IMPROVED SPIN DYNAMICS SIMULATIONS
OF MAGNETIC EXCITATIONS

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Using Suzuki-Trotter decompositions of exponential operators we describe new algorithms for the numerical integration of the equations of motion for classical spin systems. These techniques conserve spin length exactly and, in special cases, also conserve the energy and maintain time reversibility. We investigate integration schemes of up to eighth order and show that these new algorithms can be used with much larger time steps than a well-established predictor-corrector method. These methods may lead to a substantial speedup of spin dynamics simulations, however, the choice of which order method to use is not always straightforward.

1. Introduction

Our understanding of static behavior near phase transitions is now mature and has resulted largely from the investigation of simple model spin systems such as the Ising, the XY, and the Heisenberg model. These models are equally valuable for the investigation of dynamic critical behavior and dynamic scaling. Realistic models of magnetic materials can be constructed from these simple spin models, however, the theoretical analysis of experimentally accessible quantities, such as the dynamic structure factor, is usually too demanding for analytical methods. Computer simulations are beginning to provide important information about dynamic critical behavior and material properties of model magnetic systems.

These simulations use model Hamiltonians with continuous degrees of freedom represented by a three-component spin \( S_k \) with fixed length \( |S_k| = 1 \) for each lattice site \( k \). A typical model Hamiltonian is then given by

\[
H = -J \sum_{<k,l>} (S_k^x S_l^x + S_k^y S_l^y + \lambda S_k^z S_l^z) - D \sum_k (S_k^z)^2,
\]

where \( J \) is the exchange integral, \( <k,l> \) denotes a nearest-neighbor pair of spins \( S_k \), \( \lambda \) is an anisotropy parameter, and \( D \) determines the strength of a single-site or crystal field anisotropy.

Modelling specific magnetic materials may require additional interactions in the

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Hamiltonian, such as two-spin exchange interactions between more distant neighbors, three spin exchange interactions, or even biquadratic coupling.

The thermodynamic properties can be obtained from a Monte-Carlo simulation and the dynamical properties of the spin system are provided by solutions to the equations of motion given by

$$\frac{d}{dt} S_k = \frac{\partial H}{\partial S_k} \times S_k$$

(2)

These equations must be integrated numerically, where a Monte-Carlo simulation of the model provides equilibrium configurations as initial conditions for Eq.(2). The most important quantity to be extracted from the numerical results is the dynamic structure factor \(S(q, \omega)\), which is given by the space-time Fourier transform of the spin-spin correlation function

$$G^{\alpha, \beta}(r_k - r_l, t - t') \equiv \langle S^\alpha_k(t) S^\beta_l(t') \rangle,$$

(3)

where \(\alpha, \beta = x, y, z\), \(r_k\) and \(r_l\) are lattice vectors, and the average \(\langle \ldots \rangle\) must be taken over a large number of independent initial equilibrium configurations. (This procedure is appropriate since the typical time over which Eq.(2) can be integrated is much shorter than typical timescales set by other excitations.)

To speed up the numerical integration of Eq.(2) it is desirable to use the largest possible time step; however, with standard methods the size of the time step is severely limited by the accuracy within which the conservation laws of the dynamics are obeyed. It is evident from Eq.(2) that the total energy is conserved, and if, for example, \(D = 0\) and \(\lambda = 1\) (isotropic Heisenberg model) the magnetization \(M = \sum_k S_k\) is also conserved. For the anisotropic Heisenberg model, i.e., \(\lambda \neq 1\) or \(D \neq 0\) only \(M_z\) is conserved. Conservation of spin length and energy is particularly crucial, because the condition \(|S_k| = 1\) is a major part of the definition of the model and the energy of a configuration determines its statistical weight. It would therefore also be desirable to devise an algorithm which conserves these two quantities exactly.

In the remaining sections we describe a 4th-order predictor-corrector method and a new integration procedure, which is based on Trotter-Suzuki decompositions of exponential operators. We compare both schemes with special regard to speed and the accuracy within which the conservation laws hold.

