Conservation laws preserving algorithms for spin dynamics simulations

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Abstract

We propose new algorithms for numerical integration of the equations of motion for classical spin systems with fixed spatial site positions. The algorithms are derived on the basis of a mid-point scheme in conjunction with the multiple time staging propagation. Contrary to existing predictor-corrector and decomposition approaches, the algorithms introduced preserve all the integrals of motion inherent in the basic equations. As is demonstrated for a lattice ferromagnet model, the present approach appears to be more efficient even over the recently developed decomposition method.
The prediction of collective phenomena in magnetic materials was the subject of many investigations in theory and computer experiment [1–6]. These investigations dealt mainly with static properties, in particular, with phase transitions, critical behavior and scaling. The theoretical description of dynamic properties presents a much more difficult problem which, at the present time, cannot be solved quantitatively even for the simplest lattice systems such as the Ising, XY, and Heisenberg models. Until now, the method of molecular dynamics (MD) can be considered as the main tool for quantitative studies of dynamic critical behavior, dynamic scaling, and processes of spin relaxation.

The construction of stable and efficient MD algorithms for systems with spin (orientational) degrees of freedom remains a current problem. The traditional numerical methods [6] on integrating differential equations are unsuitable because of their high instability on MD scales of time. For this reason, standard predictor-corrector schemes were utilized in recent years for MD simulations of classical XY and Heisenberg models in $d = 2$ and of Heisenberg ferro- and antiferromagnets in $d = 3$ dimensions [8–12]. However, the requirement on total energy conservation restricts these schemes to be used with very little step sizes only.

Quite recently, new spin dynamics algorithms have been devised [13–15]. They are based on the Suzuki-Trotter (ST) decompositions of exponential operators and unlike usual methods preserve the total energy to within machine accuracy. It was shown that these algorithms allow much larger time steps than the predictor-corrector schemes and thus may lead to a substantial speedup of MD simulations. However, the decomposition integrators destroy the conservation of magnetization vector. Moreover, they are applicable, in fact, only to spin systems when the decomposition into noninteracting sublattices is possible and cannot be used for models with arbitrary lattice structures.

In this report we solve the problems just mentioned and derive algorithms which preserve all the conservation laws imposed by the equations of motion. The algorithms are tested and compared with previous approaches.

Let us consider a collection of $N$ spins represented by continuous three-component vectors $s_i = (s^x_i, s^y_i, s^z_i)$ with the fixed length $|s_i| = 1$ for each site $i$. A typical model Hamiltonian
for such a system can be cast in the form

$$H = -\sum_{i<j}^{N} J_{ij} (s_i^x s_j^x + s_i^y s_j^y + \lambda s_i^z s_j^z) - C \sum_{i=1}^{N} (s_i^z)^2$$  \hspace{1cm} (1)$$

where $J_{ij}$ is the exchange integral for a pair $(i,j)$ of spins, $\lambda$ is the exchange anisotropy parameter, and $C$ denotes the strength of single-site field anisotropy. At $C = 0$, Eq. (1) represents the isotropic ($\lambda = 1$) or anisotropic ($\lambda \neq 1$) Heisenberg ferro- or the corresponding antiferro-magnet for $J > 0$ and $J < 0$, respectively. For $\lambda = C = 0$, Eq. (1) reduces to the XY model. We do not restrict ourselves to lattice systems with the nearest-neighbor interaction, and the results presented below can be used for continuum models with arbitrary spatial spin distributions as well. Therefore, we indicate explicitly by the subscripts $i, j$ that the exchange integral $J_{ij}$ depends on spatial positions (which are fixed but not necessarily periodic) of spin sites.

