambda(t)$ becomes weak at small ω . Further, because the average rates at all frequencies are the same (this will be explicitly shown in the next section), the KMC steps on average are of the same size at small frequencies, so the simulation time should be proportional to the period length. Thus, because on average the longer the period is the more KMC steps are needed to cover it, the algorithm acceleration should be sought in reducing the number of simulated KMC steps.

IV. THINNING THE NOVOTNY ALGORITHM

One way of reducing the number of KMC steps in thinning algorithms is to use a tighter majorization, e.g., including more steps in piecewise-constant functions. This improves the performance at moderately low frequencies, as shown in Figs. 3 and 4. However, even in stationary systems when the BKLA is fully rejectionless, the simulation of the magnetization switching in metastable states encounters a severe slowdown due to the low rate of nucleation of the opposite spin domains [21]. A solution to this problem was suggested in Ref. [11] using the observation that at low temperatures the KMC evolution is plagued by back and forth fluctuations between a small number s of transient states close to the fully ordered one without advancing the growth of nucleation droplets. However, the linear master equation with an $s \times s$ matrix of transition rates governing the fluctuations between a small number of states can be integrated faster, even analytically in some cases, than simulated by KMC methods. When out of the subspace the simulation proceeds by the standard BKLA [11]. We call this intermittent use of the BKLA and MCAMC the Novotny algorithm.

In simulations of hysteresis this approach can be even more useful because the system spends most of the time near one of two stable free energy minima where the fluctuations are completely unproductive. This is because the total magnetization reversal is virtually impossible in even small nanostructures.

In the present study we adapt an appropriately modified NA formalism to hysteresis simulation as follows. First, we use stochastic matrices in continuous time instead of the discrete-time Markov chains. Second, we deal with nonstationary Hamiltonians. Finally, to accelerate the algorithm we use thinning and call it the TNA. For simplicity, its implementation is illustrated for the simplest case $s = 2$, but generalization to larger s should be feasible along similar lines.

Before proceeding, it is important to make a remark about our notation. Because the ferromagnetic Ising model has two ordered states with positive and negative magnetizations, our notation e_0 is ambiguous, so it would be natural to distinguish the states, e.g., by using a superscript such as $e_0^\pm$. However, we need many quantities to describe the evolution of states $e_0 - e_s$, which would all have to carry the superscript. So for brevity we develop a formalism for one of the ordered states

which can be modified to use in the other state via a simple reversal of spin directions.

In the $s = 2$ case we have only two states e_0 and e_1 which satisfy the continuous-time evolution equation with a 2×2 matrix of nonstationary rates $R(t)$,

$$\frac{d\psi_k(t, t_0)}{dt} = R(t)\psi_k(t, t_0), \quad (17)$$

where ψ_k , $k = 0, 1$, are two independent two-component vectors

$$\psi_0(t, t_0) = \begin{bmatrix} p_1(t, t_0) \\ 1 - p_1(t, t_0) \end{bmatrix}, \quad (18)$$

$$\psi_1(t, t_0) = \begin{bmatrix} 1 - p_0(t, t_0) \\ p_0(t, t_0) \end{bmatrix}. \quad (19)$$

The evolution is initiated by $p_k(t_0, t_0) = 0$ so that vectors $\psi_k(t_0, t_0)$ can be identified with states e_k , $k = 0, 1$; p_1 is the probability of finding reversed spin when the evolution starts at e_0 and similarly for p_0 . Explicitly,

$$R(t) = \begin{bmatrix} -r_q(t) & Nr_0(t) \\ r_q(t) & -Nr_0(t) \end{bmatrix}, \quad (20)$$

where the underlined subscripts are the rates (3) which have the underlined number of NN spins pointing in the direction opposite to spin i and $q = 2D$ is the coordination number.

Our generalization of the algorithm of Refs. [11] proceeds as follows. If at time t_e the system state is e_0 , further evolution will follow the $e_0 \rightleftharpoons e_1$ fluctuations described by Eq. (17) for $\psi_0(t, t_e)$ until the second spin is reversed, in which case, following Ref. [11], the simulation proceeds via the TBKLA until a new occurrence of state e_0 . Because in the PP two spins cannot reverse simultaneously, the two-spin state can appear only when at least one reversed spin is already present in the system. Thus, the second reversal is given by the product of the probability of having one reversed spin $p_1(t, t_{e_0})$ multiplied by the rate of the second spin reversal in state e_1 ,

$$\lambda(t) = p_1(t, t_{e_0})r_{1 \rightarrow 2}(t), \quad (21)$$

where [23]

$$r_{1 \rightarrow 2} = [(N - q - 1)r_0 + qr_1] \quad (22)$$

is the rate of the second spin reversal in the presence of one reversed spin. Although only $p_1(t, t_{e_0})$ is needed in the TNA, the problem is that it depends on two arguments, which means that a two-parameter surface would have to be calculated and/or stored. This can be a computationally demanding task, so to facilitate it we invoke the transition matrix formalism [42] as explained in Appendix B.

V. LIFETIME OF METASTABLE STATES

To illustrate the superior performance of the TNA over the MCAMC, we consider the decay of metastable states in the stationary KIM [23,33,34,43,44]. In this case all r_i are time independent, so the integrals in Eqs. (B8) and (B11) are easily taken to give

$$p_1(t, t_0) = \mu^{-1}Nr_0(1 - e^{-\mu(t-t_0)}), \quad (23)$$

where μ , as defined in Eq. (B9), is time independent in the stationary case. Substituting this in Eq. (21), we find

$$\begin{aligned}\lambda(t) &= p_1(t, t_{e_0})[(N - q - 1)r_0 + qr_1] \\ &= \frac{r_0}{\mu}N[(N - q - 1)r_0 + qr_1](1 - e^{-\mu(t-t_{e_0})}).\end{aligned}\quad (24)$$

As it can be seen, by omitting the negative term in the second set of parentheses we can obtain a constant majorization for $\lambda(t)$ as

$$\bar{\lambda} = \frac{r_0}{\mu}N[(N - q - 1)r_0 + qr_1].\quad (25)$$

Moreover, the inequality $\bar{\lambda} \geq \lambda(t)$ is quite tight because the neglected term quickly turns to zero as $t - t_{e_0}$ grows. By assuming that N is fixed, it is easy to see that as $T \rightarrow 0$, $\bar{\lambda} \rightarrow 0$ because both rates in the numerator r_0 and r_1 vanish in this limit while $\mu \rightarrow 1$, as it can be seen from Eq. (B9), where the dominant rate $r_q \rightarrow 1$. Thus, at sufficiently low temperatures the random time difference generated with the use of $\bar{\lambda}$ in Eq. (7) will be on average much larger than $\mu^{-1} \simeq 1$, so the term with minus sign in Eq. (24) will be negligible. This means that in a typical time step at low enough temperature the rejections are very rare.

For comparison purposes we have applied the TNA (in conjunction with the conventional BKLA because of the stationary Hamiltonian) to determine the nucleation times $\langle \tau \rangle$ in two metastable systems simulated in Ref. [23] within the NA. Also, KMC simulations have been compared with the theoretical predictions of Refs. [23,32,34], according to which the nucleation time is equal to the mean time of escape over an energy barrier. In the case of single-domain (SD) nucleation the latter depends on the barrier height Γ_D as

$$\langle \tau \rangle = \frac{A_D}{v_0 N} \exp \frac{\Gamma_D}{T},\quad (26)$$

where the dependence of A_D on T is weaker than in the Arrhenius law and at low temperatures is negligible. The prefactor $1/N$ comes from the fact that SD nucleation rate, which is the inverse of τ , is proportional to the number of nucleation sites in the system N .