2. Integration Methods

2.1. Predictor-corrector methods

Predictor-corrector methods have been quite effective for the numerical integration of spin equations of motion; however, in order to limit truncation errors small time steps \(\delta t\) must be used with at least a fourth-order scheme. In a more symbolic form Eq.(3) can be written as \(\dot{y} = f(y)\) with the initial condition \(y(0) = y_0\), where \(y\) is a short-hand notation of a complete spin configuration. The initial equilibrium
configuration is denoted by $y_0$. The predictor step of the scheme used here, the explicit Adams-Bashforth four-step method \textsuperscript{8} is

$$y(t + \delta t) = y(t) + \frac{\delta t}{24} [55f(y(t)) - 59f(y(t - \delta t)) + 37f(y(t - 2\delta t)) - 9f(y(t - 3\delta t))]$$

which has a local truncation error of the order $(\delta t)^5$. The corrector step consists of typically one iteration of the implicit Adams-Moulton three-step method \textsuperscript{8}

$$y(t + \delta t) = y(t) + \frac{\delta t}{24} [9f(y(t + \delta t)) + 19f(y(t)) - 5f(y(t - \delta t)) + f(y(t - 2\delta t))]$$

which also has a local truncation error of the order $(\delta t)^5$. (Values for $y(\delta t)$, $y(2\delta t)$, and $y(3\delta t)$ in addition to $y(0) = y_0$ can be provided by three successive integrations of $\dot{y} = f(y)$ (see Eq.	extsuperscript{4}) by the 4th-order Runge-Kutta method \textsuperscript{8}.) This method requires that spin configurations at the last four time steps must be kept in memory.

This predictor-corrector method is very general and is independent of the special structure of the right-hand side of the equations of motion (see Eq.	extsuperscript{4}). The conservation laws discussed earlier will only be observed within the accuracy set by the truncation error of the method. In practice, this limits the time step to typically $\delta t = 0.01/J$ in $d = 3$ for the isotropic model ($D = 0$) \textsuperscript{4}, where the total integration time is typically $600/J$ or less.

2.2. **Suzuki-Trotter decomposition methods**

The motion of a spin may be viewed as a precession of the spin $S$ around an effective axis $\Omega$ which is itself time dependent. The lattice can be decomposed into two sublattices such that a spin on one sublattice precesses in a local field $\Omega$ of neighbor spins which are all located on the other sublattice. For the Hamiltonian in Eq.	extsuperscript{1} there are only two such sublattices if the underlying lattice is simple cubic.

To illustrate the method, we consider first the $D = 0$ case. The basic idea of the algorithm is to rotate a spin about its local field $\Omega$ by an angle $\alpha = |\Omega|\delta t$, rather than directly integrate Eq.	extsuperscript{1}. This procedure guarantees the conservation of the spin length $|S|$ and energy to within machine accuracy. Denoting the two sublattices by $\mathcal{A}$ and $\mathcal{B}$, respectively, we can express the local fields acting on the spins on sublattice $\mathcal{A}$ and $\mathcal{B}$ as $\Omega_\mathcal{A}[[S]]$ and $\Omega_\mathcal{B}[[S]]$, respectively. The set of equations of motion for spins on one sublattice reduces to a linear system of differential equations if the spins on the other sublattice are kept fixed. Thus an *alternating* update scheme may be used, i.e., the spins $S_{k \in \mathcal{A}}$ are rotated for the given values of $S_{k \in \mathcal{B}}$ and vice versa. (The scalar products $S_{k \in \mathcal{A}} \cdot \Omega_\mathcal{A}[[S]]$ remain constant during the update of $S_{k \in \mathcal{A}}$ and the scalar products $S_{k \in \mathcal{B}} \cdot \Omega_\mathcal{B}[[S]]$ remain constant during the update of $S_{k \in \mathcal{B}}$). Note, that each sublattice rotation is performed with the *actual* values of the spins on the other sublattice, so that only a single copy of the spin configuration is kept in memory at any time. However, the magnetization will not be conserved during the above rotation operations. Since the two alternating rotation operations do not commute, a closer examination of the sublattice decomposition of the spin rotation is required.
We now decompose a full configuration into two sublattice components \( y_A \) and \( y_B \), i.e. \( y = (y_A, y_B) \), and denote by matrices \( A \) and \( B \) the generators of the rotation of the spin configuration \( y_A \) on sublattice \( A \) at fixed \( y_B \) and of the spin configuration \( y_B \) on sublattice \( B \) at fixed \( y_A \), respectively. The update of the configuration \( y \) from time \( t \) to \( t + \delta t \) is then given by an exponential (matrix) operator

\[
y(t + \delta t) = e^{(A+B)\delta t} y(t).
\]  

