Energy balance and energy correction in dynamics of classical spin systems

Dmitry A. Garanin
Department of Physics, Herbert H. Lehman College and Graduate School,
The City University of New York, 250 Bedford Park Boulevard West, Bronx, New York 10468-1589, USA

Energy-correction method is proposed as an addition to mainstream integrators for equations of motion of systems of classical spins. This solves the problem of non-conservation of energy in long computations and makes mainstream integrators competitive with symplectic integrators for spin systems that for different-site interactions conserve the energy explicitly. The proposed method is promising for spin systems with single-site interactions for which symplectic integrators do not conserve energy and thus have no edge against mainstream integrators. From the energy balance in the spin system with a phenomenological damping and Langevin fields, a formula for the dynamical spin temperature in the presence of single-site anisotropy is obtained.

I. INTRODUCTION

As computing capabilities grow, models of classical spins on a lattice receive unfading attention. They allow description of both magnetic structures at low temperatures and thermal disordering effects, including phase transitions. The latter is an advantage compared to the more traditional approach, micromagnetics, that struggles to incorporate the temperature. The fastest method to compute the thermodynamics of magnetic systems is, of course, Monte Carlo. However, more versatile is the dynamical approach to classical magnetic systems using the equation of motion [1] for lattice spins, in which the temperature can be introduced either via the phenomenological Landau-Lifshitz damping [1] and stochastic Langevin fields [2] simulating the heat bath or microscopically via the coupling to the elastic system of the solid.

The stochastic equations of motion for classical spins are usually solved numerically by the Heun method with a small integration step $\delta t$ [3] (for a review, see Ref. [4]). For this method, the step error is $\delta t^3$ and thus the accumulated error is $\delta t^2$. However, in the important case of a weak coupling to the bath, one can replace the continuous Langevin noise by the pulse noise [5] and, between the regular noise pulses, use more accurate and efficient integrators such as the classical fourth-order Runge-Kutta (RK4) method (step error $\delta t^5$) or even Butcher’s RK5 method having a step error $\delta t^8$ (for a general introduction to ordinary differential equations, see Ref. [6]; the RK5 code can be found, e.g., in the Appendix of Ref. [5]). This allows one to solve the Landau-Lifshitz-Langevin equation with the same computing speed as the usual Landau-Lifshitz equation and in particular to efficiently solve the problem of non-uniform thermal activation of a magnetic particle considered as a system of many spins [7, 8]. The idea of splitting the deterministic and stochastic parts of the spin motion was proposed earlier [9] using the Suzuki-Trotter (ST) decomposition of the evolution operators.

The latter is a part of a major development in computational physics: implementation of symplectic integrators that have some important advantages in comparison with classical ordinary differential equations (ODE) solvers. The main advantage of symplectic methods is explicit energy conservation for conservative systems. For classical spin systems, the algorithm consists in sequential rotating spins around effective fields acting on them. This explicitly conserves the spin length. If the effective field depends on the other spins, this rotation also conserves the energy of the system. The energy conservation is very important. Long computations on conservative systems using non-energy-conserving solvers cause energy drift that accumulates to significant values if the integration step is not very small. This can be interpreted as a positive or negative fictitious damping in the system. Sometimes instabilities develop in computations, which results in the system warming up and becoming disordered. This cannot happen if the numerical method conserves energy.

There are different types of Suzuki-Trotter decomposition of evolution operators for spin systems [10–15]. The simplest second-order Suzuki-Trotter decomposition (ST2) is easy to program and fast in the execution. Its accuracy is not great, with a step error $\delta t^3$, but the energy conservation makes the method viable. Accurate treatment of the energy also improves the accuracy of other physical quantities. This is probably why currently in most cases the second-order decomposition is used (see, e.g., [16–19]). The fourth-order decomposition (ST4) (step error $\delta t^5$) is computation-intensive and cumbersome to program. Also worth mentioning is the implicit spherical mid-point rule [20, 21].