The dynamic properties of the system can be obtained from MD simulations by numerical integrating the following equations of motion [8–13]:

$$\dot{s}_i \equiv \frac{d}{dt}s_i = \frac{1}{\hbar} \frac{\partial H}{\partial s_i} \times s_i(t) \equiv \Omega_i(t) \times s_i(t),$$  \hspace{1cm} (2)$$

where $\Omega_i = -\frac{1}{\hbar} (\sum_{j \neq i} J_{ij} (s_j^x s_i^x + s_j^y s_i^y, \lambda s_j^z s_i^z) + 2C(0,0, s_i^z))$ denotes the local Larmor frequency. Since the effect of collective thermal excitations (e.g., phonons) is not described by the Hamiltonian (1), Monte-Carlo (MC) simulations must be employed additionally [13] to generate equilibrium configurations as initial conditions to Eq. (2). This procedure is justified by the fact that in magnetic systems the characteristic time intervals corresponding to varying spin variables are much shorter than typical time scales of the thermal excitations.

In view of the symmetry $J_{ij} = J_{ji}$, it follows from Eqs. (1) and (2) that the total energy $E \equiv H$ is an integral of motion, i.e. $dE/dt = 0$. The magnetization $\mathbf{M} = \sum_i s_i$ is also conserved during the spin evolution of the isotropic Heisenberg model. For the anisotropic case ($\lambda \neq 1$ and/or $C \neq 0$) only the component $M_z$ of $\mathbf{M}$ will unchange in time. In addition, the structure of Eq. (2) imposes also the conservation of individual spin lengths. Existing MD algorithms do not fulfill these conservation laws simultaneously. Thus, in order to
reproduce the dynamical behavior properly it is required that the deviations of conservative quantities from their exact values to remain within an acceptable level of precision. This leads to obvious limitations on the size of time steps which can be used in MD simulations. It would, therefore, be very desirable to derive algorithms which conserve all the integrals of motion exactly or, at least, within machine accuracy.

The basic idea of our approach consists in the following. Suppose that an initial spin configuration \( \{ s_i(t) \} \) has been specified and we would like to obtain values of \( s_i \) at time \( t + \tau \) within \( O(\tau^3) \) truncation terms, where \( \tau \) denotes the step size. This can be realized using a mid-point scheme, \( s_i(t + \tau) = s_i(t) + \dot{s}_i(t + \tau/2)\tau + O(\tau^3) \). The time derivative can be determined applying the usual interpolation formula \( \dot{s}_i(t + \tau/2) = \frac{1}{2}[\dot{s}_i(t) + \dot{s}_i(t + \tau)] + O(\tau^2) \). Such a formula, however, does not maintain the unit norm of \( s_i(t + \tau) \) and thus needs in modifications. Since \( \dot{s}_i \) depends on both the local frequency \( \Omega_i \) and spin orientation \( s_i \), it is more natural to apply the interpolation with respect to these two dynamical variables separately rather than to the function \( \dot{s}_i \) as a whole. In doing so we obtain \( \dot{s}_i(t + \tau/2) = \frac{1}{4}[(\Omega_i(t) + \Omega_i(t + \tau)) \times (s_i(t) + s_i(t + \tau))] + O(\tau^2) \), resulting in the implicit spin propagation

\[
 s_i^{(n+1)}(t + \tau) = s_i(t) + \frac{\tau}{2} [\tilde{\Omega}_i^{(n)} \times (s_i(t) + s_i^{(n)}(t + \tau))] + O(\tau^3),
\]

where \( \tilde{\Omega}_i^{(n)} = \frac{1}{2}[\Omega_i(t) + \Omega_i^{(n)}(t + \tau)] \). As far as the mid-step frequency \( \tilde{\Omega}_i^{(n)} \) depends itself on (generally speaking) all spin orientations at time \( t + \tau \), Eq. (3) constitutes a set of \( N \) quadratic equations for \( \{ s_i(t + \tau) \} \) which can be solved iteratively \( (n = 0, 1, 2, \ldots) \) putting \( s_i^{(0)}(t + \tau) = s_i(t) + \Omega_i(t) \times s_i(t)\tau \) as the initial guess (note that iterative solutions are inherent in predictor-corrector and decomposition schemes too). Already one iteration is enough to reach the required \( O(\tau^3) \) accuracy. The necessity of performing further several updates of Eq. (3) will be motivated latter.

