Landau-Lifshitz-Gilbert-Brown

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arXiv : 1412.6497

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Plan

- Macromagnetism: the stochastic Landau-Lifshitz-Gilbert-Brown (sLLGB) equation (precession, dissipation, noise and torque).
- Discretisation schemes for multiplicative white noise (Markov) stochastic differential equations. Asymptotic measure and drift term.
- Back to the sLLGB equation, analytic approach:

  drift term & functional formalism in Cartesian and spherical coordinates ; exact results.
- Back to the sLLGB equation, numerical simulations:

  analysis of a benchmark.
- Future work.

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Magnetisation precession

Bloch equation

Evolution of the time-dependent $3d$ magnetisation density per unit volume, $\mathbf{M} = (M_x, M_y, M_z)$, with constant modulus $M_s = |\mathbf{M}|$

$$\boxed{\mathrm{d}_t\mathbf{M} = -\gamma_0\, \mathbf{M} \wedge \mathbf{H}_{\mathrm{eff}}}$$

$\gamma_0 \equiv \gamma\mu_0$ is the product of $\gamma = \mu_B g/\hbar$, the gyromagnetic ratio, and μ_0, the vacuum permeability constant (μ_B Bohr's magneton and g Lande's g-factor)

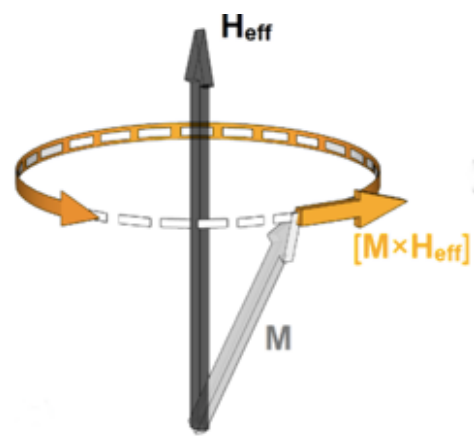
For the initial condition $\mathbf{M}(t_{\mathrm{i}}) = \mathbf{M}_{\mathrm{i}}$

the magnetisation precesses around $\mathbf{H}_{\mathrm{eff}}$

with $2\mathbf{M} \cdot \mathrm{d}_t\mathbf{M} = \mathrm{d}_t|\mathbf{M}|^2 = 0$

and $\mathrm{d}_t(\mathbf{M} \cdot \mathbf{H}_{\mathrm{eff}}) = 0$ (if $\mathbf{H}_{\mathrm{eff}} =$ ct)

Bloch 32



Dissipative effects

Landau-Lifshitz & Gilbert equations

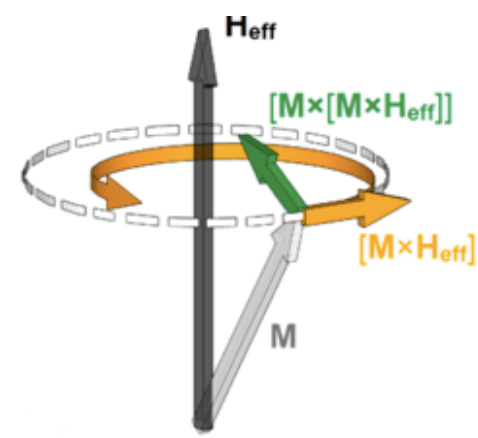
$$\mathrm{d}_t\mathbf{M} = -\frac{\gamma_0}{1+\eta^2\gamma_0^2}\,\mathbf{M}\wedge\left[\mathbf{H}_{\mathrm{eff}} + \frac{\eta\gamma_0}{M_s}\left(\mathbf{M}\wedge\mathbf{H}_{\mathrm{eff}}\right)\right]$$

Landau & Lifshitz 35

$$\mathrm{d}_t\mathbf{M} = -\gamma_0\,\mathbf{M}\wedge\left(\mathbf{H}_{\mathrm{eff}} - \frac{\eta}{M_s}\mathrm{d}_t\mathbf{M}\right)$$

Gilbert 55

2nd terms in RHS: dissipative mechanisms slow down the precession and push $\mathbf{M}$ towards $\mathbf{H}_{\mathrm{eff}}$ with $2\mathbf{M}\cdot\mathrm{d}_t\mathbf{M} = \mathrm{d}_t|\mathbf{M}|^2 = 0$ and $\mathrm{d}_t(\mathbf{M}\cdot\mathbf{H}_{\mathrm{eff}}) > 0$