The first simulated system was a 2D KIM that has the largest size $L = 200$ and the highest nucleation barrier among 2D models studied in long-time simulations in Ref. [23] within the $s = 3$ MCAMC (NA in our terminology). Although we have used only the $s = 2$ TNA, we succeeded in simulating nucleation at temperatures lower than shown in Fig. 1 of Ref. [23] (see also Fig. 5 herein). The lowest temperature was $0.25J$ in our simulations and approximately $0.325J$ in Ref. [23]. In terms of the nucleation times, this amounts to a five order of magnitude difference because of large $\Gamma_2 = 13.5J$ in Eq. (26). The computer time needed for the simulation is proportional to the nucleation time and in our case it was less than 1.5 min per nucleation, which means that dealing with even lower temperatures should be feasible.

Another example is a three-dimensional KIM with $H_0 = 3.9J$ studied within the MCAMC in Ref. [23], where the small- T interpolation was not quite straightforward (see Fig. 4 in that reference). This particular case is of interest because in Ref. [23] the zero-temperature limit of the measured barrier

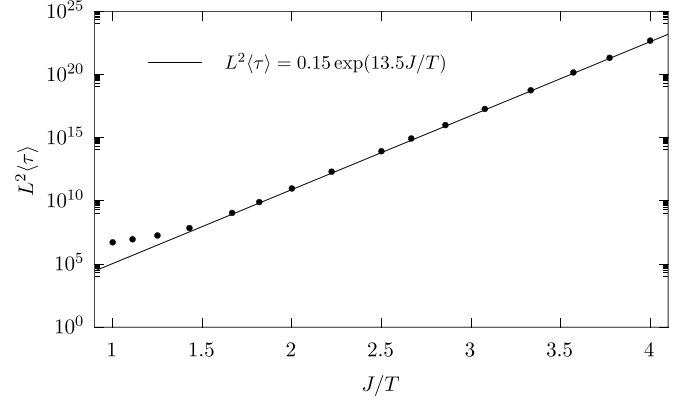


FIG. 5. Mean lifetimes of a 2D KIM of size $L = 200$ with $H = 3J/4$ as in Fig. 1 of Ref. [23] simulated with the use of the TNA (circles); the straight line is the low-temperature theoretical prediction [Eqs. (53)–(56)].

height

$$\Gamma_3(T) = T \ln(L^3 \langle \tau \rangle)\quad (27)$$

was predicted to be

$$\Gamma_3(0) = 28J - 6H_0 = 4.6J,\quad (28)$$

in strong disagreement with the $\Gamma_3(0) = J$ predicted in other studies. However, the lowest temperature $T = 0.09J$ in the simulations of Ref. [23] was rather high and in view of large statistical errors the interpolated value at $T = 0$ was not determined precisely despite the use of up to $s = 4$ MCAMCs.

Figure 6 shows our results of the $s = 2$ TNA simulations extended down to $T = 0.01J$. As it is seen, excellent agreement with Eq. (28) has been found. The average time of simulation for one nucleation event grew from 0.5 s at the highest temperature in the figure to approximately 10 min at $T = 0.01J$. Because the nucleation events are completely

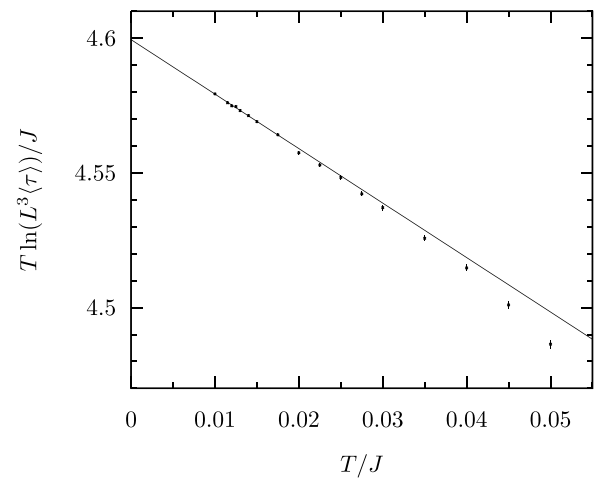


FIG. 6. Simulation of nucleation from the metastable state with the use of the $s = 2$ TNA in the simple cubic system with $L = 32$ and $|H_0| = 3.9J$ [23] at low temperatures. The number of nucleations N_{nuc} at each T is 10^3 ; the function at the vertical axis is the RHS of Eq. (27). Linear interpolation (thin solid line) is done over the points with $T \leq 0.015J$.

independent, statistics can be improved with the use of parallel architecture, so the simulations could have been performed even at lower temperatures. However, at about 33% lower temperature the double-precision arithmetic will overflow, so going to even lower temperatures would require the use of a multiple-precision arithmetic. It is important to note that because of the form of Eq. (27), according to the error propagation formula, the statistical errors scale with the number of nucleation events N_{nucl} as $T/\sqrt{N_{\text{nucl}}}$. Therefore, at $T = 0.01J$ the same accuracy as at $0.1J$ could have been achieved with 100 times less nucleation. However, in Fig. 6 the statistics were gathered over $N_{\text{nucl}} = 10^3$ at all temperatures in order to assess the algorithm performance. It may be expected that even faster simulations are possible with the use of $s > 2$ algorithms [11,24].

The slope of the linear fit in Fig. 6 is the logarithm of the prefactor in Eq. (26), which has been estimated as $A_3 \approx 0.13$. Unfortunately, there is no theoretical prediction for comparison because $|H_0|$ exceeds $2J$ [23].

Thus, our simulations show that the TNA is more efficient than the MCAMC. This is attributed to the fact that in the MCAMC one effectively deals with solving a discrete analog of Eq. (6), which is computationally more time consuming in comparison with the thinning method.

Low-temperature kinetics and thinning algorithms

Our simulations in this section and in Sec. III (see Figs. 2, 5, and 6) show that at low temperatures the TBKLA and TNA outperform previously used algorithms [20,23]. This can be qualitatively understood as follows. Due to the weakening of thermal disorder, the spin orientations are governed by the system energy. The spin reversal requires overcoming an activation barrier $E_A > 0$, where we assume that the external field satisfies the condition (16) and E_A is some ensemble- or time-averaged value sufficient for qualitative estimates. The spin-reversal probability satisfies the Arrhenius law $p_{\text{flip}} \propto \exp(-E_A/T)$, so when $T \rightarrow 0$ the MA acceptance rate becomes low and the number of attempts needed for the reversal to occur grows as $\exp(E_A/T)$. This is the reason for the MA slowdown at lowering temperature, as is seen in Fig. 2.

The integration of the exact equation (6) even in the discrete-time approximation [11] would not solve the problem because the integration range would be

$$\Delta t^{\text{flip}} \sim \Delta t^{\text{MA}} e^{E_A/T} \quad (29)$$

and $O(e^{E_A/T})$ integration steps would be necessary to solve the equation.

In the simplest implementation of thinning with a constant majorization function that we have used in the simulations, the exact rate $\lambda(t)$ is bounded by a constant $\bar{\lambda}$ satisfying $\lambda(t) \leq \bar{\lambda} < \bar{\lambda}^{\text{MA}}$, which leads to a longer average interarrival time $\langle \Delta t \rangle = 1/\bar{\lambda} > \Delta t^{\text{MA}}$. At low temperatures one can choose $\bar{\lambda} \ll \bar{\lambda}^{\text{MA}}$, thus considerably accelerating the simulation in the TBKLA due to lower number of MC steps needed to cover the Δt^{flip} time span.