It can be shown readily that for the isotropic model the magnetization is conserved exactly during the spin dynamics propagation given by Eq. (3). Indeed, summation of Eq. (3) over the spin numbers and taking into account the explicit expression for \( \tilde{\Omega}_i^{(n)} \) yields
\[ \mathbf{M}^{(n+1)}(t + \tau) = \mathbf{M}(t) + \Delta \mathbf{M}^{(n)}, \]

where \( \Delta \mathbf{M}^{(n)} = \frac{\tau}{\hbar} \sum_{i \neq j} J_{ij} [s_i^{(n)}(t) + s_i^{(n)}(t + \tau)] \times [s_j^{(n)}(t) + s_j^{(n)}(t + \tau)]. \)

The term \( \Delta \mathbf{M}^{(n)} \) is canceled because of the invariance of the double sum with respect to the transformation \( i \leftrightarrow j \), and of the obvious equality \( \mathbf{a} \times \mathbf{b} + \mathbf{b} \times \mathbf{a} = 0 \) which is valid for arbitrary vectors \( \mathbf{a} \) and \( \mathbf{b} \). Thus, \( \mathbf{M}(t + \tau) = \mathbf{M}(t) \) within each iteration. The proof of the conservation \( M_z(t + \tau) = M_z(t) \) for the anisotropic case is similar.

Another important feature of the mid-point propagation is that it conserves the total energy within machine accuracy \( \mathcal{O}(\varepsilon) \), where \( \varepsilon \) denotes the iterative precision, i.e., \( |s_i^{(n+1)}(t + \tau) - s_i^{(n)}(t + \tau)| < \varepsilon \). To show this, let us perform a scalar multiplication of Eq. (3) with the vector \( \tilde{\mathbf{\Omega}}_i = \frac{1}{2} [\mathbf{\Omega}_i(t) + \mathbf{\Omega}_i(t + \tau)] \). Then using the equality \( [\mathbf{a} \times \mathbf{b}] \cdot \mathbf{a} = 0 \) one obtains

\[ s_i(t + \tau) \cdot [\mathbf{\Omega}_i(t) + \mathbf{\Omega}_i(t + \tau)] = s_i(t) \cdot [\mathbf{\Omega}_i(t) + \mathbf{\Omega}_i(t + \tau)], \]

where \( \mathcal{O}(\varepsilon) \) terms have been neglected. Summing up the last relation leads to \( E(t + \tau) = \frac{\hbar}{2} \sum_i s_i(t + \tau) \cdot \mathbf{\Omega}_i(t + \tau) = \frac{\hbar}{2} \sum_i s_i(t) \cdot \mathbf{\Omega}_i(t) + \Delta E \), where \( \Delta E = \frac{\hbar}{2} \sum_i [s_i(t) \cdot \mathbf{\Omega}_i(t + \tau) - s_i(t + \tau) \cdot \mathbf{\Omega}_i(t)] \). The term \( \Delta E \) is canceled again because of the linear dependency of \( \mathbf{\Omega}_i \) on spin components, and of the symmetry \( J_{ij} = J_{ji} \), so that \( E(t + \tau) = E(t) + \mathcal{O}(\varepsilon) \). The uncertainty \( \varepsilon \) can be reduced to a negligibly small value at a given \( \tau \) by adjusting the number \( l > 1 \) of iterations for Eq. (3). The rapid convergence \( \varepsilon \to +0 \) is guaranteed by the power dependence \( \varepsilon \sim \mathcal{O}(\tau^{l+2}) \) and by the smallness of \( \tau \). Of course, the iterative solutions require additional computational efforts, but they are compensated completely by using larger time steps. For instance, spending the same amount of computer time, we could try to reduce the energy deviations within only one iteration by decreasing the time step to \( \tau/l \). This way, however, is very inefficient because then the deviations will behave like \( \mathcal{O}((\tau/l)^3) \) and, thus, decrease with increasing \( l \) much more slower than the power dependence \( \mathcal{O}(\tau^{l+2}) \), in other words \( \tau^{l+2} \ll (\tau/l)^3 \).