Magnetic field

Conservative & non-conservative contributions

Local magnetic field $\boxed{\mathbf{H}_{\text{eff}} = \mathbf{H}^{\text{c}}_{\text{eff}} + \mathbf{H}^{\text{nc}}_{\text{eff}}}$

Conservative contribution $\boxed{\mathbf{H}^{\text{c}}_{\text{eff}} = -\mu_0^{-1} \nabla_{\mathbf{M}} U}$

with U the energy per unit volume, can originate from an external (possibly time-dependent) magnetic field $\mathbf{H}_{\text{ext}}$, and a crystal field $\mathbf{H}_{\text{ani}}$ associated to the crystalline anisotropy,

$$\boxed{U = -\mu_0 \mathbf{M} \cdot \mathbf{H}_{\text{ext}} + V_{\text{ani}}(\mathbf{M})}$$

$V_{\text{ani}}(\mathbf{M})$ is the anisotropy potential (per unit volume), e.g.

$V_{\text{ani}}(\mathbf{M}) = K \sum_{i \neq j} M_i^2 M_j^2$ (cubic crystalline structure)

$V_{\text{ani}}(\mathbf{M}) = K(M_s^2 - M_z^2)$ (uniaxial symmetry)

Bertotti, Mayergoyz & Serpico 09 ; Coffey & Kamykov 12

Magnetic field

Non-conservative component

Local magnetic field $\mathbf{H}_{\text{eff}} = \mathbf{H}^{\text{c}}_{\text{eff}} + \mathbf{H}^{\text{nc}}_{\text{eff}}$

Non-conservative contribution $\boxed{\mathbf{H}^{\text{nc}}_{\text{eff}} \neq -\mu_0^{-1}\nabla_{\mathbf{M}} U}$

Spin-torque term in Gilbert equation

$$\boxed{\mathbf{H}^{\text{nc}}_{\text{eff}} = -\frac{g\mu_B \hbar J(t)\mathcal{P}}{2M_s^2 de}(\mathbf{M} \wedge \mathbf{p})}$$

$J(t)$ the current per unit area,

$\mathcal{P}$ the (dimensionless) polarisation function of the fixed layer,

$\mathbf{p}$ is a unit vector in the direction of the current,

d the interlayer separation

e is the electric charge of the carriers.

Berger 96 ; Slonczewski 96

Thermal fluctuations

À la Langevin in Gilbert's formulation

$$\boxed{\mathrm{d}_t\mathbf{M} = -\gamma_0\mathbf{M}\wedge\left(\mathbf{H}_{\mathrm{eff}} + \mathbf{H} - \frac{\eta}{M_s}\mathrm{d}_t\mathbf{M}\right)}$$

$\mathbf{H}$ is a white random noise, with zero mean $\langle H_i(t)\rangle = 0$ and correlations

$$\langle H_i(t)H_j(t')\rangle = 2D\delta_{ij}\delta(t-t')$$

For the moment, the (diffusion) parameter D is free.

The noise $\mathbf{H}$ **multiplies** the magnetic moment $\mathbf{M}$.

This is the **Markov stochastic Landau-Lifshitz-Gilbert-Brown (sLLGB)** multiplicative white noise stochastic differential equation.

Subtleties of Markov multiplicative noise processes are now posed.

Brown 63

sLLGB

Aim

- Set up a path-integral formalism.
- Set up a numerical integrator.

Use them.

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Stochastic calculus

Discretization prescriptions

$$\mathrm{d}_t x(t) = f[x(t)] + g[x(t)]\, H(t)$$

with $\langle H(t) \rangle = 0$ and $\langle H(t) H(t') \rangle = 2D\, \delta(t - t')$ means

$$\boxed{x(t + \mathrm{d}t) = x(t) + f[\overline{x}(t)]\, \mathrm{d}t + g[\overline{x}(t)]\, H(t) \mathrm{d}t}$$

with

$$\boxed{\overline{x}(t) = \alpha x(t + \mathrm{d}t) + (1 - \alpha) x(t)}$$

and $0 \leq \alpha \leq 1$. Particular cases are $\alpha = 0$ Itō ; $\alpha = 1/2$ Stratonovich.