At high temperatures $T \gtrsim O(E_A)$ according to Eq. (29), the time interval between the spin flips becomes of the order of Δt^{MA} . Because the computations per arrival in the MA are arguably the fastest possible ones, the few rejected arrivals

at high temperatures in the MA can be less computationally costly than those needed in the implementation of thinning. Therefore, above some $T = O(E_A)$ the MA becomes more practical. The temperature value when it happens is however *a priori* unknown. For example, from Fig. 2 one may conclude that at some temperature above $T = J$ the MA will become faster than the TBKLA, but the precise value can be determined only empirically.

An important advantage of the constant majorization is that the arrival times can be found analytically from Eq. (7) (with $\bar{\lambda}$ instead of λ). This is the reason for the better performance of the TNA in comparison with the MCAMC where a discrete version of Eq. (6) has to be solved [11]. However, the temperature dependence of the acceleration in the $s = 2$ TNA is determined mainly by the probability of occurrence of the fully ordered states in the course of the evolution. For example, while the results of Ref. [10] indicate that the TBKLA should always outperform the MA below the critical temperature T_c , the TNA would be completely useless in the KIM studied in Ref. [19] with $T = 0.8T_c$ and $H_0 = 0.1J$. The reason is that the TNA is invoked when the system becomes fully ordered. However, according to Eqs. (45) and (46) from Sec. VII A below, the probability P_{e_0} of this event is $O(10^{-20})$, that is, the TNA becomes useless in this case. However, for $H_0 \gg 0.1J$ the TNA may become operative even for $T > 0.8T_c$ because a large external field tends to align spins in one direction so the probability P_{e_0} may acquire appreciable values.

VI. TNA FOR PERIODIC FIELD

If one is interested in using the TNA to study the long-time behavior of a nonstationary KIM with an arbitrary time dependence of $H(t)$, a problem arises of computing and storing transition matrices on large time intervals. A periodicity of the external field makes it possible to deal with the transition matrix known only inside one oscillation period. This is achieved with the use of the Floquet theorem, according to which the transition matrix can be cast in the form (see, e.g., Ref. [42])

$$P(t, t_0) = S^{-1}(t) e^{K(t-t_0)} S(t_0), \quad (30)$$

where S and K are periodic and constant matrices, respectively. Thus, it is sufficient to store matrix elements of S only within one period $0 \leq t < \bar{t}$. However, if a high accuracy is needed the performance of the TNA might depend on the processor memory architecture.

To simplify the simulations, in the present study we have developed a computationally easy approximate approach for low-frequency hysteresis because, as it can be seen in Figs. 3 and 4, the exact and simple implementation in the TBKLA performs quite well at higher frequencies. At low frequencies ω/ν_0 can be used as a small parameter to develop a simple and computationally efficient formalism, as it is shown below.

To facilitate numerical estimates it is convenient to switch to dimensionless quantities

$$x = \omega t, \quad (31)$$

$$\omega = \omega/\nu_0, \quad t = \nu_0 t, \quad (32)$$

$$\lambda(x) = \lambda(t)/\nu_0. \quad (33)$$

This should not cause confusion because the definitions in (32) can be viewed as simply choosing ν_0 as the frequency unit, and when using $\lambda(x)$ [Eq. (33)] one should remember that x is defined in Eq. (31). The use of x as the evolution parameter simplifies hysteresis analysis because now the oscillation period is always 2π irrespective of the frequency. In this notation Eq. (6) becomes

$$\int_{x_0}^x \lambda(x') dx' = -\omega \ln u. \quad (34)$$

As is seen, the left-hand side of this equation does not depend on ω , so $\Delta x = x - x_0 = O(\lambda)$, which shows that the number of KMC steps needed to cover the period 2π should be proportional to $2\pi/\omega = 1/\nu = \bar{\tau}$, as pointed out in the preceding section.

To compute λ [Eq. (21)] we need to calculate the probability p_1 [Eq. (B11)], which in new notation reads

$$p_1(x, x_{e_0}) = [\hat{p}_1(x) - \chi(x, x_{e_0})\hat{p}_1(x_{e_0})], \quad (35)$$

where

$$\hat{p}_1(x) = \omega^{-1} \int_0^x \exp\left(-\omega^{-1} \int_{x'}^x \mu(x'') dx''\right) a_1(x') dx' \quad (36)$$

[see Eq. (B8)] and

$$\chi(x, x_{e_0}) = \exp\left(-\omega^{-1} \int_{x_{e_0}}^x \mu(x') dx'\right). \quad (37)$$

Similar to the stationary case of Sec. V, the majorizing rate for λ [Eq. (21)] can be obtained by neglecting the negative second term in square brackets in Eq. (35) as

$$\bar{\lambda}^0(x) = \hat{p}_1(x) r_{1 \rightarrow 2}(x). \quad (38)$$

However, unlike in the stationary case, the majorizing function is not a constant but depends on x in a nontrivial manner. This would make the thinning with its use almost as difficult as with the exact rate.

Therefore, the majorizing function $\bar{\lambda}^0$ is further approximated by a piecewise-constant function $\bar{\lambda}^{\text{st}}$ as follows [26,28]. First, to facilitate the implementation of the binary search algorithm, the dimensionless period $(0, 2\pi)$ is divided into 2^n equal intervals of length $\Delta x = 2\pi/2^n$. At each point $x_i^0 = \Delta x k$, $k = 0, \dots, 2^n - 1$, values $\bar{\lambda}_k^0 = \bar{\lambda}^0(x_k^0)$ are calculated and used as majorizing constants within the intervals; to this end, among two values of $\bar{\lambda}_k^0$ at the interval ends the larger one has to be chosen and $\bar{\lambda}^{\text{st}}(x)$ is set equal to this value within the interval. Next the piecewise majorizing function integrated over x is calculated, resulting in a piecewise linear cumulative majorizing function

$$\bar{\Lambda}(x) = \int_0^x \bar{\lambda}^{\text{st}}(x') dx', \quad (39)$$

which is easily calculated with the knowledge of Δx and of the sequence $\{\bar{\lambda}_k^{\text{st}}\}$. It is used to generate the arrival times via an algorithm described in Refs. [26,28]. The arrivals to be thinned are generated according to Eq. (6), written as

$$\bar{\Lambda}(x) - \bar{\Lambda}(x_0) = \int_{x_0}^x \bar{\lambda}^{\text{st}}(x') dx' = -\omega \ln u \quad (40)$$

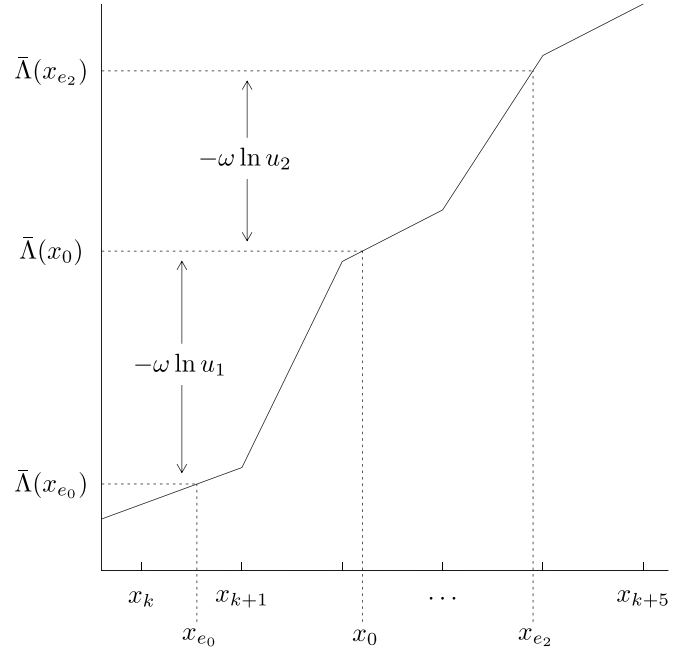


FIG. 7. Schematic illustration of the $s = 2$ TNA hysteresis simulation with the use of a piecewise linear cumulative majorizing function $\bar{\Lambda}(x)$ [Eq. (39)]. It is assumed that at the point x_{e_0} the TBKLA simulation reaches a fully ordered state e_0 . Then $\bar{\Lambda}(x_{e_0})$ is calculated as described in the text and a random variate u_1 is generated. The next arrival point x_0 is determined and another random variate u'_1 is generated to test the acceptance criterion (9). If the arrival is rejected, yet another random variate u_2 is generated and x_{e_2} is found as above. Here the subscript e_2 is chosen because this time we assume that u'_2 satisfies the acceptance criterion so the configuration should contain two reversed spins. From this point the simulation proceeds by the TBKLA.