Although the exponential operator in Eq.\((6)\) rotates each spin of the configuration, it has no simple explicit form, because the rotation axis for each spin depends on the configuration itself; however, the operators \( e^{A\delta t} \) and \( e^{B\delta t} \) which rotate \( y_A \) at fixed \( y_B \) and \( y_B \) at fixed \( y_A \), respectively, do have a simple explicit form. We demonstrate this for the case \( \lambda = 1 \) and \( D = 0 \) in Eq.\((1)\). For each \( k \in A \) we find

\[
\Omega_A([S]) = -J \sum_{l=NN(k)} S_l \equiv \Omega_k,
\]  

where \( NN(k) \) denotes the nearest neighbors of \( k \) (which belong to \( y_B \)). Eq.\((7)\) can be readily generalized for \( \lambda \neq 1 \), the case \( D \neq 0 \) will be discussed below. The explicit rotation of spins on each sublattice reads (see also Watson \textit{et al}.\(9\))

\[
S_k(t+\delta t) = \frac{\Omega_k(\Omega_k \cdot S_k(t))}{\Omega_k^2} + \left[ S_k(t) - \frac{\Omega_k(\Omega_k \cdot S_k(t))}{\Omega_k^2} \right] \cos(|\Omega_k|\delta t) + \frac{\Omega_k \times S_k(t)}{|\Omega_k|} \sin(|\Omega_k|\delta t).
\]  

Note that according to Eq.\((8)\) \( \Omega_k \cdot S_k(t+\delta t) = \Omega_k \cdot S_k(t) \) and energy is thus conserved. The alternating update scheme for the integration of the equations of motion amounts to the replacement \( e^{(A+B)\delta t} \to e^{A\delta t}e^{B\delta t} \) in Eq.\((3)\), which is only correct up to order \( (\delta t)^2 \). The magnetization will therefore only be conserved up to terms of the order \( \delta t \) (global truncation error), but one can employ higher order Suzuki-Trotter decompositions of the exponential operator in Eq.\((3)\) to decrease the local truncation error of the algorithm and thus improve the conservation. The simplest possible improvement is given by the 2nd-order decomposition

\[
e^{(A+B)\delta t} = e^{A\delta t/2}e^{B\delta t}e^{A\delta t/2} + \mathcal{O}(\delta t^3).
\]  

which is equivalent to the midpoint integration method applied to the equations of motion (see also Watson \textit{et al}.\(9\)). We can also use the \( m \)-th order decomposition

\[
e^{(A+B)\delta t} = \prod_{i=1}^{n} e^{p_iA\delta t/2}e^{p_iB\delta t}e^{p_iA\delta t/2} + \mathcal{O}(\delta t^{m+1})
\]  

where \( n = 5 \) for 4th-order and \( n = 15 \) for 8th-order and the parameters \( p_i \) are given by Suzuki and Umeno\(10\).

The additional computational effort needed to evaluate higher order expressions can be compensated to some extent by using larger time steps. The evaluation of the trigonometric functions in Eq.\((8)\) can also be avoided since the above decompositions...
Improved spin dynamics simulations are only correct to within a certain order in $\delta t$ and it is therefore sufficient to replace $\sin x$ and $\cos x$ by appropriate Taylor polynomials; alternatively a Cayley transform could be used (up to 2nd and 4th-order, it corresponds to $\sin x = x / (p(x) + (x/2)^2)$, with $p(x) = 1$ and $p(x) = 1 - x^2 / 12$, respectively; determining $\cos x$ from $\sin^2 x + \cos^2 x = 1$ ensures spin-length conservation). For a 4th-order method the Cayley transform was $10 - 20\%$ faster, depending upon the machine. Note that the decompositions maintain the time inversion property of $e^{(A+B)\delta t}$. The inclusion of next-nearest neighbor bilinear interactions on a simple cubic lattice can be treated within the above framework if the lattice is decomposed into four sublattices. This approach can also be extended to the case $D \neq 0$, but in contrast to the isotropic case, the equation of motion for each individual spin on each sublattice is nonlinear. In practice, the best form of solution is via iterative numerical methods. For the sublattice decomposition of the spin rotation the requirement for energy conservation in the presence of a single site anisotropy is

$$\Omega_k \cdot S_k(t + \delta t) - D [S^z_k(t + \delta t)]^2 = \Omega_k \cdot S_k(t) - D [S^z_k(t)]^2 \quad (11)$$

for $k \in A$ and $k \in B$, where $\Omega_k$ is given by Eq.(7). In order to perform a rotation operation in analogy to Eq.(8) we have to identify an effective rotation axis. This can be achieved by rewriting Eq.(11) in the form $\tilde{\Omega}_k \cdot (S_k(t + \delta t) - S_k(t)) = 0$, where

$$\tilde{\Omega}_k = \Omega_k - D (0, 0, S^z_k(t) + S^z_k(t + \delta t)) \quad (12)$$

Since the rotation requires knowledge of $S^z_k$ at the future time $t+\delta t$, this problem can be solved iteratively starting from the initial value $S^z_k(t+\delta t) = S^z_k(t) + (\Omega_k \times S_k(t))^z \delta t$ in Eq.(12) and performing several updates according to the decompositions given by Eqs.(9) or (10), respectively, in order to improve energy conservation according to Eq.(11). Both the degree of conservation and the execution time depend to some extent on the number of iterations used. The initial value for $S^z_k(t + \delta t)$ used here yields a better energy conservation (at almost no extra CPU time) than using the initial value $S^z_k(t + \delta t) = S^z_k(t)$, with the same number of iterations. Biquadratic interactions can be treated by the same iterative scheme, but inclusion of three-spin interaction would require reconsideration of the sublattice decomposition.