The **chain rule** for the time-derivative is

$$\boxed{\mathrm{d}_t Y(x) = \mathrm{d}_t x\, \mathrm{d}_x Y(x) + D(1 - 2\alpha)\, g^2(x)\, \mathrm{d}_x^2 Y(x)}$$

For $\alpha = 1/2$ (Stratonovich) one recovers the usual expression.

Stratonovich 67 ; Gardiner 96 ; Øksendal 00 ; van Kampen 07

Stochastic calculus

Fokker-Planck & stationary measure

The Fokker-Planck equation

$$\begin{aligned}\partial_t P(x,t) &= -\partial_x[(f(x)+2D\alpha g(x)\mathrm{d}_x g(x))P(x,t)] \\ &\quad +D\,\partial_x^2[g^2(x)P(x,t)]\end{aligned}$$

has the stationary measure

$$P_{\rm st}(x) = Z^{-1}\,[g(x)]^{2(\alpha-1)}\,e^{\frac{1}{D}\int^x \frac{f(x')}{g^2(x')}} = Z^{-1}e^{-\frac{1}{D}U_{\rm eff}(x)}$$

with $U_{\rm eff}(x) = -\int^x \frac{f(x')}{g^2(x')} + 2D(1-\alpha)\ln g(x)$

Remark : the potential $U_{\rm eff}(x)$ depends upon α and $g(x)$.

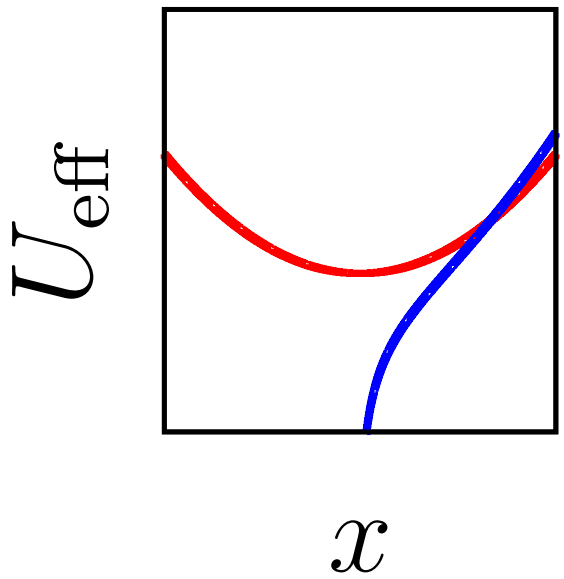
Noise induced phase transitions

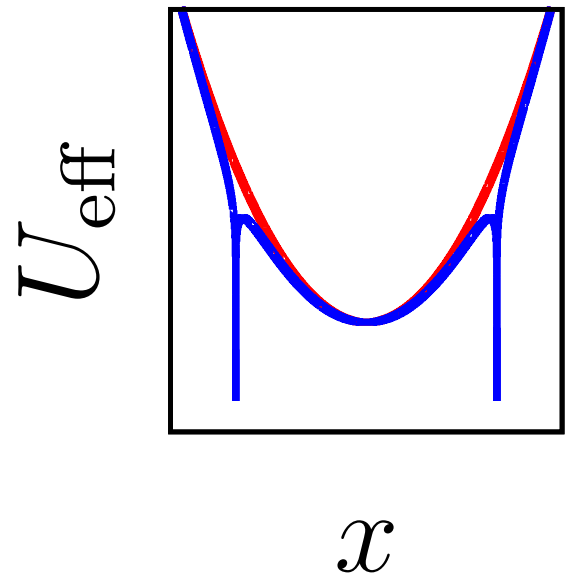
Stratonovich 67 ; Sagués, Sancho & García-Ojalvo 07

Stochastic calculus

Fokker-Planck & stationary measure

e.g. $U_{\text{eff}}(x) = V(x) + 2D(1-\alpha)\ln g(x)$





x^2 + $2D(1-\alpha)\ln x$

$g(x) = x$

x^2 + $2D(1-\alpha)\ln(1-x^2)$

$g(x) = (1-x^2)$

Stochastic calculus

Drift

The **Gibbs-Boltzmann equilibrium**

$$P_{\mathrm{GB}}(x) = Z^{-1}\, e^{-\beta U(x)}$$

is approached if

$$\boxed{f(x) \mapsto \underbrace{-g^2(x)\mathrm{d}_x U(x)}_{\text{Potential}}\ \underbrace{-2D\alpha g(x)\mathrm{d}_x g(x)}_{\text{drift}}}$$

Remark: the drift is also needed for the Stratonovich mid-point scheme.