and cast in the form

$$\bar{\Lambda}(x) = \bar{\Lambda}(x_0) - \omega \ln u. \quad (41)$$

Now, given x_0 , the interval k to which it belongs is found simply as the integer part of $x_0/\Delta x$. Then $\bar{\Lambda}(x_0)$ is found by simple linear interpolation within the interval. Next, having generated u to obtain $\bar{\Lambda}(x)$, one finds x by first determining the interval to which the $\bar{\Lambda}(x)$ value belongs by bracketing it via a binary search algorithm and then finding x using inverse linear interpolation within the interval. Two steps of the algorithm of Ref. [28] adapted to the present case are shown in Fig. 7.

Numerical implementation

Unlike in the stationary case of the preceding section, in the oscillating field the quadratures in Eqs. (36) and (37) can be taken only numerically. The equations are exact, so the computations in principle can be performed with an arbitrary precision. However, numerical integration with high accuracy requires significant computational resources, which will slow down the performance of the algorithm. However, in long-time simulations the execution speed is of major importance. Therefore, to avoid generation of stochastic time increments, in the MA simulations of Refs. [11,19,20] the authors chose a constant increment (11), which means that arrival times

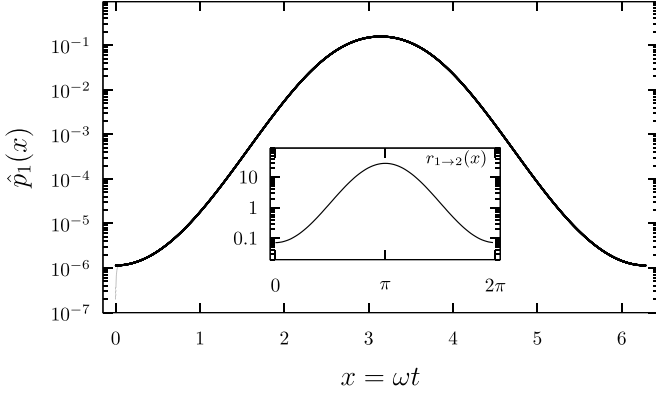


FIG. 8. The solid line shows the numerical integration in Eq. (B8) compared to the approximate analytic expression (43) (dots). The 2D KIM parameters were $L = 64$, $T = 0.5J$, $H = 1.5J$, and $\omega = 10^{-2}v_0$; the inset shows the rate $r_{1 \rightarrow 2}$ Eq. (22) in units of v_0 .

cannot be determined with an accuracy better than Δt^{MA} . In a slowly varying external field with the frequencies satisfying Eq. (12), this should be irrelevant.

Constant majorization would not be efficient in the case of functions that strongly vary in time, such as λ [Eq. (21)] and $\bar{\lambda}^0$ [Eq. (38)]. To simplify the simulation of arrivals in this case we use the fact that the TNA is not needed at high frequencies where the exact TBKLA is sufficient (see Figs. 3 and 4). At low frequencies, on the other hand, the closeness to the stationary case $\omega = 0$ makes frequency a natural expansion parameter which can be used to calculate the rates with a desirable precision. To this end we first note that the integration range in Eqs. (6) and (40) $x - x_0 = O(\omega)$. Thus, if the rates in the equations will be known to $O(\omega)$ accuracy, the error δx in the dimensionless arrival time will be $O(\omega^2)$; hence, according to Eq. (31),

$$\delta t = O(\omega). \quad (42)$$

Thus, the accuracy of determination of arrival times will improve as frequency lowers and eventually should exceed the accuracy of approximation (11).

The quadratures in the first of two terms in p_1 [Eq. (35)] can be performed to $O(\omega)$ precision using the Laplace form of the integral. According to Appendix C, at small ω it can be approximated as

$$\hat{p}_1(x) = \frac{a_1(x)}{\mu(x)} + O(\omega), \quad (43)$$

where higher-order terms in ω can also be determined [45].

The quality of the approximation (43) has been tested by a numerical integration over 10^4 points in Eq. (B8) for the sinusoidal field (2). From Fig. 8 it can be seen that even at relatively high frequency $\omega = 0.01$ the worst discrepancy is restricted to a narrow interval $\Delta x \sim O(\omega)$ near $x = 0$ where the exact value should vanish while the approximation is finite. This means that the errors will be $O(\omega)$, in agreement with the chosen level of approximation. The error introduced by the discrepancy is further reduced by the prefactor $r_{1 \rightarrow 2}$ in the NHPP rate (21), as can be seen in Fig. 8. To estimate the quadrature in Eq. (37) we first point out its difference from similar integration in Eq. (36). In the latter case it may cover

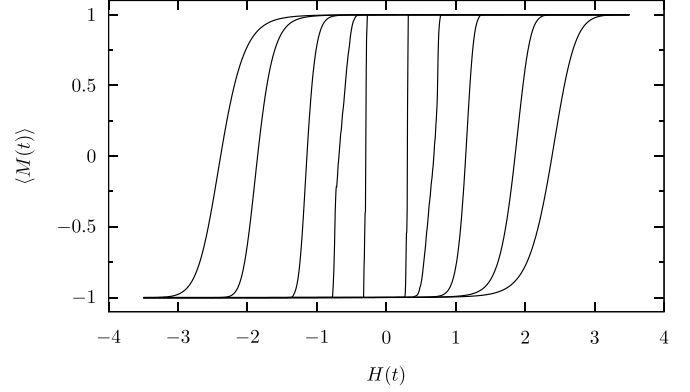


FIG. 9. Hysteresis loops for a 2D KIM with $L = 64$ [19], $H_0 = 3.5J$, and $T = J$ for frequencies (in order of decreasing area) $v/v_0 = 10^{-2}$ (10^6), $10^{-2.5}$ (10^6), $10^{-3.5}$ (10^5), 10^{-5} (10^4), and 10^{-10} (6); in parentheses is the number of simulated loops.

an arbitrarily large part of the oscillation period 2π , that is, is an $O(1)$ quantity, while in Eq. (37) x and x_e differ by a quantity $O(\omega)$. This can be seen from Eq. (34), which contains the exact rate λ so it generates the accepted arrival $x = x_{e_2}$, which terminates the simulation of $e_0 \rightleftharpoons e_1$ fluctuations. State e_2 with two reversed spins should be further simulated with the TBKLA. Thus, arrival x simulated with the use of a majorizing rate is always smaller than or equal to x_{e_2} and so also is at an $O(\omega)$ distance from x_e . This is illustrated in Fig. 7 for simulation with the use of a piecewise-constant majorizing rate.

Further, because in Eq. (B9) $\mu(x) = O(\omega^0)$ and $\Delta x = x - x_{e_0} = O(\omega)$, the integral in Eq. (37) can be approximated by a single step of the trapezoidal rule. Corrections to the latter are of order $(\Delta x)^2 = O(\omega^2)$, which divided by ω makes errors in Eq. (37) to be $O(\omega)$. This is sufficient at our level of approximation.