A drawback of symplectic integrators for spin systems is that they are hardly suitable for systems with single-site interactions, such as a crystal field. The effective field produced on the spin by the single-site anisotropy depends on the spin itself and changes as the spin is precessing around it. Considering this effective field to be constant and equal to its value for the starting orientation of the spin leads to nonconservation of energy. The second-order Suzuki-Trotter decomposition loses one order of accuracy, so the step error becomes $\delta t^2$ and the accumulated error becomes $\delta t$. If the single-site anisotropy is much smaller than the exchange, this could be tolerated at short times, but without the exact energy conservation
the approach loses its edge and cannot be called symplectic. The problem of a nonconstant effective field was solved by iterations \[10, 11\], but this makes the method cumbersome and causes slowdown. This difficulty had been overcome in a rather unexpected way: Researchers could not sacrifice the popular numerical method and instead abandoned models with single-site anisotropy. For pure spin models, an anisotropic exchange is used instead of the latter. In the models unifying spin and lattice dynamics, spin-lattice interaction is introduced via the dependence of the exchange coupling on the distance between the neighboring atoms, modified by lattice deformations, and/or via the pseudodipolar coupling, in which the distances and directions are also modified by phonons (see, e.g., \[17\]).

The purpose of this work is to rehabilitate the traditional methods of solving equations of motion for classical spins that have no problems with single-site interactions. The nonconservation of the spin length, accumulating at large times, can be easily corrected by normalization of all spins from time to time. Correcting the energy is less trivial and it is discussed in detail. The idea is the following. If the expected energy of the system is known (e.g., in isolated conservative systems it remains the same, and in non-isolated systems it increases by the amount of the absorbed energy and decreases by the amount of the dissipated energy), one can change the state of the system by a small amount to compensate for the mismatch between the target (expected) energy and the actual energy subject to drift as the result of accumulating numerical errors or slowly developing instability. For the systems of particles having kinetic energy, the energy correction is quite simple: It is sufficient to multiply all momenta of particles having kinetic energy, the energy correction is obtained by

\[\dot{\mathbf{H}}_{\text{eff},i} = -\frac{\partial \mathcal{H}}{\partial \mathbf{s}_i} = \sum_i J_{ij} \mathbf{s}_j + D (\mathbf{n}_i \cdot \mathbf{s}_i) \mathbf{n}_i + \mathbf{H}(t),\]

where \(J_{ij}\) is the exchange coupling, \(D\) is the uniaxial anisotropy that can be coherent or random, depending on the directions of the local anisotropy axes \(\mathbf{n}_i\), and \(\mathbf{H}(t)\) is the time-dependent magnetic field in energy units. The dynamics of this system is described by the Landau-Lifshitz-Langevin equation that phenomenologically accounts for the interaction of spins with a heat bath:

\[\hbar \dot{\mathbf{s}}_i = \mathbf{s}_i \times (\mathbf{H}_{\text{eff},i} + \zeta_i) - \alpha \mathbf{s}_i \times (\mathbf{s}_i \times \mathbf{H}_{\text{eff},i}),\]

where \(\alpha\) is the dimensionless damping constant \([1]\), and \(\zeta_i\) are the Langevin white-noise fields satisfying

\[\langle \zeta_i(t)\zeta_j(t') \rangle = 2\alpha \hbar T \delta_{ij} \delta_{\alpha \beta} \delta(t - t').\]

The time derivative of the system’s energy is given by

\[\dot{\mathcal{H}} = -\dot{\mathbf{H}}(t) \cdot \sum_i \mathbf{s}_i - \frac{1}{\hbar} \sum_i \mathbf{H}_{\text{eff},i} \cdot (\mathbf{s}_i \times \zeta_i) - \frac{\alpha}{\hbar} \sum_i (\mathbf{s}_i \times \mathbf{H}_{\text{eff},i})^2.\]

Here the first term is the power input into the spin system by the time-dependent magnetic field, the second term is the power input in the system by the heat bath, and the last term is the dissipated power. In a large system, the second term has to be averaged over the realizations of the Langevin fields \(\zeta_i\). Calculation in the Appendix results in the energy balance equation

\[\dot{\mathcal{H}} = -\dot{\mathbf{H}}(t) \cdot \sum_i \mathbf{s}_i + \frac{\alpha T}{\hbar} \left\{ 2 \sum_{i,j} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j + D \left[ 3 (\mathbf{n}_i \cdot \mathbf{s}_i)^2 - 1 \right] \right\} - \frac{\alpha}{\hbar} \sum_i (\mathbf{s}_i \times \mathbf{H}_{\text{eff},i})^2.\]

The first and last terms on the right-hand side of this equation are the absorbed power of the applied field and the dissipated power,

\[P_{\text{abs}} = -\dot{\mathbf{H}}(t) \cdot \sum_i \mathbf{s}_i,\]

\[P_{\text{diss}} = \frac{\alpha}{\hbar} \sum_i (\mathbf{s}_i \times \mathbf{H}_{\text{eff},i})^2.\]

