LETTER TO THE EDITOR

Thermally activated processes in magnetic systems consisting of rigid dipoles: equivalence of the Ito and Stratonovich stochastic calculus

D V Berkov[1] **and N L Gorn**

INNOVENT e.V., Pruessingstrasse 27B, D-07745, Jena, Germany

E-mail: db@innovent-jena.de

Abstract
We demonstrate that the *Ito* and the *Stratonovich* stochastic calculus lead to identical results when applied to the stochastic dynamics study of magnetic systems consisting of dipoles with the *constant* magnitude, despite the *multiplicative* noise appearing in the corresponding Langevin equations. The immediate consequence of this statement is that *any* numerical method used for the solution of these equations will lead to the physically correct results.

Study of thermally activated processes in magnetic systems is currently an extremely important research topic not only from the fundamental point of view (as it always was [1]), but also due to the miniaturization of magnetic devices (such as heads and sensors) [2], increasing density of magnetic storage [3] and development of novel magnetic technologies like MRAM [4]. In all these cases the decreasing size of magnetic elements makes thermally activated processes extremely important because the activation barrier decreases with the volume of a magnetic unit whose magnetization should be reversed, thus setting fundamental limits on the smallest size of reliable magnetic devices.

The most straightforward way to study the system dynamics taking into account thermal fluctuations is by the solution of the corresponding stochastic (Langevin) equations. In the overwhelming majority of models developed for the description of magnetic systems, the *magnitude* of magnetic moments is assumed to be *constant*. This is the case, e.g., for the classical Heisenberg model, in models describing RKKY spin glasses and fine-magnetic-particle systems [1] and in standard micromagnetic formalism [5] commonly used to analyse the behaviour of ferromagnetic materials (the last example represents probably the most relevant research area from the practical point of view).

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[1] Author to whom any correspondence should be addressed.

In all these cases magnetic moments $\boldsymbol{\mu}_i$ of the system are allowed only to *rotate* and thus their dynamics can be described by the stochastic Landau–Lifshitz–Gilbert equation [6]

$$\frac{\mathrm{d}\boldsymbol{\mu}_i}{\mathrm{d}t} = -\gamma[\boldsymbol{\mu}_i \times (\boldsymbol{H}_i^{\mathrm{det}} + \boldsymbol{H}_i^{\mathrm{fl}})] - \gamma\frac{\lambda_i}{\mu_i}[\boldsymbol{\mu}_i \times [\boldsymbol{\mu}_i \times (\boldsymbol{H}_i^{\mathrm{det}} + \boldsymbol{H}_i^{\mathrm{fl}})]], \quad (1)$$

where $\gamma(>0)$ denotes the precession constant and λ the reduced damping rate. Standard magnetic interactions (with the external field, magnetocrystalline anisotropy, exchange and dipolar fields) are included in the *deterministic* effective field $\boldsymbol{H}_i^{\mathrm{det}}$ acting on the i—the magnetic moment. Thermal fluctuations are taken into account via the so-called 'fluctuation field' $\boldsymbol{H}_i^{\mathrm{fl}}(t)$ whose Cartesian components have the well known statistical properties [6]

$$\langle H_{\alpha,i}^{\mathrm{fl}} \rangle = 0, \qquad \langle H_{\alpha,i}^{\mathrm{fl}} H_{\beta,j}^{\mathrm{fl}} \rangle = 2D\delta_{ij}\delta_{\alpha\beta} \quad (2)$$

where i, j are the moment indices, α, $\beta = x$, y, z and the noise power D is proportional to the system temperature T [6, 7].

It is because of this fluctuation field that equation (1) can*not* be treated as a 'usual' differential equation, because the integral of the random field $\boldsymbol{H}_i^{\mathrm{fl}}(t)$ represents a Wiener process and hence is not differentiable, with the result that the derivative on the left-hand side of (1) does not exist. Equation (1) should be considered rather as an informal way of introducing the so-called stochastic integral [8] which can be interpreted self-consistently in framework of the corresponding mathematical formalism.