An additional surprising property of the mid-point integration is the conservation of spin lengths. Implicit evaluations given by Eq. (3) achieve this conservation in iterative sense, i.e., \( |\mathbf{S}_i(t + \tau)| = 1 + \mathcal{O}(\varepsilon) \). In order to maintain spin lengths exactly, the iteration process should be reconstructed. Considering the quantity \( \tilde{\mathbf{\Omega}}_i^{(n)} \) as a parameter, Eq. (3) can be
solved analytically,

\[
s^{(n+1)}_i(t + \tau) = \frac{1}{1 + \frac{\tau^2}{4} (\tilde{\Omega}^{(n)}_i)^2} \left[ s_i(t) + \tilde{\Omega}^{(n)}_i \times s_i(t) \tau 
\right. \\
+ \frac{\tau^2}{4} \left( 2 \tilde{\Omega}^{(n)}_i (\tilde{\Omega}^{(n)}_i \cdot s_i(t)) - (\tilde{\Omega}^{(n)}_i)^2 s_i(t) \right) \right],
\]

(4)

and further iterated because of the explicit dependence of \( \tilde{\Omega}_i \) on spin orientations \( \{ s_i(t + \tau) \} \).

Obviously, such a modified iterative scheme will conserve the magnetization and total energy (to within machine accuracy) like the usual spin evaluation (3) (since Eq. (4) was obtained from Eq. (3) by the exact transformation). Moreover, as can be verified easily, Eq. (4) presents the unitary propagation \( s_i(t + \tau) = D_i(t, \tau) s_i(t) \), where \( D_i(t, \tau) \) is an orthonormal matrix which rotates the vector \( s_i(t) \) on angle \( \varphi = \arcsin(\tilde{\Omega}_i \tau / (1 + \tau^2 \tilde{\Omega}^2_i / 4)) \) around axis \( \tilde{\Omega}_i \).

Therefore, the modified scheme will maintain the unit norm of spin lengths perfectly, i.e. \( |s_i(t + \tau)| = |s_i(t)| = 1 \), for each iteration. This may lead to more efficient computations, despite a somewhat complicated structure of the RHS of Eq. (4) with respect to that of Eq. (3).

The convergence of Eq. (4) can be improved significantly by using an advanced iterative method. Namely, recalculating a current \((i = 1, 2, \ldots, N)\) value of \( s^{(n+1)}_i(t + \tau) \) within the \( n \)th iteration, it is necessary to take into account the already obtained quantities \( s^{(n+1)}_k(t + \tau) \) for \( k = 1, 2, \ldots, i - 1 \) when forming the RHS of Eq. (4). The advanced method is preferable for lattice systems with the nearest-neighbor convention, when the computer time per iteration required for the recalculations of spin values (according to Eq. (4)) dominates over the time needed to update the mid-step Larmor frequencies. Further optimizations are also possible for each specific model. This completes our mid-point spin dynamics (MPSD) algorithm of the second-order.

A way to construct higher-order versions of the MPSD integrator lies in employing a multiple staging technique used earlier [13] in the framework of the ST approach. We have realized that this technique is applicable for our approach too and obtained the following result.
\[ s_i(t + \tau) = \prod_{p=1}^{P} D_i(t, \xi_p \tau) s_i(t) + \mathcal{O}(\tau^{m+1}), \]

where the coefficients \( \xi_p \) are chosen at a given number \( P \) in such a way to provide the highest possible value for \( m \). The desired fourth-order \((m = 4)\) algorithm (MPSD4) can be directly derived from Eq. (5) using \( P = 5 \) and the coefficients \( \xi_1 = \xi_2 = \xi_4 = \xi_5 \equiv \xi = 1/(4 - 4^{1/3}) \), and \( \xi_3 = 1 - 4\xi \). That is very interesting, these coefficients coincide with those obtained within the ST decomposition of exponential operators [16].