II. THE MODEL AND THE ENERGY BALANCE

Consider a classical spin system on the lattice described by the Hamiltonian

\[\mathcal{H} = -\frac{1}{2} \sum_{i,j} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j - \frac{D}{2} \sum_i (\mathbf{n}_i \cdot \mathbf{s}_i)^2 - \mathbf{H}(t) \cdot \sum_i \mathbf{s}_i,\]

Substituting the equation of motion, one obtains

\[\begin{align*}
\dot{\mathcal{H}} &= -\dot{\mathbf{H}}(t) \cdot \sum_i \mathbf{s}_i - \frac{1}{\hbar} \sum_i \mathbf{H}_{\text{eff},i} \cdot (\mathbf{s}_i \times \zeta_i) - \frac{\alpha}{\hbar} \sum_i (\mathbf{s}_i \times \mathbf{H}_{\text{eff},i})^2.
\end{align*}\]
At equilibrium $\dot{\mathbf{H}}(t) = 0$ and $\dot{\mathcal{H}} = 0$, so the energy input from the heat bath via the Langevin fields is equal to the energy dissipated to the heat bath. This implies that $T = T_S$, where $T_S$ is the dynamical spin temperature defined by

$$T_S = \frac{\sum_i (\mathbf{s}_i \times \mathbf{H}_{\text{eff},i})^2}{2 \sum_{i,j} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j + D_R \sum_i [3 (\mathbf{n}_i \cdot \mathbf{s}_i)^2 - 1]}. \tag{9}$$

If all spins are aligned with their effective fields, $\mathbf{s}_i \times \mathbf{H}_{\text{eff},i} = 0$ and thus $T_S = 0$. If spins are totally disordered, then for a large system both terms in the denominator average to zero, and $T_S = \infty$. Equation (9) without the single-site anisotropy was obtained in Ref. [22], also by the Langevin formalism. The validity of this formula is more general. For instance, one can create a spin state by Monte Carlo at the temperature $T$ also by the Langevin formalism. Theorem (9) does not require the single-site anisotropy.

III. THE ENERGY CORRECTION

Integrating Eq. (7), one obtains the time dependence of the system’s energy due to different processes. The integrals of the three terms on the right-hand side are robust in the numerical solution. The work done on the system is counted and does not change with time. On the contrary, the energy on the left-hand side is not robust and drifts because of the accumulation of numerical errors. It is especially clear for the isolated conservative system when the rhs is trivially zero but the lhs is slowly drifting because of numerical errors if spins are moving and the integrator does not conserve the energy explicitly. However, if high-accuracy ODE solvers are used, the energy drift is very small and can be compensated for by the energy-correction procedure repeated from time to time. This procedure changes the system’s energy by the small amount

$$\delta E = E_{\text{target}} - E, \tag{10}$$

where $E_{\text{target}}$ is the precise target value of $E$ obtained by integrating the rhs of Eq. (7) and $E$ is the imprecise value of the energy subject to drift and determined from the instantaneous spin state. The proposed change of the spin state is

$$\delta \mathbf{s}_i = \xi \mathbf{s}_i \times (\mathbf{s}_i \times \mathbf{H}_{\text{eff},i}), \tag{11}$$

where the factor $\xi$ is chosen so that the energy changes by $\delta E$. To first order, the change of system’s energy is given by

$$\delta E = - \sum_i \mathbf{H}_{\text{eff},i} \cdot \delta \mathbf{s}_i = \xi \sum_i (\mathbf{s}_i \times \mathbf{H}_{\text{eff},i})^2. \tag{12}$$

where from

$$\xi = \frac{\delta E}{\sum_i (\mathbf{s}_i \times \mathbf{H}_{\text{eff},i})^2}. \tag{13}$$

The new spins $\mathbf{s}_i + \delta \mathbf{s}_i$ should be normalized. This energy-correction method works as a compensative damping or antidamping. It is efficient if the fictitious damping due to numerical errors is not too high that is satisfied in high-accuracy computations.