3. Results and Comparisons

For a quantitative analysis of the integration methods outlined above we restrict ourselves to the Hamiltonian given by Eq.(1) for $\lambda = 1$ in $d = 3$. The underlying lattice is simple cubic with $L = 10$ lattice sites in each direction and periodic boundary conditions in all cases discussed below.

In order to compare the different integration methods we first investigate the accuracy within which the conservation laws are fulfilled. The initial configuration is a well equilibrated one from a Monte-Carlo simulation for $\lambda = 1$ at a temperature $T = 0.8T_c$ for $D = 0$ and $D = J$, where $T_c$ refers to the critical temperature of the isotropic model ($D = 0$). The magnetization of such a configuration is
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non-zero and provides an indicator for the numerical quality of the magnetization conservation. We integrate the equations of motion to \( t = 800/J \) and monitor the energy \( e(t) \equiv E(t)/(JL^3) \) of the configuration per spin and the modulus \( m(t) \equiv |M(t)|/L^3 \) of the magnetization per spin for the isotropic case \( D = 0 \) and its \( z \)-component \( m_z(t) \equiv M_z(t)/L^3 \) for the strongly anisotropic case \( D = J \) as functions of time. Note that for these tests both integration methods are started from identical initial configurations.

For \( D = 0 \) the implementation of Eqs. (9) and (10) using Eq. (8) is straightforward. The Taylor polynomial for \( \sin x \) is chosen as \( \sin x = x - x^3/6 \) for Eq. (9) and up to (and including) the terms \( x^5/120 \) and \( x^9/9! \) for the 4th- and 8th-order decompositions in Eq. (10), respectively, in order to reduce the magnetization fluctuations. Fig. 1 shows that \( e(t) \) for the predictor-corrector method increases linearly with time whereas the decomposition methods both yield \( e(t) = \text{const} \). Thus, \( \delta t = 0.01/J \) is about the largest value that can be used without introducing substantial non-conservation of the energy. Fig. 2 displays the magnetization conservation for the 2nd-, 4th- and 8th-order decomposition methods, all with the same time step \( \delta t = 0.1/J \). The predictor-corrector method conserves \( m(t) \) exactly, whereas the decomposition methods cause fluctuations of \( m(t) \) on all time scales. It is also clear that the second-order method is unstable with such a large time step. The temporal structure of \( m(t) \) for the eighth-order decomposition methods with different time steps is displayed in Fig. 3. Even with a time step as large as \( \delta t = 0.25/J \), the magnetization is rather well conserved out to a time of \( t_{\text{max}} = 800J^{-1} \). The three different decomposition methods can be made to produce fluctuations of the same magnitude, e.g. of \( 2 \times 10^{-5} \), by adjusting the value of \( \delta t \) to be \( 0.007J^{-1} \) for

![Fig. 1. Energy \( e(t) = E(t)/(JL^3) \) per spin for the predictor-corrector method (see Eqs. (4) and (5)) for several time steps and \( D = 0 \).](image-url)
Fig. 2. Magnetization $m(t) = |M(t)|/L^3$ per spin for different order decomposition schemes for $D = 0$ and time step $\delta t = 0.1/J$: (dotted line) 2nd-order scheme; (solid line) 4th-order scheme; (dashed line) 8th-order method.