Important choice: if one wants the dynamics to approach thermal equilibrium independently of α and g the drift term has to be added.

Stochastic calculus

Path-integral representation

The initial state at time $-\mathcal{T}$ is drawn from a probability distribution $P_{\rm i}(x_{-\mathcal{T}})$.

The noise generates random trajectories with probability density $P(x;\alpha)$.

$P(x;\alpha) = \langle \prod_t \delta(x_t - x_t^{\rm sol}) \rangle$ where $x_t^{\rm sol}$ is a solution to the Langevin equation and depends on the noise H.

The constraint can be written $J\ \delta(\prod_t \mathsf{Eq}_t[x,H;\alpha])$ with the Jacobian

$$J = \det_{tt'} \left[\frac{\delta \mathsf{Eq}_t[x,H;\alpha]}{\delta x_{t'}} \right]$$

Using the exponential representation of the delta $\delta(y) \propto \int d\hat{y}\ e^{{\rm i}\hat{y}y}$

We write the probability density of a trajectory x_t from $t=-\mathcal{T}$ to $t=\mathcal{T}$

$$P(x;\alpha) \quad = \quad P_{\rm i}(x_{-\tau})\ \langle\ J \int \mathcal{D}[\hat{x}]\ e^{\int_{-\mathcal{T}}^{\mathcal{T}} {\rm d}t\ {\rm i}\hat{x}_t\ \mathsf{Eq}_t[x,H;\alpha]}\ \rangle$$

Stochastic calculus

Path-integral representation

$$P(x;\lambda,\alpha) \propto \int \mathcal{D}[\hat{x}]\, P(x,\hat{x};\lambda,\alpha) = \int \mathcal{D}[\hat{x}]\, e^{S(x,\mathrm{i}\hat{x};\lambda,\alpha)}$$

and the **Martin-Siggia-Rose-Janssen 79** action

$$S(x,\mathrm{i}\hat{x};\lambda,\alpha) \equiv \ln P_{\mathrm{i}}(x_{-\mathcal{T}},\lambda_{-\mathcal{T}})$$
$$+ \int \Big[\mathrm{i}\hat{x}_t(\mathrm{d}_t x_t - f_t + \underbrace{2D\alpha g_t \mathrm{d}_x g_t) + D(\mathrm{i}\hat{x}_t)^2 g_t^2 - \alpha \mathrm{d}_x f_t}_{\text{From the Jacobian and the integration over the noise}}\Big]$$

cfr. **Langouche, Roekaerts & Tirapegui 79 ; Lau & Lubensky 07**

Remark: The action depends on α and g.

Observable averages can now be calculated as

$$\langle A(x_t)\rangle = \int \mathcal{D}[x]\, P(x;\lambda,\alpha) A(x_t)$$ (and do not depend on α)

Path probabilities

Path-integral representation

$$\frac{P(\mathcal{T}x, \mathcal{T}\hat{x}; \overline{\lambda}, \overline{\alpha})}{P(x, \hat{x}; \lambda, \alpha)} = e^{\Delta S(x, \hat{x}; \lambda, \alpha)}$$

where $\mathcal{T}x$ and $\mathcal{T}\hat{x}$ are transformed trajectories,

$\overline{\lambda}$ the transformed parameter in the potential,

$\overline{\alpha}$ a different discretization parameter ;

and from here obtain relations between observables by averaging this relation : equilibrium fluctuation dissipation ($\Delta S = 0$), or out of equilibrium theorems ($\Delta S \neq 0$).