One can ask what the accuracy of the energy-correcting transformation is and whether it changes the order of the ODE solver. Indeed, reinstating the energy value, one possibly can sacrifice the accuracy of other physical quantities. To clarify this, for the step error of the ODE solver one can write $\delta s_i^{(p)} \sim \delta t^{p+1}$, where $p$ is the accuracy order of the method. The error accumulated over $n$ integration steps that require the time $t = n \delta t$ is given by $\delta s_i^{(p)} \sim n \delta s_i^{(p)} \sim t \delta t^{(p)}$. The energy-correcting transformation of the first order given above compensates for the first-order term in the energy due to the accumulated errors in spin vectors. One has $\delta E \sim \delta s_i^{(p)}$ and then for the energy-correcting spin changes one obtains $\delta s_i \sim \xi \sim \delta E \sim \delta s_i^{(p)}$. This means that the deformations of trajectories due to the energy-correcting transformation are of the same order as the accumulated errors, that is, the order of the ODE solver is not affected.

The restoration of the energy is incomplete as there are also quadratic terms in the energy expansion: $\delta^2 E \sim \delta s_i^{(p)} \sim \left[ \delta s_i^{(p)} \right]^2$. These residual terms are very small, especially for high-order integrators and a not too long interval between the energy-restoring procedures, $n$. One can do another energy-correcting transformation to eliminate this term too. Then the residual term would be \left[ \delta s_i^{(p)} \right]^3. This iteration procedure converges very quickly. However, in practical cases, one iteration is sufficient.

The interval between energy corrections depends on the required accuracy of the energy. If only one iteration is done, the remaining error in the energy is \left[ \delta s_i^{(p)} \right]^3 \sim \left[ n \delta s_i^{(p)} \right]^3. For high-order integrators, the step error $\delta s_i^{(p)}$ is small, and thus $n$ can be large, which reduces the computing load. In any case, there is no need to perform the energy correction after each integration step of the basic ODE solver.

IV. CHECKING THE ENERGY-CORRECTING METHOD FOR A TOY MODEL

To see how the energy-correction method works with mainstream ODE integrators for classical-spin systems, consider a toy model of two coupled spins with uniaxial anisotropy

$$\mathcal{H} = -J \mathbf{s}_1 \cdot \mathbf{s}_2 - \frac{D}{2} (s_{1z}^2 + s_{2z}^2). \tag{14}$$
The equations of motion for the spins have the form
\[ \hbar \frac{d\mathbf{s}_1}{dt} = \mathbf{H}_{\text{eff}},_1 = \mathbf{s}_1 \times (J \mathbf{s}_2 + D \mathbf{e}_z s_{1z}) \]
\[ \hbar \frac{d\mathbf{s}_2}{dt} = \mathbf{s}_2 \times \mathbf{H}_{\text{eff}},_2 = \mathbf{s}_2 \times (J \mathbf{s}_1 + D \mathbf{e}_z s_{2z}). \] (15)

The state of this system is specified by four angles: \( \theta_1, \varphi_1, \theta_2, \) and \( \varphi_2. \) There are two integrals of motion: \( \mathbf{H} \) and \( S_z = s_{1z} + s_{2z}. \) Thus the equations of motion can be represented via only two dynamical variables. The general solutions should be complicated though.

An approximate analytical solution is possible in the limit \( D \ll J \) where there is a fast precession of spins around the total spin and a slow precession of the total spin around \( z \) axis. In terms of new variables
\[ \mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2, \quad \mathbf{\sigma} = \mathbf{s}_1 - \mathbf{s}_2 \] (16)
the equations of motion become
\[ \hbar \frac{d\mathbf{S}}{dt} = \frac{1}{2} D \mathbf{S} \times \mathbf{e}_z S_z + \frac{1}{2} D \mathbf{\sigma} \times \mathbf{e}_z \sigma_z \] (17)
\[ \hbar \frac{d\mathbf{\sigma}}{dt} = \frac{1}{2} J \mathbf{\sigma} \times \mathbf{S}. \] (18)

where in the second equation the small terms with \( D \) are discarded. One can see that the motion of the total spin \( \mathbf{S} \) is slow. In the equation for \( \mathbf{S}, \) the second term has to be averaged over the fast precession of \( \mathbf{\sigma} \) around \( \mathbf{S} \). After some vector algebra one obtains the resulting equation of motion for the total spin
\[ \hbar \frac{d\mathbf{S}}{dt} = \mathbf{\Omega} \times \mathbf{S}, \quad \hbar \mathbf{\Omega} = \frac{D}{4} s_{1z}^2 + 3 s_{1z} \cdot s_{2z} + 1 + s_{1z} \cdot s_{2z}. \] (19)

The direction of precession of \( \mathbf{S} \) depends not only on \( S_z, \) but also on the angle \( \theta_{12} \) between the two spins. For \( s_{1z} \cdot s_{2z} = \cos \theta_{12} = -1/3, \) that is, for \( \theta_{12} \approx 110^\circ, \) the total spin is frozen.