Fig. 3. Magnetization $m(t)$ per spin for $D = 0$ using the eighth-order decomposition method (see Eq. (10)) with different time steps.
the 2nd-order method, $0.1J^{-1}$ for 4th-order and $0.25J^{-1}$ for 8th-order. A single integration of the equations of motion using Eq.(9) (2nd-order decomposition) is about twice as fast as the predictor-corrector method. The 4th- and 8th-order decompositions (see Eq.(10)), however, are respectively about 2.5 and 9 times slower than the predictor-corrector method. Taking the change in time step by factors of 0.7, 10, and 25, respectively, into account, we find that the 2nd-, 4th- and 8th-order decomposition methods yield a speedup of the integration of the equation of motion by factors of approximately 1.5, 4, and 2.5, respectively. Using time steps $\delta t = 0.04/J$ and $0.2/J$ for the 2nd- and 4th-order methods, respectively, yields in both cases an eightfold speedup as compared to the predictor-corrector method with $\delta t = 0.01/J$. If the overall quality of the magnetization conservation is also taken into account, there is a clear advantage for the 4th-order decomposition according to Eq.(10) for the isotropic case $D = 0$. Somewhat surprisingly, with the current implementation, the 8th-order method is not competitive. For strong anisotropy, $D = J$, the predictor-corrector method can be applied as before, but the decomposition scheme must be modified because the spin rotation axis depends on the spin value $S^z_k$ at the future time $t + \delta t$ (see Eq.(12)). As described in Sec. 2.2 this self-consistency problem is solved iteratively, where the quality of the energy conservation depends on the number of iterations performed. For the 2nd-order decomposition with $\delta t = 0.04/J$ two iterations are sufficient to obtain a better energy conservation than the predictor-corrector method. Thus a time integration step using the 2nd-order decomposition takes twice as long as for $D = 0$, so that its advantage in speed only comes from the increase in the time step, which is still a factor of four. For the 4th-order decomposition with $\delta t = 0.2/J$ six iterations are needed to obtain energy conservation to within six significant digits, so one integration becomes 15 times slower than one with the predictor-corrector method. From the increase of $\delta t$ by a factor 20 only a 30% gain in speed is obtained. The number of iterations needed decreases with $\delta t$, but this decrease does not compensate the loss in speed due to the smaller time step. However, one still obtains a greatly improved energy conservation. All methods behave similarly, the change in energy is basically linear with time (see Fig.4). The reason for this is the iterative nature of all four methods in the case $D \neq 0$. The overall accuracy of the magnetization conservation appears to be independent of $D$ for all decomposition methods. Considering both overall energy conservation and speed, the 2nd-order decomposition has some advantages over the predictor-corrector method.

Lastly, in Fig.5 we show spin dynamics data for the dynamic structure factor in the (100) direction for the isotropic Heisenberg ferromagnet ($D = 0$) on a simple cubic lattice ($L = 10$) at $T = 0.8T_c$ obtained with the second-order decomposition method (see Eq.(9), $\delta t = 0.04/J$). The equations of motion have been integrated to $800/J$ and averages have been taken over 1000 initial configurations, where the time displaced correlation functions have been measured to $400/J$. A spin wave peak is located at $\omega_0 = 0.25J$ and the shoulder like feature at $\omega \simeq 0.5J$ in $S_i(q, \omega)$ (see Fig.5) is due to multi-spin-wave processes, the description of which is beyond
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Fig. 4. Energy $e(t)$ per spin for different order decomposition schemes for $D = J$: (solid line) predictor-corrector method; (dot-dashed line) 2nd-order scheme; (dashed line) 4th-order scheme; (dotted line) 8th-order method. The number of iterations performed are marked next to each line.

Fig. 5. Dynamic structure factor of an isotropic Heisenberg ferromagnet for $T = 0.8T_c$ and $|q| = \pi/5$ in the (100) direction on a simple cubic lattice ($L = 10$) obtained with the 2nd-order decomposition method for time step $\delta t = 0.04/J$. The longitudinal component is $S_l(q, \omega)$ and the transverse component is $S_t(q, \omega)$. 
the scope of this article.

4. Summary

We have described a set of algorithms which is based on Suzuki-Trotter decompositions of exponential operators and compared their relative performance with each other as well as with a predictor-corrector method. The advantages of the predictor-corrector method are its versatility and its capability to conserve the magnetization exactly. The decomposition of the lattice into sublattices, which is the basis for the decomposition method, depends on the range of the interactions, so that this approach is less general than the predictor-corrector method. Crystal field anisotropies leave the performance of the predictor-corrector method almost unaffected, whereas the decomposition method suffers from a drastic reduction in speed.

The advantage of the decomposition method is its ability to handle large time steps and to conserve spin length exactly. In the absence of anisotropies it also conserves the energy exactly and maintains reversibility. For anisotropic Hamiltonians energy conservation and reversibility can be obtained to a high accuracy using iterative schemes. Exact magnetization conservation, however, is lost. The time steps which can be used far exceed those used by the predictor-corrector method. In simple cases the 4th-order decomposition yields very accurate results even for time steps, which are an order of magnitude larger than typical time steps used for the predictor-corrector method. The 8th-order algorithm improves the conservation significantly but at the cost of greatly increased execution time.

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