Such integrals have a very non-trivial feature: their *value* depends, generally speaking, on the positions of intermediate points chosen for the evaluation of the integrand inside the small intervals used to take the limit of the stochastic partial sums (analogues to the Darby sums by the construction of the standard Riemann integrals). The two most common choices are to take these points (i) at the beginning of the intervals, leading to the Ito stochastic integral and (ii) in the middle of the intervals, which leads to the Stratonovich stochastic calculus. It is well known [9] that if the noise in the stochastic equation is *multiplicative*—i.e., the random term is *multiplied* by some function of the system variables—then the Ito and Stratonovich interpretations of this equation lead to *different* solutions (a simple, but impressive example is given in [9]). It was also shown that in this case the Stratonovich interpretation provides physically correct results, recovering, e.g., some important properties of physical random processes obtained using more general methods [9].

The noise in the Langevin equation (1) is obviously multiplicative, because due to the vector products the projections of the random field $\boldsymbol{H}_i^{\mathrm{fl}}$ are *multiplied* by the magnetic moment projections. This fact was noted already in the pioneering paper of Brown [6] who suggested that the Stratonovich interpretation of the this equation should be used to obtain physically consistent results. For quite a long time afterwards, the question was abandoned because analytical solutions of (1) are available only in a few simplest cases and computers were not powerful enough to enable numerical studies of really interesting magnetic systems.

During the last decade, however, corresponding numerical simulations became available and many research groups have performed studies of remagnetization processes in various systems using the Langevin formalism based on the solution of equation (1)—see [7, 10–14] etc. For such simulations, the question concerning the choice of the stochastic calculus (Ito or Stratonovich) is of primary importance, because different numerical methods converge to *different* kinds of stochastic integral: the Euler scheme and the simple implicit methods obviously converge to the Ito solution, the Heun and Milstein schemes are known to converge to the Stratonovich integral [15] and the Runge–Kutta schemes can converge to anything (including the cases in between) depending on the coefficients used there [16]. Most authors [7, 11, 12] and commercial micromagnetic packages [17, 18] use the Heun and Runge–Kutta methods converging to the Stratonovich solution (simply because they are far more stable

than the Euler method), but several groups employ the Ito-converging Euler [10,13] and implicit schemes [14]. The last two cited papers were seriously criticized in the recent paper [7] where it has been claimed once again that only the Stratonovich interpretation ensures a physically correct solution of the basic equation (1) and that thus results obtained with methods converging to the Ito integrals should be discarded as incorrect.

In this letter we prove analytically—and support our proof with numerical experiments—that if the time evolution of the system is governed by the stochastic equation (1), then *there is no difference* between the system behaviours for Ito and Stratonovich interpretations of this equation.

First of all, we note that the fluctuation field in the dissipation term on the right-hand side of this equation can be omitted; although the particular realizations of the system trajectories will be different then, the average system properties (which are the only ones of practical interest) remain the same if the noise power D is rescaled correspondingly—see, e.g., [7, 19]. Thus we can restrict ourselves to the study of a simpler equation

$$\frac{\mathrm{d}\boldsymbol{m}_i}{\mathrm{d}\tau} = -[\boldsymbol{m}_i \times (\boldsymbol{h}_i^{\mathrm{det}} + \boldsymbol{h}_i^{\mathrm{fl}})] - \lambda_i[\boldsymbol{m}_i \times [\boldsymbol{m}_i \times \boldsymbol{h}_i^{\mathrm{det}}]], \tag{3}$$

where we have introduced the unit magnetization vector $\boldsymbol{m} = \boldsymbol{\mu}/\mu$, the reduced field $\boldsymbol{h} = \boldsymbol{H}/M_S$ (M_S being the saturation magnetization of the material) and absorbed all constants except λ into the reduced time $\tau = t\gamma M_S$.

The most straightforward way to show why the *multiplicative* noise in (3) does not lead to any difference between the Ito and Stratonovich interpretations of this equation is to analyse the additional drift term appearing as a result of the transition between the Ito and Stratonovich forms. That is, it is well known [8] that if one adds to the system of stochastic ODEs

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = A_i(\boldsymbol{x}, t) + \sum_k B_{ik}\xi_k \tag{4}$$

the *deterministic* drift term $D \sum_{jk} B_{jk}(\partial B_{ik}/\partial x_j)$, then the Ito solution of this new system