For the initial spin state \( \{s_1, s_2\} = \{(0, 0, 1), (1, 0, 0)\} \) one has \( s_1 \cdot s_2 = 0, \) and \( S_z = 1, \) and Eq. (19) yields
\[ \hbar \mathbf{\Omega} = \frac{D}{4}. \] (20)

For the initial state \( \{(-1/\sqrt{2}, 0, 1/\sqrt{2}), (1, 0, 0)\} \) one has \( s_1 \cdot s_2 = -1/\sqrt{2}, \) and \( S_z = 1/\sqrt{2}, \) and Eq. (19) yields
\[ \hbar \mathbf{\Omega} = \frac{D \sqrt{2} - 3}{4 \sqrt{2} \sqrt{2} - 1} \simeq -0.677 D. \] (21)
Figure 1 shows the numerical solution of the system of equations (15) in both cases above for $D/J = 0.01$. For such a small anisotropy, the curves for $S_x$ and $S_y$ are visibly perfect sinusoids, while $S_z$ is a straight line. In the first case, the period is $T = 2513$ (in units of $\hbar/J$), in perfect accordance with the value $T = 2\pi/\Omega = 2513$ following from Eq. (20). In the second case, the precession goes in the other direction with the period $T = 936$, in reasonable accordance with the result $T = 928$ of Eq. (21) (in this case, the approximation made in the derivation of $\Omega$ works less well). The fast motion of the difference spin $\sigma$ is not seen in this figure. For larger anisotropies, such as $D/J \gtrsim 0.1$, the numerical solution shows a more complicated behavior with both types of motion.

This toy model is well suited for checking the methods of integrating equations of motion for classical spin systems. As in the real systems, here there is fast precession of spins around each other with the exchange frequency $\omega_{ex} \sim J/\hbar$ that in real systems becomes important at high excitation, in particular, at elevated temperatures. At the same time, there is a slow motion of the observed macroscopic quantities, driven by the interactions much weaker than the exchange. Although the latter are of interest, the integration step $\delta t$ in the numerical solution is dictated by the fast motion and is typically $\delta t \sim 0.1$ in the units of $\hbar/J$. This leads to very long computations even for physically fast processes. In such computations, numerical errors tend to accumulate. This is why the energy-conserving symplectic integrators have become widely accepted.

To demonstrate that the method of energy correcting proposed above is efficient in long computations using RK4 and RK5 ODE solvers, computations on the toy model with $D/J = 0.01$ and the initial spin configuration $\{s_1, s_2\} = \{(0, 0, 1), (1, 0, 0)\}$ were performed over 100 periods of the precession of the total spin, $T = 2\pi/\Omega$ specified by Eq. (20).

Figure 2 shows the energy drift computed with the corrected and uncorrected RK4 and RK5 methods, as well as with the second-order Suzuki-Trotter decomposition for comparison (all spins are rotated sequentially by half-angles around their effective fields and then the same in the opposite order [18], with no attempt to solve the problem of a non-constant effective field by iterations [10, 11]). In the case of ST2, the energy decreases very fast and saturates at $\Delta E/J = -1$, which corresponds to the angle between the spins decreasing from its initial value $90^\circ$ to zero (see Fig. 6). This confirms an extreme inaccuracy of the ST2 method for systems with uniaxial anisotropy that in this case acts as an effective damping. As said in the Introduction, ST2 straightforwardly applied to such systems has, in fact, a step error $\delta t^2$, which is inferior to that of RK4 having a step error $\delta t^5$. Still, over this huge integration time, the RK4 energy drift is also significant, $\Delta E/J \simeq -0.0874$.