Jarzinsky 97, Crooks 00, & many others

Stochastic calculus

Transformations in the path-integral representation

Let us define

$$\mathrm{d}_t^{(\alpha)} x_t \equiv \mathrm{d}_t x_t - 2\beta^{-1}(1-2\alpha) g_t \mathrm{d}_x g_t$$

and group two terms in the action due to the coupling to the bath

$$S_{\mathrm{diss}}[x, \mathrm{i}\hat{x}] = \int \mathrm{i}\hat{x}_t \, [\mathrm{d}_t^{(\alpha)} x_t + \beta^{-1} \mathrm{i}\hat{x}_t g_t^2]$$

This expression suggests to use the generalized transformation on the time-dependent variables $\{x_t, \mathrm{i}\hat{x}_t\}$

$$\mathcal{T}_c = \begin{cases} x_t & \mapsto & x_{-t} \ , \\ \mathrm{i}\hat{x}_t & \mapsto & \mathrm{i}\hat{x}_{-t} - \beta g_{-t}^{-2} \mathrm{d}_t^{(\alpha)} x_{-t} \ , \end{cases}$$

Stochastic calculus

Consequences of the transformation

For initial conditions drawn from $P_{\rm i}(x) = Z^{-1} e^{-\beta U(x)}$ and

$$\boxed{f(x) = -g^2(x) {\rm d}_x U(x) + 2D\alpha g(x) {\rm d}_x g(x)}$$ one proves

$$S_{\rm det+jac}[\mathcal{T}_c {\rm i}\hat{x}, \mathcal{T}_c x; \overline{\alpha}] = S_{\rm det+jac}[{\rm i}\hat{x}, x; \alpha]$$

that implies

$$P[\mathcal{T}_c {\rm i}\hat{x}, \mathcal{T}_c x; \overline{\alpha}] = P[{\rm i}\hat{x}, x; \alpha]$$

From this result we can prove exact equilibrium relations such as the **fluctuation-dissipation theorem**

$$\boxed{R(t,t') = \left.\frac{\delta \langle x_t \rangle}{\delta h_{t'}}\right|_{h=0} = \beta\, \partial_{t'} \langle x_t x_{t'} \rangle\, \theta(t-t')}$$

Stochastic calculus

Consequences of the transformation

For initial conditions drawn from $P_{\rm i}(x) = Z^{-1} e^{-\beta U(x)}$ and

$$\boxed{f(x,\lambda_t) = -g^2(x)\partial_x U(x,\lambda_t) + 2D\alpha g(x) {\rm d}_x g(x)}$$

one proves

$$\frac{P[\mathcal{T}_c {\rm i}\hat{x}, \mathcal{T}_c x; \overline{\alpha}, \overline{\lambda}_t]}{P[{\rm i}\hat{x}, x; \alpha, \lambda_t]} = e^{\beta W - \beta \Delta F}$$

with

$$\begin{aligned} W &= \int {\rm d}t \, {\rm d}_t \lambda_t \, \partial_\lambda U(x,\lambda) \\ \Delta F &= \ln Z(\lambda_{\mathcal{T}}) - \ln Z(\lambda_{-\mathcal{T}}) \end{aligned}$$

the work, and free-energy difference between initial and fictitious final states.

Exact out of equilibrium relations such as the **Jarzinsky relation** follow

$$\boxed{\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}}$$

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Magnetisation dynamics

Conservation of magnetisation modulus

$$\mathrm{d}_t\mathbf{M} = -\gamma_0\mathbf{M}\wedge(\dots) \qquad \rightarrow \qquad \mathbf{M}\cdot\mathrm{d}_t\mathbf{M} = 0$$

but

$$\mathrm{d}_t|\mathbf{M}|^2 = \mathrm{d}_t M_s^2 = 4D(1-2\alpha)\frac{\gamma_0^2}{1+\eta^2\gamma_0^2}M_s^2 \neq 0$$

because of the α-dependent **chain rule** associated to the Markov Landau-Lifshitz-Gilbert-Brown **stochastic equation**.

The sLLGB equation has to be modified to ensure the modulus conservation. This is achieved by replacing the derivative by the operator

$$\boxed{\mathrm{d}_t \mapsto \mathrm{D}_t^{(\alpha)} = \mathrm{d}_t + 2D(1-2\alpha)\frac{\gamma_0^2}{1+\eta^2\gamma_0^2}}$$

Magnetisation dynamics

Fokker-Planck equation and Gibbs-Boltzmann equilibrium

With this change, the probability density $P(\mathbf{M}, t)$ is determined by an α**-independent** Fokker-Planck equation.