Thus, by neglecting $O(\omega)$ terms, the NHPP rate (21) can be found without resource-intensive numerical integrations and/or interpolations.

VII. HYSTERESIS SIMULATION

Because at sufficiently low frequencies the hysteresis loops shrink, the hysteretic behavior eventually becomes stochastic. Its exhaustive description requires many statistics to be gathered and analyzed, which necessitates the acquisition of large volumes of data and poses nontrivial storage problems [19]. Because our primary goal is the algorithm's performance, in our simulations we gathered only a simple statistic of average hysteresis loops. Several of them are shown in Fig. 9. The simulation time of one loop scales inversely proportional to the frequency; therefore, averages have been performed over 10^6 loops at the highest frequencies to only 6–10 loops at the lower end of the frequency range due to computer time restrictions. Data have been gathered in 2^{12} bins of equal width.

The loops presented in Fig. 9 were simulated with both the TNA and the pure TBKLA (except at the lowest frequency where the TBKLA was too slow) and no difference was discernible at the scale of the drawing. This was a test of our

additional approximation in using the TNA where we set the magnetizations to their saturated values to further accelerate simulations of $e_0 \rightleftharpoons e_1$ fluctuations. The soundness of this approximation and the range of validity will be discussed below.

A. Parameter dependence of the TNA accuracy

The steepest variation of magnetization in the hysteresis loops occurs in the vicinity of $\pm H_c$ where the dynamic coercive field H_c can be defined as the absolute value of the external field when the magnetization changes sign, that is, when $M = 0$ (see Fig. 9). In these regions the errors in simulated M will be the largest. To assess them we note that at low frequencies the magnetization reversal occurs in a single nucleation event [19] with M at low temperatures switching from $\pm m_0$ to $\mp m_0$ with $|m_0| \simeq 1$. Therefore, at $H \simeq \pm H_c$ magnetizations M will be the averaged random sequences of $M \approx \pm 1$, which means that the mean dispersion will be approximately 1. The statistical error in this case will scale as the inverse square root of the number of simulated loops $\delta M \simeq 1/\sqrt{N_{\text{loops}}}$, which we will use as a reference in further estimates.

A straightforward estimate of the magnetization change during $e_0 \rightleftharpoons e_1$ fluctuations can be obtained by assuming that the flipped spin contributing $\pm 2/N$ to the total magnetization $M = \pm 1$ stays reversed throughout the fluctuation time span. The contribution can be considered negligible when it does not exceed $\delta M \simeq N_{\text{loops}}^{-1/2}$ at the switching points, which would take place when

$$N_{\text{loops}} \lesssim N^2/4 \approx 4 \times 10^6, \quad (44)$$

where the numerical value is for $N = 64^2$. It should be noted that fluctuations with more than one reversed spin are simulated within the TBKLA and their contributions to the magnetization are taken into account exactly.

The inequality (44) can be improved by weakening the underlying assumption. In deriving it we have assumed that in the course of fluctuations $e_0 \rightleftharpoons e_1$ the probability of e_1 is unity, though in reality it is usually small. At low frequencies we may assess the probability P_{e_1} of e_1 occurrence by invoking the adiabatic approximation [19] and using the ergodicity principle. It should be noted that such an estimate will give only an upper bound on the probability of e_1 in $e_0 \rightleftharpoons e_1$ fluctuations because during the latter e_1 appears only from the $e_0 \rightarrow e_1$ process while the equilibrium P_{e_1} accounts also for the $e_2 \rightarrow e_1$ process, which we treat within the exact TBKLA.

The probability can be estimated in the mean-field approximation (MFA) of equilibrium statistics, which is quite reliable at low temperatures (see, e.g., Ref. [46]). In the MFA all spins are assumed to be independent, so the probability is a product of probabilities over all sites, which in the case of e_0 is

$$P_{e_0} = (p_0^{\text{eq}})^N \quad (45)$$

because in a homogeneous system all sites are equivalent. For the Ising model on the square lattice the MFA gives

$$p_0^{\text{eq}} = (1 + e^{-2\beta(4J+H)})^{-1}. \quad (46)$$

Here we have assumed that the ordered state corresponds to positive magnetization $M \approx 1$ and that the expression is

also valid for metastable states because in the MFA both behave similarly in the vicinity of the saturated magnetization [20,47,48]. Hence,

$$P_{e_0}(H, T, N) = [1 - p_1^{\text{eq}}(H, T)]^N \simeq e^{-N p_1^{\text{eq}}(H, T)}, \quad (47)$$

where in the second equality we have assumed $p_1^{\text{eq}} \equiv 1 - p_0^{\text{eq}} \simeq e^{-2\beta(4J+H)}$ to be small. Similarly,

$$P_{e_1}(H, T, N) = N p_1^{\text{eq}} (p_0^{\text{eq}})^{N-1} \simeq N p_1^{\text{eq}} e^{-N p_1^{\text{eq}}}. \quad (48)$$

As is easily seen, the last function of p_1^{eq} is unimodal with maximum value $1/e$ occurring at $p_1^{\text{eq}} = 1/N$. Thus, using the formula

$$\delta M = (2/N) P_{e_1}, \quad (49)$$

one may obtain instead of Eq. (44)

$$N_{\text{loops}} \lesssim (e/2)^2 N^2 \approx 3 \times 10^7, \quad (50)$$

which is an order of magnitude larger number.

The value of external field H_m where P_{e_1} reaches its maximum can be found by solving the equation $p_1^{\text{eq}}(T, H_m) = 1/N$ at small p_1^{eq} as

$$H_m = -4J + 0.5T \ln N. \quad (51)$$

However, H_m may not be reachable by the oscillating field because it is restricted to $-H_0 \leq H(t) \leq H_0$. In such cases $P_{e_1}(H, T, N)$ will attain its maximum at one of the boundaries $\pm H_0$ where the probability, hence δM , will be smaller than at H_m .

For example, in the model with the parameters of Fig. 4, $H_m \simeq -1.9J$ while $-H_0 = -1.5J > H_m$. From Eq. (49) $\delta M(0.5J, -1.5J) \simeq 7.5 \times 10^{-5}$, which means that approximately 2×10^8 loops have to be simulated to make this correction comparable to the statistical error at H_c . This is arguably only a lower bound for N_{loops} because at low frequencies the metastable state would hardly survive down to $H = -1.5J$.

In the model of Fig. 9 $H_m \approx 0.16J$ is within the oscillation range $-3.5J \leq H \leq 3.5J$. By Eq. (49) $\delta M = 2/eN \approx 2 \times 10^{-4}$ at H_m , while in the most stable state $\delta M(3.5J, J) \simeq 6 \times 10^{-7}$, which is three orders of magnitude smaller. This disparity of values can be used to accelerate simulations even when small corrections due to the single spin flips are important, e.g., in small systems. Because $O(10^{-7})$ accuracy can rarely be demanded in MC simulations, a threshold value of δM^{min} can be chosen to invoke the computation of the correction only when δM^{min} is exceeded. The MFA expressions (48) and (49) and suitably modified equation (51) should be sufficient for this purpose.

B. Hysteresis loop areas

The frequency dependence of the loop areas for $T = J$ case is shown in Fig. 10. The area dispersion has been calculated only for the lowest frequency where all six loops have been measured. Arguably, the resulting error is the largest one because the number of simulated loops grew up to 10^6 at higher frequencies. The change of the curve slope seen in Fig. 10 has been attributed to the transition from stochastic to the deterministic regime as the dynamic coercive field grows [19,21].