Figure 3 shows a close-up of the energy drift. Correcting the energy every half-period $T/2$ of the slow precession with the RK4 integrator yields a constant energy deviation $\Delta E/J \simeq -0.7 \times 10^{-3}$ that is not that bad, especially as it is not growing with time. This energy deviation accumulates over the time $T/2$, after which the energy each time returns to its target value. As here $T/2 \approx 1257$ and the integration step is $0.1$, energy corrections are performed extremely rarely and in fact can be done much more frequently, further reducing the energy deviation. Uncorrected RK5 computation has much better accuracy than the uncorrected RK4 one, as can be seen in Fig. 3. Energy corrections for RK5 make errors in the energy invisible on this scale.
Energy plays a profound role in the dynamics, affecting other physical quantities, as the value of the energy defines the region of the phase space that the system is allowed to visit. The negative energy drift in the present uncorrected computations causes the spins to move closer to the anisotropy axis. As a result, there is a positive drift in the integral of motion $S_z$ and a positive drift in the slow precession frequency. Figure 4 shows the numerical results for $S_z$. Indeed, for the uncorrected RK4 and RK5 solvers $S_z$ increases, and for RK4 this increase is very pronounced ($S_z = 1.0834$ at the end of the integration interval). RK4 with energy correction yields a small $S_z$ drift, even decreasing with time. Using RK5 with energy correction makes $S_z$ errors invisible on this scale.

The frequency drift shown in Fig. 5 is similar to the $S_z$ drift. In the uncorrected RK4 computation, the frequency $\Omega$ becomes $0.0035J$ at the end of the integration time, which is a huge deviation from the correct value of $\Omega$. The accurate numerical calculation yields $\Omega$ slightly higher than the theoretical value $0.0025J$. The reason for this is that Eq. (19) is an approximate analytical result and there should be corrections to it.

Finally, the time dependence of the length of the total spin $m = |S| = \sqrt{2(1 + s_1 \cdot s_2)}$ is shown in Fig. 6. Applying ST2 makes the two spins, initially perpendicular to each other, become parallel, reducing the energy (see Fig. 2). The drift of $m$ in the uncorrected RK4 computation is also substantial. In the uncorrected RK5 computation, there is also a positive drift of $m$; however, invisible on this scale. In the corrected RK4 and RK5 computations, there is no $m$ drift but, upon zooming in, one can see fast oscillations with a very small amplitude, as $m$ is not conserved in this model.

V. ENERGY CORRECTION IN SYSTEMS WITH DAMPING AND PUMPING

If the spin system is damped, $\alpha > 0$, and $T = 0$, so that there is no thermal agitation, the system will relax fast to its ground state, so that no significant error will accumulate during the relaxation, if the integrator is accurate enough. The problem of accumulation of errors arises in the case of continuous pumping, which causes nontrivial dynamics during an extended time. The absorbed and dissipated energies

$$E_{\text{abs}}(t) = \int_0^t dt' P_{\text{abs}}(t'),$$

$$E_{\text{diss}}(t) = \int_0^t dt' P_{\text{diss}}(t'),$$

(22)

where $P_{\text{abs}}$ and $P_{\text{diss}}$ are given by Eq. (8), are robust quantities. The contributions to them obtained by the integration up to the current time are recorded and do not change any more. The only change of $E_{\text{abs}}(t)$ and $E_{\text{diss}}(t)$ is due to the further evolution. On the contrary, the energy of the system $H$ is subject to drift because of the accumulation of errors in the numerical solution of the system’s dynamics that is on during the whole computation. If $H$ strongly deviates from its accurate value, the state of the system changes so that $P_{\text{abs}}$ and $P_{\text{diss}}$ become wrong, and the whole computation breaks down. The key to the correct computation is in correcting the energy change $\Delta E(t) \equiv H(t) - H(0)$ so that it satisfies the energy balance condition (7) integrated over the time, i.e.,

$$\Delta E(t) = E_{\text{abs}}(t) - E_{\text{diss}}(t).$$

(23)

Thus, in Eq. (10) $E_{\text{target}} = H(0) + E_{\text{abs}}(t) - E_{\text{diss}}(t)$, and the required energy correction becomes

$$\delta E = E_{\text{abs}}(t) - E_{\text{diss}}(t) - \Delta E(t).$$

(24)

Such a strategy was applied in recent work [26], where the absorption of microwave energy in a large system of classical spins with random anisotropy was studied. Although no phenomenological damping was included, as the system of many interacting spins has its own internal damping, this work illustrates well the power of the energy-correcting procedure. With accurate numerical integration in Eqs. (22) and the energy correction, the evolution of the system can be traced up to unlimited times. With the use of the RK 5 integrator, the integration was performed with a time step of $\delta t = 0.1$ up to $t = 100000$ in units of $\hbar/J$.