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = A_i(\boldsymbol{x}, t) + D \sum_{jk} B_{jk}\, \partial B_{ik}/\partial x_j + \sum_k B_{ik}\xi_k \tag{5}$$

is equivalent to the Stratonovich solution of the initial system (4). Comparing the standard form (4) with the LLG system (3) which we are interested in, we can immediately see that in our case the matrix **B** has the form $B_{ik} = -\sum_j \epsilon_{ijk}m_j$, so the drift term $D \sum_{jk} B_{jk}\, \partial B_{ik}/\partial m_j$ reduces to

$$\frac{\mathrm{d}\boldsymbol{m}_i}{\mathrm{d}\tau} = -2D\boldsymbol{m}_i. \tag{6}$$

Hence this drift contributes to the field component *along* the magnetic moment $\boldsymbol{m}_i$ only, thus trying to change the *magnitude* of this moment which is forbidden by the model. For this reason this term must be discarded, which means that *for stochastic dynamics of models with rigid dipoles (dipoles with constant magnitudes) there is no difference between the Ito and Stratonovich solutions of corresponding stochastic ODEs.*

The mathematical reason for the multiplicative noise present in (3) not leading to a difference between its Ito and Stratonovich interpretations is that *Cartesian* coordinates of magnetic moments are *not* independent variables: due to the condition that the magnitude of each dipole moment should be constant, they are subject to the restriction $m_{i,x}^2 + m_{i,y}^2 + m_{i,z}^2 = 1$. The independent variables in this case are *spherical* coordinates of the magnetic moment unit

vector (θ_i, ϕ_i). After the transition to these coordinates, the *stochastic* part of the system (3) which we have to analyse reads [6, 19]

$$\frac{d\theta}{d\tau} = h_\phi^{fl}$$
$$\frac{d\phi}{d\tau} = -\frac{1}{\sin\theta} h_\theta^{fl},$$

(7)

(where we have omitted the moment index i for the sake of simplicity), so the matrix **B** responsible for the drift mentioned above is

$$\mathbf{B} = \begin{pmatrix} B_{\theta\theta} & B_{\theta\phi} \\ B_{\phi\theta} & B_{\phi\phi} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1/\sin\theta & 0 \end{pmatrix}$$

(8)

and it is straightforward to verify that this drift is exactly zero: $D \sum_{jk} B_{jk}(\partial B_{ik}/\partial x_j) \equiv 0$ (here $i, j, k = 1, 2$ and $x_1 = \theta$, $x_2 = \phi$). Hence we arrive at the same result that Stratonovich and Ito stochastic integrals are equivalent in this case.

At this point we would like to mention that the opposite statement was made in [7], where the authors claimed to show that Ito and Stratonovich stochastic calculus are *not* equivalent for the micromagnetic calculation. The authors of [7] have used the formalism of the Fokker–Planck equation (FPE) which describes the temporal and spatial evolution of the probability distribution of the magnetization orientation $P(\boldsymbol{m}, t)$. They have demonstrated that an additional drift term $\partial(\boldsymbol{m}P)/\partial\boldsymbol{m}$ arises in the FPE derived from the Ito interpretation of the Langevin equation when compared with the Stratonovich one (see p 14 940 in [7]). Unfortunately, Garcia-Palacios and Lazaro [7] did not take into account exactly the point which we have emphasized in our study: that Cartesian coordinates of magnetic moment are *not* independent variables. For this reason one can*not* use the FPE written in these coordinates to compare the Ito and Stratonovich forms without introducing the restriction $|\boldsymbol{m}| = 1$ explicitly. In particular, the additional drift term $\partial(\boldsymbol{m}P)/\partial\boldsymbol{m}$ which appears in the Ito interpretation of the FPE should be excluded from this equation because it leads to the drift of the probability density *along* the magnetization vector: this can be clearly seen after transition to *spherical* coordinates of $\boldsymbol{m}$: $(m_x, m_y, m_z) \rightarrow (m, \theta, \phi)$, where this drift term reduces to $\partial[mP(m, \theta, \phi)]/\partial m$. This means that the corresponding term tries to change the moment magnitude, which is *forbidden* by the model. We would also like to add that this mistake does not influence the interesting physical results obtained in the paper [7], which contains a comprehensive study of the single-particle thermodynamics and is, in general, of really high scientific quality.