If only conservative fields are applied $\boxed{\mathbf{H}_{\text{eff}} = \mu_0^{-1} \nabla_{\mathbf{M}} U}$ one proves that its asymptotic solution is of the Gibbs-Boltzmann form

$$P_{\text{GB}}(\mathbf{M}) = Z^{-1}\, e^{-\beta V U(\mathbf{M})}$$

with V the sample volume and U the potential energy per unit volume, *provided* the diffusion coefficient in the noise-noise correlation be chosen to satisfy

$$\boxed{D = \frac{\eta k_B T}{M_s V \mu_0}}$$

Formalism

Choices

Path-integral construction :

Landau-Lifshitz & Gilbert formalism ; Cartesian & spherical coordinates.

Aron, Barci, LFC, González-Arenas & Lozano 14

Generic results on equilibrium and out of equilibrium theorems :

We preferred to use the Gilbert formalism in Cartesian coordinates.

Aron, Barci, LFC, González-Arenas & Lozano 14

Numerical simulations.

We preferred to use the Landau-Lifshitz formalism in spherical coordinates.

Romá, LFC & Lozano 14

The action

in the Gilbert formalism in Cartesian coordinates

$$S_G = S_{G,\mathrm{det}} + S_{G,\mathrm{diss}} + S_{G,\mathrm{jac}}$$

with

$$\begin{aligned}
S_{G,\mathrm{det}} &= \ln P_{\mathrm{i}}[\mathbf{M}(t_{\mathrm{i}}), \mathbf{H}_{\mathrm{eff}}(t_{\mathrm{i}})] + \int \mathrm{i}\hat{\mathbf{M}}_{\parallel} \cdot \mathrm{D}_t^{(\alpha)}\mathbf{M} \\
&\quad + \int \mathrm{i}\hat{\mathbf{M}}_{\perp} \cdot \left(M_s^{-2}\, \mathrm{D}_t^{(\alpha)}\mathbf{M} \wedge \mathbf{M} + \gamma_0 \mathbf{H}_{\mathrm{eff}} \right) \\
S_{G,\mathrm{diss}} &= \int \gamma_0 \mathrm{i}\hat{\mathbf{M}}_{\perp} \cdot \left(D\gamma_0 \mathrm{i}\hat{\mathbf{M}}_{\perp} - \frac{\eta}{M_s}\, \mathrm{D}_t^{(\alpha)}\mathbf{M} \right) \\
S_{G,\mathrm{jac}} &= \frac{\alpha\gamma_0}{1+\eta^2\gamma_0^2} \frac{1}{M_s} \int \Big[2\eta\gamma_0 \mathbf{M} \cdot \mathbf{H}_{\mathrm{eff}} + M_s \epsilon_{ijk} M_k \partial_j H^{\mathrm{nc}}_{\mathrm{eff}_i} \\
&\qquad - \eta\gamma_0 (M_s^2 \delta_{ij} - M_i M_j) \partial_j H_{\mathrm{eff}_i} \Big]
\end{aligned}$$

The transformation

in the Gilbert formalism in Cartesian coordinates

$$\mathcal{T}_c = \begin{cases} \mathbf{M}_t & \mapsto & -\mathbf{M}_{-t} \\ \gamma_0 \, \mathrm{i}\hat{\mathbf{M}}_t^{\perp} & \mapsto & -\gamma_0 \, \mathrm{i}\hat{\mathbf{M}}_{-t}^{\perp} - \beta V \mu_0 \, \mathrm{d}_t \mathbf{M}_{-t} \\ \mathrm{i}\hat{\mathbf{M}}_t^{\parallel} & \mapsto & \mathrm{i}\hat{\mathbf{M}}_{-t}^{\parallel} \end{cases}$$

and

$$\overline{\alpha} = 1 - \alpha$$

if one simultaneously changes the sign of the effective field

$$\mathbf{H}^{\mathrm{c}}_{\mathrm{eff}\,t} \mapsto -\mathbf{H}^{\mathrm{c}}_{\mathrm{eff}\,-t} \; .$$

This change is a consequence of the transformation $\mathbf{M}_t \mapsto -\mathbf{M}_{-t}$ when the effective field derives from a potential $\mathbf{H}_{\mathrm{eff}} = -\mu_0^{-1} \nabla_{\mathbf{M}} U$ with U an even function of $\mathbf{M}$.

The transformation

in the Gilbert formalism in Cartesian coordinates

With this formalism one proves

the equilibrium **fluctuation-dissipation theorem**.

out of equilibrium **fluctuation relations**.