Of course, there will be some error accumulation because of inaccuracies of the numerical integration in the formulas for $E_{\text{abs}}(t)$ and $E_{\text{diss}}(t)$ [Eqs. (22)]. However, these errors just slightly renormalize the pumping and damping and cannot result in any drastic effects.
If the pumping and damping are strong, the non-conservation of the system’s energy resulting from the inaccuracy of the ODE solver is not very important as it only slightly shifts the tight and fast establishing balance between pumping and damping. The energy correction becomes necessary when pumping and damping are weak, so the process is so long that the accumulated errors in the system’s energy due to the inaccuracy of the ODE solver become noticeable.

In the case of nonzero temperature \( T \), one should keep in mind that the energy-balance equation (7) is averaged over the fluctuations of the phenomenological stochastic fields. The equations to solve are stochastic equations, the solution of which is fluctuating around the average value at a given time. Also, the system’s energy is fluctuating and because of this it cannot be corrected as was described above. On the other hand, thermal agitation tends to restore the average system’s energy in a natural way. The result of numerical errors will be just a small deviation of the dynamical spin temperature \( T_\beta \) from the temperature of the bath \( T \) and there will be no error accumulation. Thus, having a sufficiently accurate ODE solver, one can forget about the energy correction for \( T > 0 \).

An efficient method of solving the stochastic Landau-Lifshitz-Langevin equation for classical spins, especially in the realistic case of weak damping \( \alpha \ll 1 \), is replacing the continuous noise by a pulse noise [5] acting at time intervals \( \Delta t \). Within these intervals, the motion of the system is noiseless and it can be solved by high-accuracy ODE solvers such as RK4 or RK5. This is an important advantage in comparison with the standard approach using the original continuous noise that requires using the low-accuracy Heun (a variant of RK2) integrator with a very small integration step. Within the pulse-noise scheme, one can implement the energy correction at the end of each interval \( \Delta t \) to ensure a proper energy behavior within this interval.

VI. DISCUSSION

It was shown that mainstream ODE solvers, not explicitly conserving the energy for conservative classical-spin systems, can be used for solving the equations of motions for spins over very long times, if the energy-correction procedure is employed in the algorithm. This procedure, executed from time to time, returns the value of the energy of the spin system to its target value computed from the initial energy and the energy injected into and dissipated in the system, which are not subject to drift. In particular, one can use the classical fourth-order Runge-Kutta solver or the Butcher’s fifth-order Runge-Kutta solver. For many-spin systems, these solvers can be written in the vector form so that the code looks like that for one differential equation. Correcting the energy also makes other computed physical quantities more accurate.

The energy-correction method can be implemented both for the pure spin dynamics with the phenomenological damping and Langevin stochastic fields simulating the heat bath (if the pulse-noise model [5] is used) and for the combined spin-lattice dynamics. In both cases, the target energy of the spin system can be computed.

The method is especially useful for spin systems with single-site anisotropy for which the popular symplectic integrators based on the Suzuki-Trotter decomposition of exponential operators do not conserve energy and thus become inefficient. Even in the absence of single-site interactions, mainstream methods with energy correction are competitive with symplectic methods. For instance, the second-order Runge-Kutta (RK2) solver makes two function evaluations per integration step, while the most used second-order Suzuki-Trotter solver, ST2, also makes two effective function evaluations per step, only it does it sequentially for all spins. The RK4 solver has the fourth order of accuracy and makes four evaluations per step but the ST4 solver makes \( 5 \times 2 = 10 \) [10, 11] effective function evaluations per step. It is inferior to Butcher’s RK5 that makes six function evaluations per step.

How frequently energy corrections have to be done depends on the error accumulated during the time between the corrections. The latter depends on the particular problem and on the integration step. Thus, before the definitive computation is run, different variants have to be tested.

Considering the energy balance in classical spin systems allowed us to obtain the formula for the dynamic spin temperature in the presence of single-site anisotropy, generalizing the previously obtained results for different-site interactions. This formula is useful in studying spin dynamics.