Clearly, the fourth-order version is energy- and magnetization-preserving and conserves spin lengths (since the conservations are achieved at each stage \( p \)). The solutions generated by the MPSD/MPSD4 algorithms are also time reversible (because past and future values of \( s_i \) and \( \Omega_i \) enter symmetrically into the interpolated function \( \dot{s}_i \), and because \( \xi_p \) appear symmetrically in Eq. (5)). The reproduction of the last feature is particularly important as well since the numerical stability of an algorithm is directly connected with its time reversibility [17].

In our MD simulations we considered a simple cubic lattice in \( d = 3 \) with \( N = 1000 \) sites imposing periodic boundary conditions to each direction. The strongly anisotropic case \( C = J \) with \( J > 0 \), \( J_{ij} = J \delta_{ij} \) and \( \lambda = 1 \) was chosen to describe spin interactions (Eq. (1)), where \( \delta_{ij} = 1 \) for the nearest neighbor \( j \) of site \( i \), and \( \delta_{ij} = 0 \) otherwise. All test runs were started from an identical well equilibrated configuration prepared by us with the help of MC simulations at a temperature \( T = 0.8T_c \), where \( T_c = 1.442929 \ J/k_B \) is the critical temperature of the isotropic model \((C = 0)\). The simulations were performed on the Origin 2000 workstation at the Linz University. The equations of motion were integrated using the Adams-Bashforth-Moulton (ABM) predictor-corrector integrator [7] at \( \tau^* = \tau J/\hbar = 0.01 \), the ST decomposition schemes [13] of the second (STD) and forth (STD4) orders at \( \tau^* = 0.04 \) and 0.2, respectively, as well as using our MPSD and MPSD4 algorithms (Eqs. (4) and (5)) at \( \tau^* = 0.04, 0.1, 0.2, \) and 0.4.

Examples on the total energy \( E^* = E/J \) and magnetization \( M_z \) conservations are shown in Fig. 1. The huge energy drift (see dashed curve in Fig. 1a) indicates clearly that the ABM
algorithm is unsuitable for long-duration observations even at the smallest time step. This is explained by the irreversibility of the ABM integrator and the fact that it destroys the unit norm of spin lengths. At the same time, the STD/STD4 algorithms allow much larger step sizes, that is in the self-consistency with a conclusion of Ref. [13]. Three iterations were sufficient for the STD algorithm to obtain a level of energy conservation presented in Fig. 1a. Correspondingly 5 and 6 iterations were required for the STD and STD4 algorithms to conserve the total energy within machine accuracy ($\varepsilon \sim 10^{-9}$ in our program code). The STD/STD4 integrators, however, do not conserve the magnetization (see Fig. 1b) which fluctuates quite visibly especially in the STD case. These fluctuations are caused by the $\mathcal{O}(\tau^3)$ (or $\mathcal{O}(\tau^5)$) truncation errors and will increase drastically with further increasing $\tau$.

The pattern is different for the MPSD/MPSD4 algorithms because they can conserve both the total energy and magnetization at, in principle, arbitrary time steps. We have determined the following values for the number $l$ of iterations needed for obtaining the conservation to within machine accuracy: $l = 5, 8, 11,$ and 18 for the MPSD as well as $l = 4, 6, 7,$ and 11 for the MPSD4 integrators, corresponding to the time steps $\tau^* = 0.04, 0.1, 0.2,$ and 0.4, respectively (note that the advanced method was used to iterate Eq. (4)). The MPSD (MPSD4) algorithm required at $\tau^* = 0.04$ ($\tau^* = 0.2$) approximately the same computer time as that of the STD (STD4) scheme for the integration over the fixed $t^* = tJ/\hbar = 1000$ interval. However, the MPSD/MPSD4 algorithms can be used with larger time steps ($\tau^* > 0.04/\tau^* > 0.2$) in view of their energy- and magnetization-preserving properties. Taking into account that the number $l$ increases with increasing $\tau$ slower than linearly, these algorithms will lead to an improvement efficiency of the computations. Of course, we cannot apply too large step sizes ($\tau^* \sim 1$), because then the microscopic solutions will deviate considerably from exact trajectories. The final decision on using the biggest possible values of step sizes for the MPSD/MPSD4 algorithms can be done in each specific case by direct MD measurements of macroscopic observable quantities.
Our measurements were performed for the dynamic structure factor