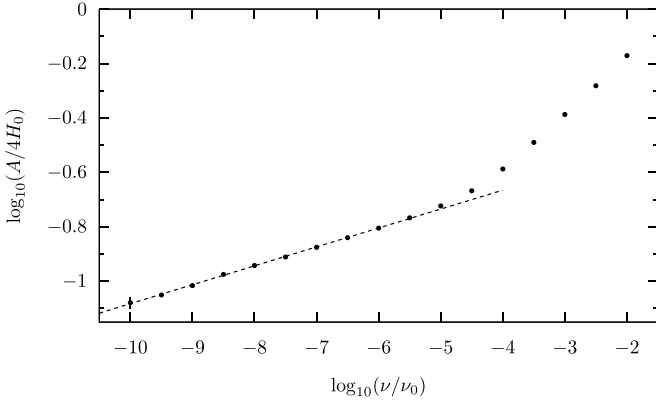


FIG. 10. Circles show the simulated frequency dependence of the hysteresis loop area A for a KIM with the same parameters as in Fig. 9. The dashed line is the power-law fit to the dependence proportional to ω^γ , with $\gamma \simeq 0.07$ at low frequencies. The error bar at the leftmost point is the standard deviation of approximately 5%, which for six simulated loops amounts to a standard error of approximately 2%, which we assess to be the largest error among all data points.

As can be seen in Fig. 3, the TNA performance at $T = J$ is only about one order of magnitude faster than that of the simple TBKLA with constant majorization. We see two plausible causes for that. First, the closeness of $H_0 = 3.5J$ to $H_{\text{DSP}}(0) = 4J$ makes the purely constant majorization inefficient, so the piecewise-constant majorization should accelerate the TBKLA part of the algorithm. Second, at higher temperatures the number of flipped spins in the ground state grows. This can enhance fluctuations within a set of states with more reversed spins than one, so the use of the $s > 2$ TNA may significantly improve the algorithm performance [11].

As expected, at $T = 0.5J$ it is possible to simulate much lower frequencies because the acceleration provided by the TNA is considerably higher, as can be seen from the comparison of the lower and the upper curves in Figs. 3 and 4. The simulation data shown in Fig. 11 are obtained by averaging loop areas over 10 – 10^6 hysteresis cycles with the number growing from the lowest to the highest frequencies. As in the case $T = J$, at the lowest frequencies the statistics have been gathered over individual loops and the standard deviation has been found to be approximately 1.5%, hence the standard error less than the size of the symbols in Fig. 11. As it is shown in the next section, the dispersion grows weakly with the increased frequency. However, because the number of simulated loops has been growing faster, the estimated errors at higher frequencies have been assessed to be negligible.

The lowest frequency $\nu/\nu_0 = 10^{-16.5} = 3.16 \times 10^{-17}$ simulated at $T = 0.5J$ would correspond in physical terms to $\nu \sim 30$ nHz if the lowest estimated $\nu_0 = 1$ GHz would be used, which is much smaller than in previous hysteresis simulations [19]. Going to even lower frequencies encounters not only the problem of the fast growing computation time (approximately 16 h per period) but also problems of arithmetic precision. As it has been argued earlier, from Eq. (34) it follows that a typical step size $\Delta x = O(\omega)$. Thus, to pass an oscillation period one would have to add Δx to x of order

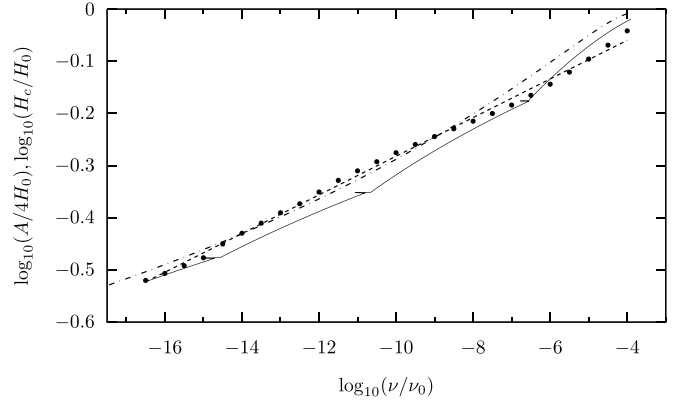


FIG. 11. Circles show the simulated frequency dependence of the hysteresis loop area of a 2D KIM at $T = 0.5J$ with $H_0 = 1.5J$; the dashed line shows the power-law fit to ω^γ , with $\gamma \simeq 0.037$; the dash-dotted line shows the frequency dependence on the dynamic coercive field H_c [Eq. (62)]; and the solid line shows the adiabatic approximation [19] with the use of Eqs. (53)–(56).

of the period length 2π . However, $\omega/2\pi = \nu$, so with $\nu < 3.16 \times 10^{-17}$ we are already below the double-precision machine epsilon value 2.22×10^{-16} . Thus, simulations at lower frequencies would require the use of a multiple-precision arithmetic.

C. Low-temperature theory

Because $T = J$ is a relatively high temperature, theoretical interpretation of the data in Fig. 10 should be sought within the approach of Ref. [19], which, however, requires some heuristic input. On the other hand, in Refs. [23,34] it was found that the fully analytic low-temperature theories of Refs. [33,34,43,44] can be valid up to $T = 0.5J$ – $0.6J$. Though the nucleation theories in these studies, in particular, Eq. (26), were developed for the stationary case, they can be adapted to a low-frequency hysteresis within the adiabatic approximation [19]. It should be noted that in the above theories it was assumed that the system is in a metastable state, while during hysteresis it spends most of the time in stable states. Therefore, the range of validity of Eq. (26) in our case is restricted to such values of τ when the external field is directed oppositely to the system magnetization. In addition, because at low frequencies the magnetization switch predominantly occurs within each half-period [49], the external field (2) will be directed oppositely to it when $\omega t = 2\pi n + \pi/2 + \omega\tau$, where n is an integer and $0 < \omega\tau < \pi$, where for concreteness we assumed that initially the system magnetization was negative. Within this time interval, according to Eq. (2),

$$H(\tau) = H_0 \sin(\omega\tau) > 0. \quad (52)$$

In the 2D case at a frequency sufficiently low for the adiabatic approximation to be adequate [19,22] the rate of a droplet nucleation λ_n can be estimated as the inverse of the average nucleation time (26), which for the 2D KIM reads [23,33,34,50]

$$\lambda_n(\tau) = (L^2/A_2)e^{-\Gamma_2(\tau)/T}, \quad (53)$$

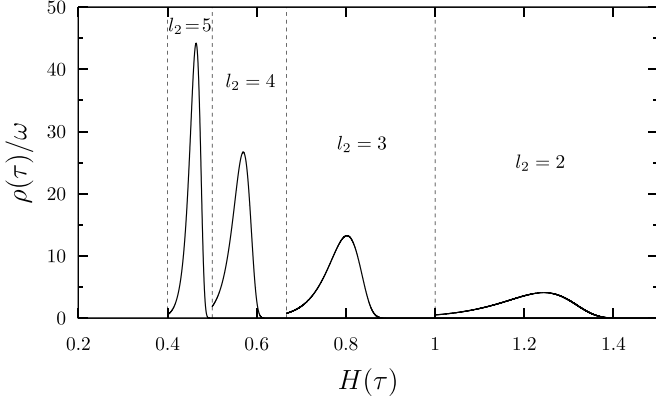


FIG. 12. Probability density rate of the magnetization switch (A4) with $\lambda_n(\tau)$ [Eq. (53)]. Only the first quarter-period after the field reversal at $\tau = 0$ is shown. The curves from right to left are drawn for $l_2 = 2, 3, 4, 5$, respectively, where the corresponding distribution maxima occur at frequencies $\nu/\nu_0 = 10^{-5}, 10^{-9}, 10^{-13}, 10^{-16}$ in the same order. The values correspond to four segments of the solid line in Fig. 11.

where [44]

$$A_2 = 3/(8l_2 - 4), \quad (54)$$

$$\Gamma_2(\tau) = 8Jl_2 - B_2H(\tau), \quad (55)$$

$$B_2 = 2(l_2^2 - l_2 + 1), \quad (56)$$

and

$$l_2(\tau) = [2J/H(\tau)] + 1. \quad (57)$$

The first term on the RHS of (57) is the integer part, which means that $l_2(\tau)$ is discontinuous at integer values of $2J/H(\tau)$ while being τ independent in between.