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APPENDIX

In the term \( \mathbf{H}_{\text{eff},i} \cdot (\mathbf{s}_i \times \mathbf{\zeta}_i) \) in Eq. (6), the Langevin field \( \mathbf{\zeta}_i \) directly correlates with \( \mathbf{s}_i \) and, in the presence of single-site interactions, with \( \mathbf{H}_{\text{eff},i} \). Thus, averaging over realizations of \( \mathbf{\zeta}_i \), one has to calculate two terms:

\[
\langle \mathbf{H}_{\text{eff},i} \cdot (\mathbf{s}_i \times \mathbf{\zeta}_i) \rangle = A + B,
\]

where

\[
A \equiv \mathbf{H}_{\text{eff},i} \cdot (\mathbf{s}_i \times \mathbf{\zeta}_i), \quad B \equiv \langle \mathbf{s}_i \cdot (\mathbf{H}_{\text{eff},i} \times \mathbf{s}_i) \rangle. \tag{26}
\]

One can use the implicit solution

\[
s_{i\alpha}(t) = \frac{1}{\hbar} \int_{t_0}^{t} dt' e_{\alpha\beta\gamma} s_{i\beta}(t') \mathbf{\zeta}_{i\gamma}(t') + \ldots \tag{27}
\]
for the dependence of $s_i$ on $\zeta_i$ that follows from Eq. (2). Then in $A_i$ one has

$$\langle (s_i(t) \times \zeta_i(t)) \rangle = e_{\alpha\mu\nu} s_{i\mu}(t) \zeta_i(t)$$
$$= \frac{1}{\hbar} \int_{t_0}^t dt' e_{\alpha\mu\nu} e_{\mu\beta\gamma} s_{i\beta}(t') \zeta_i(t') + \ldots$$

(28)

Using the identity $e_{\mu\nu\alpha} e_{\mu\beta\gamma} = \delta_{\nu\beta} \delta_{\alpha\gamma} - \delta_{\nu\gamma} \delta_{\alpha\beta}$, one can rewrite this as

$$\frac{1}{\hbar} \int_{t_0}^t dt' (\delta_{\nu\beta} \delta_{\alpha\gamma} - \delta_{\nu\gamma} \delta_{\alpha\beta}) \zeta_i(t') s_{i\beta}(t') \zeta_i(t') =$$
$$\frac{1}{\hbar} \int_{t_0}^t dt' [\zeta_{i\beta}(t) s_{i\beta}(t') \zeta_i(t') - \zeta_i(t) s_{i\alpha}(t') \zeta_i(t')].$$

(29)

Here the correlator of the Langevin fields is equal to 1/2 of the value given by Eq. (4) as $t' = t$ is the upper limit of the integral. Thus one obtains

$$\langle (s_i(t) \times \zeta_i(t) \rangle = \alpha T s_{i\alpha}(t) - 3 \alpha T s_{i\alpha}(t) = -2 \alpha T s_{i\alpha}(t)$$
and

$$A \equiv \mathbf{H}_{\text{eff},i} \cdot \langle (s_i \times \zeta_i) \rangle = -2 \alpha T (\mathbf{H}_{\text{eff},i} \cdot s_i).$$

(31)

Let us calculate now the $B$-term. The contribution to $B$ comes from the uniaxial anisotropy, see Eq. (3):

$$B \equiv \langle \zeta_i \cdot \mathbf{H}_{\text{eff},i} \cdot s_i \rangle = D \langle (n_i \times s_i) \zeta_i \rangle \cdot (n_i \times s_i).$$

(32)

Similarly to the above, one writes

$$\langle (n_i \cdot s_i) \zeta_{i\alpha} \rangle = \frac{1}{\hbar} \int_{t_0}^t dt' n_{i\nu} e_{\nu\gamma\eta} s_{i\eta}(t') \zeta_{i\gamma}(t') \zeta_{i\alpha}(t)$$
$$= \alpha T n_{i\nu} e_{\nu\gamma\eta} s_{i\eta}. $$

(33)

That is,

$$\langle (n_i \cdot s_i) \zeta_i \rangle = \alpha T (n_i \times s_i)$$

(34)

and

$$B = \alpha T D (n_i \times s_i)^2 = \alpha T D \left[ 1 - (n_i \cdot s_i)^2 \right].$$

(35)

Finally, adding $A$ and $B$ and grouping the terms containing the uniaxial anisotropy, one obtains

$$\langle (\mathbf{H}_{\text{eff},i} \cdot (s_i \times \zeta_i) \rangle = -2 \alpha T \left( \mathbf{H}_{\text{eff},i} \cdot s_i \right)$$
$$- \alpha T D \left[ 3 (n_i \cdot s_i)^2 - 1 \right],$$

(36)

where $\mathbf{H}_{\text{eff},i} = \sum_j J_{ij} s_j$ is the effective field without the anisotropy term.

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