One could also apply these ideas in the Lifshitz-Landau formulation and in spherical coordinates.

Aron, Barci, LFC, González-Arenas & Lozano, arXiv:1412.7564

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Romá, LFC & Lozano 14

Magnetisation dynamics

The equations in spherical coordinates

The vector $\mathbf{M}$ defines the local basis ($\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\phi$) with $\mathbf{M} \equiv M_s\, \mathbf{e}_r(\theta, \phi)$ and the Cartesian components $M_x(t) = M_s \sin\theta(t) \sin\phi(t)$, $M_y(t) = M_s \sin\theta(t) \cos\phi(t)$ and $M_z(t) = M_s \cos\theta(t)$.

The sLLGB equation in this system of coordinates becomes $\mathrm{d}_t M_s = 0$,

$$\mathrm{d}_t\theta = \frac{D(1-2\alpha)\gamma_0^2}{1+\eta^2\gamma_0^2}\,\cot\theta + \frac{\gamma_0}{1+\eta^2\gamma_0^2}\,[H_{\mathrm{eff},\phi} + H_\phi + \eta\gamma_0(H_{\mathrm{eff},\theta} + H_\theta)]\ ,$$

$$\sin\theta\,\mathrm{d}_t\phi = \frac{\gamma_0}{1+\eta^2\gamma_0^2}\,[\eta\gamma_0(H_{\mathrm{eff},\phi} + H_\phi) - (H_{\mathrm{eff},\theta} + H_\theta)]\ ,$$

with $H_\theta = H_x \cos\theta\cos\phi + H_y \cos\theta\sin\phi - H_z \sin\theta$ and $H_\phi = -H_x \sin\phi + H_y \cos\phi$. Similarly for $\mathbf{H}_{\mathrm{eff}}$.

Magnetisation dynamics

Adimensionalisation and α-points

We introduce $\mathbf{m} = \mathbf{M}/M_s$, $\mathbf{h}_{\rm eff} = \mathbf{H}_{\rm eff}/M_s$, $\mathbf{h} = \mathbf{H}/M_s$
$\tau = \gamma_0 M_s t$, $\eta_0 = \eta\gamma_0$, and $D_0 = D\gamma_0/M_s$

We define the α-prescription angular variables

$$\theta_\tau^\alpha \equiv \alpha\theta(\tau + \Delta\tau) + (1-\alpha)\theta(\tau) \ ,$$
$$\phi_\tau^\alpha \equiv \alpha\phi(\tau + \Delta\tau) + (1-\alpha)\phi(\tau) \ ,$$

with $0 \leq \alpha \leq 1$. The effective fields at the α-point are

$$h_{{\rm eff},\theta}^\alpha \equiv h_{{\rm eff},\theta}(\theta_\tau^\alpha, \phi_\tau^\alpha) \qquad\qquad h_{{\rm eff},\phi}^\alpha \equiv h_{{\rm eff},\phi}(\theta_\tau^\alpha, \phi_\tau^\alpha)$$

We first draw the Cartesian components of the fields as $\Delta W_i = h_i \Delta\tau = \omega_i\sqrt{2D_0\Delta\tau}$ where the ω_i are Gaussian random numbers with mean zero and variance one, and we then calculate $\Delta W_\phi = h_\phi \Delta\tau$ and $\Delta W_\theta = h_\theta \Delta\tau$.

Magnetisation dynamics

The equations in spherical coordinates

The discretized dynamic equations now read $F_\theta = 0$ and $F_\phi = 0$ with

$$
\begin{aligned}
F_\theta &\equiv -\left(\theta_{\tau+\Delta\tau} - \theta_\tau\right) + D_0 \Delta\tau \frac{(1-2\alpha)}{(1+\eta_0^2)} \cot\theta_\tau^\alpha \\
&\quad + \frac{\Delta\tau}{1+\eta_0^2}\left[h^\alpha_{\mathrm{eff},\phi} + \eta_0 h^\alpha_{\mathrm{eff},\theta}\right] + \frac{1}{1+\eta_0^2}\left[\Delta W_\phi + \eta_0\, \Delta W_\theta\right] \\
F_\phi &\equiv -\left(\phi_{\tau+\Delta\tau} - \phi_\tau\right) \\
&\quad + \frac{\Delta\tau}{1+\eta_0^2}\left[\frac{\eta_0\, h^\alpha_{\mathrm{eff},\phi} - h^\alpha_{\mathrm{eff},\theta}}{\sin\theta_\tau^\alpha}\right] + \frac{1}{1+\eta_0^2}\left[\frac{\eta_0\, \Delta W_\phi - \Delta W_\theta}{\sin\theta_\tau^\alpha}\right]
\end{aligned}
$$