Equations (26) and (53) have been derived for decay of metastable states that appear after an instant reversal of the external field to favor the spin orientation opposite to the current magnetization. Therefore, in the case of hysteresis it is expected to be valid only during the first half-period after the field reversal, say, at $\tau = 0$, because the half-periods in the stable states are beyond the region of validity of the equations. In other words, the underlying picture should be that of the magnetization switching occurring every half-period which can be observed in hysteresis with sufficiently large periods (see Ref. [19] and below). The probability density can be described by Eq. (A4) with $t_0 = 0$ and $t = \tau$ as

$$\rho(\tau) = \lambda_n(\tau) \exp\left(-\int_0^\tau \lambda_n(\tau') d\tau'\right). \quad (58)$$

In Fig. 12 $\rho(\tau)$ is plotted within the first quarter-period of the oscillation where the one-to-one correspondence between the sine function and its argument has made possible to draw the $\rho - H$ dependence. The integrated probability within each of the curves shown in Fig. 12 has been found to be smaller than unity by less than approximately 10^{-4} , which supports the qualitative picture of magnetization switching every half-period. As can be seen, the probability rate distributions at small frequencies are quite narrow, so the average

value of the dynamic coercive field H_c can be estimated by the Laplace integration [45] as $H_c \equiv H(\tau_c) = H_0 \sin \omega \tau_c$, where τ_c is the most probable switching time at the maximum of $\rho(\tau)$ [Eq. (58)]. From $\rho'(\tau_c) = 0$ (prime means derivative over τ_c) one finds

$$\lambda_n'(\tau_c) = \lambda_n^2(\tau_c) \quad (59)$$

or

$$[\lambda_n^{-1}(\tau_c)]' = -1. \quad (60)$$

Substituting this in Eqs. (53) and (60), one finds an explicit equation for τ_c ,

$$(A_2/L^2)B_2(H_0/T) \cos(\omega \tau_c) e^{\Gamma(\tau_c)/T} = 1/\omega, \quad (61)$$

valid within the time intervals defined by Eq. (57) where l_2, A_2 , and B_2 remain constant. Equation (61) can be cast in a form convenient for drawing plots in Fig. 11,

$$\nu = \frac{L^2 T \exp[(B_2 H_c - 8Jl_2)/T]}{2\pi A_2 B_2 H_0 \sqrt{1 - (H_c/H_0)^2}}, \quad (62)$$

where the solid line is drawn according to this equation with the use of Eqs. (54)–(56). The cusps at integer values of l_2 have been drawn to show the infinitely narrow spikes in the values of A_0 at zero temperature; at finite temperatures they will broaden [34]. So with the broadening taken into account, the theoretical curves would approach the simulated data even closer. Furthermore, the use of an average over τ with the probability density ρ instead of using only the maximum value should smear the remaining cusps in the curves. This suggests that low-frequency hysteresis at low temperatures may be amenable to analytic treatment along the lines of Refs. [19,34].

As $\omega \rightarrow 0$, H_c also tends to zero, so the step separation in Eq. (57) becomes small and can be accurately approximated by a continuous function

$$l_2 \simeq 2J/H_c + 0.5. \quad (63)$$

Substituting this in Eqs. (54)–(56) and (62), one obtains an analytic expression plotted as the dash-dotted curve in Fig. 11. It can be easily analyzed at small H_c and the asymptotic behavior $A \propto 1/\ln \omega$ [22] can be found. Thus, despite the good agreement of the simulated data with the power-law function seen in Figs. 10 and 11, our calculation confirms the conclusion of Ref. [19] that this is just a transient phenomenon and the true asymptote is the inverse logarithm of the frequency.

VIII. SUMMARY

In this paper we have proposed a general thinning algorithm for Monte Carlo simulations of hysteresis and of the metastable state decay in the kinetic Ising models with the Glauber dynamics. This was achieved by extending the Bortz-Kalos-Lebowitz algorithm [10] and the Novotny algorithm [11] to time-dependent Hamiltonians and by accelerating the generation of arrival times in the resulting nonhomogeneous Poisson processes using the thinning method [25–28,30].

Among three implementations of the GTA developed in this work, the most useful and straightforward to implement is the thinned BKLA. The TBKLA is efficient for systems of any size and performs well at high to moderately low frequencies

of practical interest [18], as well as at temperatures where the Metropolis algorithm becomes ineffective. We have illustrated the TBKLA using the simplest case of majorization by a constant rate, which is efficient for low-magnetic-field amplitudes. However, piecewise-constant majorization suitable for arbitrary external field strength would be equally universal and readily implementable.

The efficiency of the thinned NA has been demonstrated by simulating the metastable state decay in the stationary case [21,23]. Using the $s = 2$ TNA, where $s - 1$ is the number of transient states in the algorithm [11], we succeeded in simulating lifetimes up to 177 orders of magnitude longer than those reported in Ref. [23] within the $s \geq 3$ NA. We further extended the TNA to the case of oscillating external field using thinning with a piecewise-constant majorization function. Floquet's theory guarantees that all computations can be reduced to a single oscillation period, thereby lowering storage requirements.

However, unlike in the TNA for stationary Hamiltonians where NHPP rates can be found analytically, in the sinusoidal external field the integrals in the NHPP rate can be computed only numerically. In principle, the calculations can be done to any desirable precision. However, high accuracy would require extensive computations, which would reduce the algorithm performance. Therefore, in our study we restricted the accuracy only to be not worse than the statistical errors in simulated data, namely, because the exact TBKLA is effective at high to moderately small frequencies, we restricted the accuracy to a zeroth-order approximation in the frequency. This would improve the accuracy for slower oscillations and eventually it should overcome the constant-time-step approximation used in similar studies in Refs. [19,20].

In addition, in hysteresis loops the switching between two saturated values of magnetization proceeds via stochastic nucleation events with the statistical errors scaling as the inverse square root of the number of simulated loops. Further, the contribution of a reversed spin in the single-spin fluctuations in the TNA to the saturated magnetization scales as the inverse total number of spins in the system. Therefore, for the KIM of 64^2 spins used in our simulations, this contribution is negligible when the number of loops is less than $O(10^7)$. It is pertinent to note that the largest number of loops in our study 10^6 could be easily simulated by the pure TBKLA, the TNA being indispensable only at very low frequencies where the number of simulated loops was much smaller, down to 6–10 loops at the lowest frequencies. In addition, our mean-field estimates, which are quite reliable at low temperatures, show that an even larger number of loops must be simulated in order for the single-spin-flip contributions to become noticeable. In small systems and/or for a very large number of simulated loops this contribution can be taken into account exactly, though at the cost of additional computations.

Our simulations were restricted to relatively small nanostructures, where the single-domain nucleation dominates. In principle, following Ref. [15], a large system could be divided into nonoverlapping boxes small enough for single-spin fluctuations to dominate, thus allowing the TNA to capture the relevant physics. In practice, however, this poses severe combinatorial challenges, since one would need to track not only spin pairs within some of the boxes but also boundary flips affecting rates in neighboring boxes. Restriction to only

two boxes may still be feasible. This could be relevant for simulation of nanomagnets in hyperthermia applications where optimum performance occurs near the transition from SD to many-domain nucleation [18]. It should be emphasized that the NA and TNA remain exact in systems of any size, only the probability of occurrence of the processes they describe would be reduced in large systems. An alternative to dealing with the boxes may be therefore to extend the TNA to $s > 2$, enabling simulations of larger systems and/or at higher temperatures [11].