To support our conclusion, we have performed numerical experiments simulating equilibrium (energy distribution density) and non-equilibrium (magnetic relaxation) properties of a disordered system of magnetic dipoles. We have solved the stochastic LLG equation (1) using methods converging either to its Ito (Euler scheme) or to its Stratonovich (drift-modified Euler and Heun schemes) solution. We note in passing that for numerical solution of (3) Cartesian coordinates are often preferred, because no instabilities like those observed in spherical coordinates near the polar axis ($\theta_i \approx 0$ or $\theta_i \approx \pi$) can occur. During such simulations one has to normalize the moment vector $\boldsymbol{m}_i$ after each new integration step (and also by evaluating the derivatives at the intermediate points, if necessary) in order to conserve the moment magnitude.

As the first example we have computed the equilibrium energy distribution for a single magnetic particle with the uniaxial anisotropy energy $E_{an} = -KV\cos^2\psi$ only (here V denotes the particle volume, K its anisotropy constant and ψ is the angle between the particle moment and its anisotropy axis). For this purpose we have simulated the motion of a single magnetic moment without the external field solving the stochastic equation (1) (with the relatively small damping $\lambda = 0.1$ and a moderate temperature $kT/KV = 1.0$) using different numerical
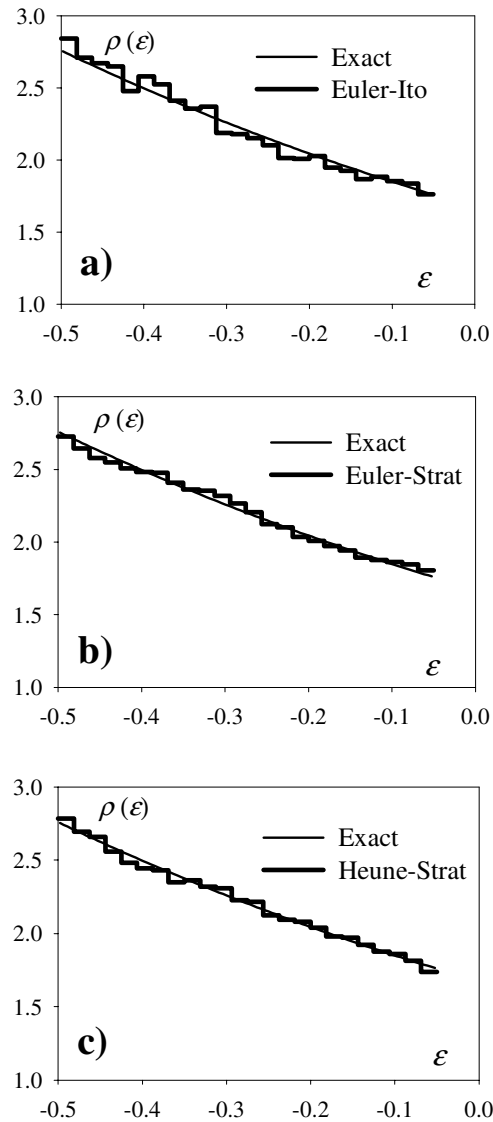
Figure 1. The equilibrium energy densities for a single-particle magnetic moment (with the uniaxial anisotropy) obtained by solving the basic equation (1) with different numerical methods converging to Ito (*a*) or Stratonovich (*b*), (*c*) solutions. The equivalence of the two approaches can be seen.

methods mentioned above. After the system reached the thermodynamic equilibrium (which may be verified, e.g., by checking that the energy does not exhibit any systematic change), we started to record the particle energy at each integration step. After a sufficiently long simulation time the distribution of these energy values must coincide (within the statistical errors) with the corresponding equilibrium Boltzmann distribution, which for such a simple system can be easily calculated analytically:

$$p(E) \propto \exp(-\epsilon/T) \frac{1}{\sqrt{-\epsilon}} \tag{9}$$
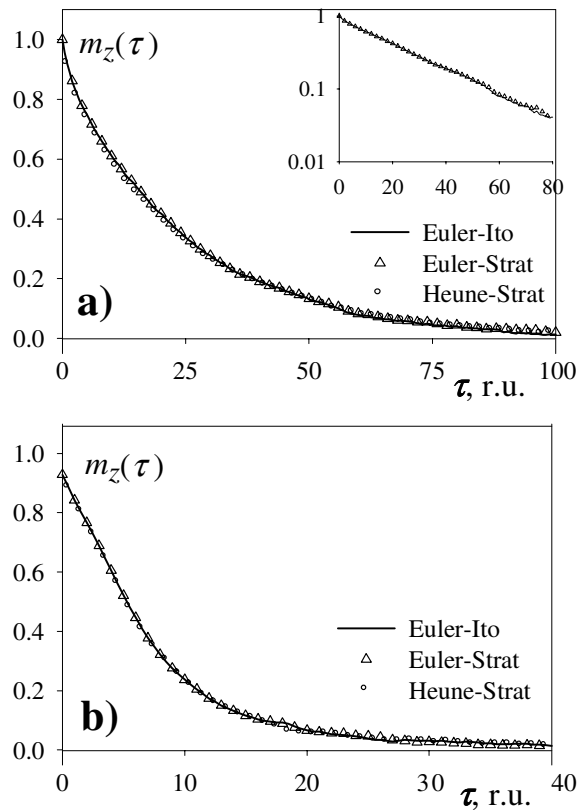
Figure 2. Magnetic relaxation curves of a system of non-interacting (*a*) and interacting (*b*) particles obtained using the same methods as in figure 1. Results obtained from the Ito and from the Stratonovich stochastic calculus coincide.

where the reduced energy $\epsilon = E/2KV = -0.5 \cos^2 \theta$ may vary in the interval $[-0.5; 0]$. The inverse square root in (9) comes from the density of states in spherical coordinates.

Energy histograms obtained from the simulations employing different integration schemes are shown in figure 1, where numerical results are compared with the analytical distribution (9) displayed as the thin solid curve; the region near the zero energy value is not shown because of the inverse-square-root singularity in (9). It can be clearly seen that all three histograms—obtained with the Euler method (Ito solution), the Euler method augmented with the drift term from (5) (Stratonovich solution) and the Heun scheme (also Stratonovich)—coincide perfectly with the correct analytical result.

The second example deals with magnetic relaxation of a disordered fine-particle system. To study such a relaxation, we have chosen a disordered system of identical particles with the same uniaxial anisotropy $E_{an} = -KV \cos^2 \psi$ and aligned anisotropy axis. For such a system *without* dipolar interaction, all particles have the same energy barrier $\Delta E = KV$ separating two energy minima along the two opposite direction of the anisotropy axes. Thus magnetic relaxation from the state where all magnetic moments are aligned along one and the same direction of the anisotropy axes should follow the exponential law $m(t) \propto \exp(-\tau/\tau_c)$, where the relaxation time τ_c depends exponentially on the relation $\Delta E/kT$. Corresponding simulation results for particles with the reduced anisotropy constant $\beta = 2K/M_S^2 = 2.0$ and the

reduced damping $\lambda = 0.1$ at the temperature $kT/KV = 0.5$ are presented in figure 2(a). Here the $m(t)$ relaxation curves obtained using the same three numerical methods as listed above are shown. Again, perfect coincidence (within the statistical errors) of the Ito and Stratonovich solutions can be seen. The inset in figure 2(a) shows the same results in semilogarithmic coordinates to demonstrate the exponential behaviour of the magnetization expected for a non-interacting system.

Results for the *interacting* system (particle volume fraction $c = 0.08$, initial metastable state prepared by quasistatic energy minimization starting from the aligned state) are shown in figure 2(b). In this case magnetodipolar interaction between the particles leads to a distribution of the corresponding energy barriers, thus resulting in non-exponential relaxation. However, the relaxation curves obtained with different numerical methods coincide again, demonstrating the equivalence of the Ito and the Stratonovich stochastic calculus for this system also.

In conclusion, we have proved analytically and shown by numerical experiments that for magnetic models where the *magnitude* of the magnetic moment at each site is *constant*, the Ito and the Stratonovich stochastic calculus lead to the same physical results despite the noise in the corresponding stochastic equation being *multiplicative*. This means that all results obtained previously using different numerical schemes are correct. A more important point is that by developing new numerical methods for solving stochastic equations for such models, one does *not* need to prove that these methods converge to the Stratonovich solution; the only consideration should be the efficiency and accuracy of these new methods.

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