\[ S(k, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left\langle \sum_{i,j} s_i^T(0) \cdot s_j^T(t) e^{i k \cdot (r_i - r_j)} \right\rangle e^{-i \omega t} dt, \]

which allows one to extract the spectrum of collective transverse spin excitations, where \( r_i \) denote the lattice vectors and \( s_i^T \) is a perpendicular to \( \mathbf{M} \) component of \( s_i \). The function \( S(k, \omega) \) is plotted in Fig. 2a in the undimensional presentation \( S^*(k, \omega) = JS(k, \omega)/\hbar \) with \( \omega^* = \omega \hbar / J, \ k^* = k/k_{\text{min}} \) and \( k_{\text{min}} = 2\pi/N^{1/3} = \pi/5 \). It was obtained within the MPSD integration at \( \tau^* = 0.04 \), and the averaging \( \langle \rangle \) was taken over the time \( t^* = 1000 \) for each of 1000 runs (with independent initial MC configurations). In order to investigate the influence of increasing step size on the spectrum, the calculations were repeated with the STD/STD4 and MPSD/MPSD4 algorithms at various step sizes. The frequency \( \omega_{\text{max}}^* \) and the relaxation time \( \tau_{\text{cor}}^* \) of the transverse waves, calculated numerically at \( k^* = 1 \) from the peak position and its half-width, respectively, are shown in Fig. 2b and 2c as the functions of the time step. As can be seen clearly, the MPSD/MPSD4 algorithms are less sensitive to increasing \( \tau \) than the STD/STD4 integrators. For instance, the level of deviations in \( \omega_{\text{max}}^* \) obtained with the STD (STD4) schemes at \( \tau^* = 0.04 \ (\tau^* = 0.2) \) can be observed with the MPSD (MPSD4) algorithms at step sizes which are approximately in factor 1.5-2.0 larger, namely, at \( \tau^* \sim 0.07 \ (\tau^* \sim 0.3) \). This gain in time is explained by additional cancellations of truncation errors due to the conservation of all the integrals of motion within our approach. For the same level of accuracy, the fourth-order versions MPSD4/STD4 allow step sizes which are nearly in 4-5 times larger than those of the second-order algorithms MPSD/STD. This compensates to some extent the additional computational efforts needed to evaluate high-order expressions. However, if very high precision is required, the fourth-order schemes become more efficient, because then the truncation errors decrease more rapidly with decreasing the step size.

In the conclusion we point out that alternative algorithms for classical spin dynamics simulations have been proposed. Their advantages over the predictor-corrector schemes are: (i) time-reversibility, (ii) exact conservation of spin lengths, and (iii) allowance of much larger time steps. The advantages over the decomposition integrators consists in (i) magnetization
conservation, (ii) allowance of larger step sizes, and (iii) applicability to systems with an arbitrary lattice structure and to continuum spin models. Moreover, the possibility of the new algorithms to preserve all the conservation laws should be considered as the chief feature which distinguishes them from all existing MD integrators. There are no other algorithms of such a kind known for any system of interacting particles. This fact may play a role in the methodology of MD and stimulate further investigations on constructing conservation laws preserving algorithms for other systems.

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Figure captions

FIG. 1. The total energy $E^*/N$ (subset (a)) and magnetization $M_z/N$ (subset (b)) per spin as functions of the time length $t^* = tJ/\hbar$ of the simulations carried out for a lattice ferromagnet model using the predictor-corrector (dashed curve, marked as ABM), decomposition (solid curves, STD/STD4), and mid-point (bold solid lines, MPSD) approaches.

FIG. 2. (a) The reduced transverse dynamic structure factor $S(k, \omega)$ of a lattice ferromagnet model; (b) and (c): The frequency peak position (b) of $S(k^*, \omega)$ and the relaxation time (c) of transverse waves as functions of the time step $\tau^*$, obtained at $k^* = 1$ within different integration schemes. Numerical errors are less than the size of symbols used in the subsets (b) and (c).