Because in comparison to the MA the implementation of thinning algorithms requires additional computations, they are most advantageous at the lowest temperatures where the MA is inefficient. However, our simulations of hysteresis were carried out at relatively high temperatures, corresponding to approximately 20% and 40% of the critical temperature of the 2D Ising model. This choice was deliberate because in Refs. [23,33,34,43,44,51] and in the present study it was found that below about 25% of the critical temperature analytic theories agree well with simulations, suggesting that low-temperature analytic theories of hysteresis should be feasible. At higher temperatures, however, both in the present study and in Ref. [19] the agreement is much poorer, making thinning algorithms more valuable. For some commonly used ferromagnetic materials, the studied temperature range includes room temperature as well as the regime relevant for hyperthermia applications [18], suggesting that suitably adapted thinning algorithms can provide a practical tool for simulations of magnetic nanostructures of practical interest.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [38].

APPENDIX A: FIRST ARRIVAL TIME

The probability distribution of the first arrival after t_0 can be derived as follows. Let the probability that no arrivals occurred in the interval (t_0, t) be $\bar{p}(t, t_0)$. Then the probability of no arrivals at time $t + \Delta t$ is $\bar{p}(t + \Delta t, t_0) = \bar{p}(t, t_0)[1 - \lambda(t)\Delta t]$, where the second term in square brackets accounts for the probability of arrival within the time interval $(t, t + \Delta t)$. With the initial condition $\bar{p}(t_0, t_0) = 1$, the solution of the ensuing differential equation is

$$\bar{p}(t, t_0) = \exp\left(-\int_{t_0}^t \lambda(t')dt'\right). \quad (\text{A1})$$

Hence, the probability that the arrival did occur within time interval (t_0, t) is

$$\begin{aligned} f(t, t_0) &= 1 - \bar{p}(t, t_0) = 1 - \exp\left(-\int_{t_0}^t \lambda(t')dt'\right) \\ &= \int_{t_0}^t \rho(t', t_0)dt', \end{aligned} \quad (\text{A2})$$

where the equality on the second line reflects the fact that in f all occurrences of the event anywhere within the time interval have been taken into account. So f is the cumulative distribution for some probability density function ρ .

The task of simulating the arrival event is solved by the theorem stating that the values of the stochastic function f in Eq. (A2) are homogeneously distributed within the interval $(0, 1)$ (see, e.g., Ref. [29], Theorem 2.1.10). So one has to generate the uniform variate $u \in (0, 1)$ and determine arrival time t by solving the equation

$$f(t, t_0) = u. \quad (\text{A3})$$

Here we note that in the PP the arrivals cannot be simultaneous, so there always is the first arrival which terminates the no-arrival time interval. Therefore, by differentiating Eq. (A2) with respect to t , we find that ρ is the rate of the first arrival [25]

$$\rho(t, t_0) = \lambda(t) \exp\left(-\int_{t_0}^t \lambda(t') dt'\right), \quad (\text{A4})$$

which is further confirmed by its unit normalization. This expression generalizes to the NHPP the exponential distribution of interarrival intervals of the conventional PP with constant λ . Moreover, the NHPP can be mapped onto the PP by a nonlinear transformation [25].

APPENDIX B: TRANSITION MATRIX

The rate matrix in Eq. (20) has the form

$$R(t) = \begin{bmatrix} -a_0(t) & a_1(t) \\ a_0(t) & -a_1(t) \end{bmatrix}, \quad (\text{B1})$$

with explicit expressions for functions a_i found in Eq. (20). The 2×2 transition matrix is defined as

$$\begin{aligned} P(t, t_0) &= \begin{bmatrix} 1 - p_0(t, t_0) & p_1(t, t_0) \\ p_0(t, t_0) & 1 - p_1(t, t_0) \end{bmatrix} \\ &= [\psi_1 \psi_0]. \end{aligned} \quad (\text{B2})$$

Its columns are vectors ψ_1 and ψ_0 , so according to Eq. (17) it satisfies the equation

$$\frac{d}{dt} P(t, t_0) = R(t) P(t, t_0) \quad (\text{B3})$$

with the initial condition

$$P(t_0, t_0) = I. \quad (\text{B4})$$

With the use of Eq. (B3) it can be shown that the matrix P also satisfies the functional equation [42]

$$P(t, t_0) = P(t, t_1) P(t_1, t_0), \quad (\text{B5})$$

where $t \geq t_1 \geq t_0$. Now assuming that the range of the time variable is $[0, \infty)$, it is easy to see from Eq. (B5) that $P(t, t_0)$

can be expressed in terms of $\hat{P}(t) \equiv P(t, 0)$ as

$$P(t, t_0) = \hat{P}(t) \hat{P}^{-1}(t_0). \quad (\text{B6})$$

Thus, a two-parameter matrix P can be calculated with the use of a one-parameter matrix $\hat{P}$ which can reduce computational overhead in KMC simulations when an analytical solution is not available. In fact, from Eq. (B2) it can be seen that only one matrix element of P is needed in Eq. (21),

$$\dot{\hat{p}}_k = -(a_0 + a_1) \hat{p}_k + a_k, \quad (\text{B7})$$

where $\hat{p}_k(t) = p_k(t, 0)$ (the arguments t of all terms in the equation have been omitted for brevity). The solution of Eq. (B7) reads

$$\hat{p}_k(t) = \int_0^t \exp\left(-\int_{t'}^t \mu(t_1) dt_1\right) a_k(t') dt', \quad (\text{B8})$$

where

$$\mu(t) = a_0(t) + a_1(t). \quad (\text{B9})$$

To invert $\hat{P}(t_0)$ in Eq. (B6) we will need its determinant

$$\det \hat{P}(t) = 1 - \hat{p}_0(t) - \hat{p}_1(t) = \exp\left(-\int_0^t \mu(t') dt'\right), \quad (\text{B10})$$

where the second equality (a particular case of the Abel-Jacobi-Liouville theorem [42]) has been obtained with the use of Eqs. (B2) and (B8). Now by using Eq. (B6), we get the probability

$$p_1(t, t_0) = \hat{p}_1(t) - \exp\left(-\int_{t_0}^t \mu(t') dt'\right) \hat{p}_1(t_0) \quad (\text{B11})$$

that enters the NHPP rate (21). An important observation concerning this expression is that dependence on t_0 on the RHS is confined to the second term, which is not positive because $\hat{p}_1 \geq 0$. Thus, the first term, which depends only on t , is a majorizing function to $\lambda(t)$ [Eq. (21)]. This means that a computationally simple one-parameter majorization is possible in this problem.

APPENDIX C: LAPLACE INTEGRAL

Equation (36) is a Laplace integral of the form

$$\begin{aligned} I(K) &= \int_a^b f(x) e^{K\phi(x)} dx \\ &= \frac{1}{K} \int_a^b \frac{f(x)}{\phi'(x)} d(e^{K\phi(x)}), \end{aligned} \quad (\text{C1})$$

with $\phi(x)$ reaching its maximum value (zero in our case) at the upper integration boundary. Integrating by parts, we find (see Ref. [45], Chap. 6.3)

$$I(K) \simeq \frac{1}{K} \frac{f(b)}{\phi'(b)} e^{K\phi(b)} + O\left(\frac{1}{K^2}\right). \quad (\text{C2})$$

Further terms of the asymptotic expansion can also be calculated [45].

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