We used a Newton-Raphson routine and we imposed $F_\theta^2 + F_\phi^2 < 10^{-10}$ to find $\phi_{\tau+\Delta\tau}$ and $\theta_{\tau+\Delta\tau}$.

To avoid singular behavior when the magnetization gets too close to the z axis we apply a $\pi/2$ rotation of the coordinate system around the y axis.

Magnetisation dynamics

The benchmark

Uniformly magnetised ellipsoid with volume $V = 6.702 \times 10^{-26}$ m^3.

The potential energy per unit volume is

$$U(\mathbf{M}) = -\mu_0 \, \mathbf{M} \cdot \mathbf{H}_{\text{ext}} + \frac{\mu_0}{2} \left(d_x^2 M_x^2 + d_y^2 M_y^2 + d_z^2 M_z^2 \right)$$

We set $\mathbf{H}_{\text{ext}} = 0$ and $d_x = d_y = 0.4132$ and $d_z = 0.0946$

After adimensionalisation

the friction coefficient becomes $\eta_0 = \eta \gamma_0 \ll 1$

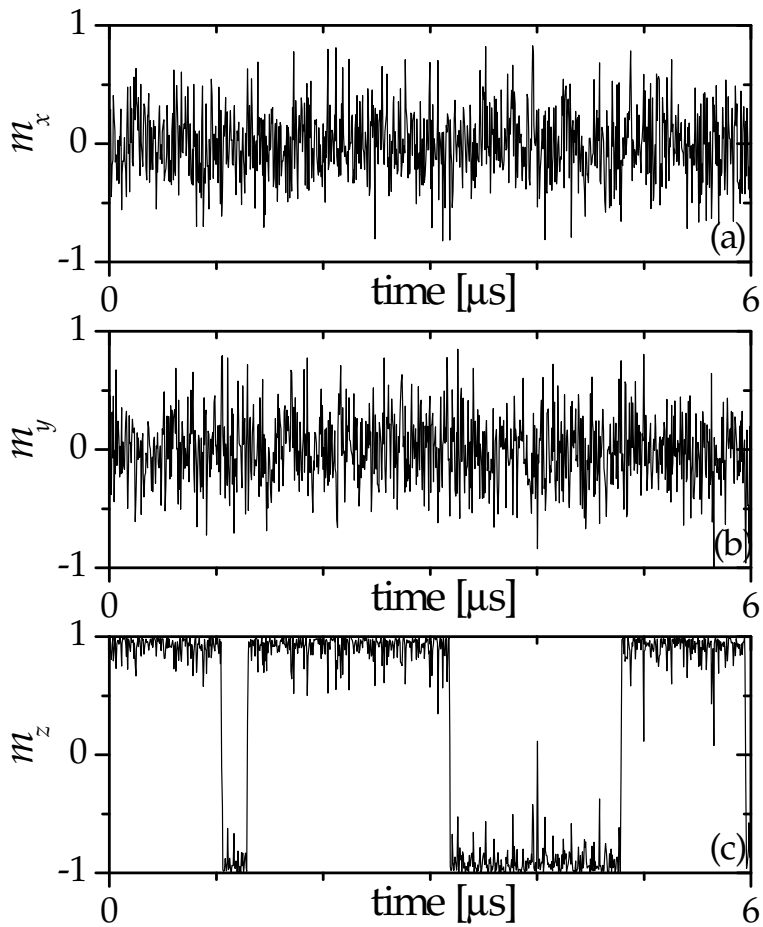
the time-step $\Delta\tau = 1$ corresponds to $\Delta t = 3.2$ ps

We set the temperature to $T = 300$ K ; then $\boxed{\dfrac{k_B T}{V \Delta U} \simeq 0.153}$

d'Aquino, Serpico, Coppola, Mayergoyz & Bertotti 06

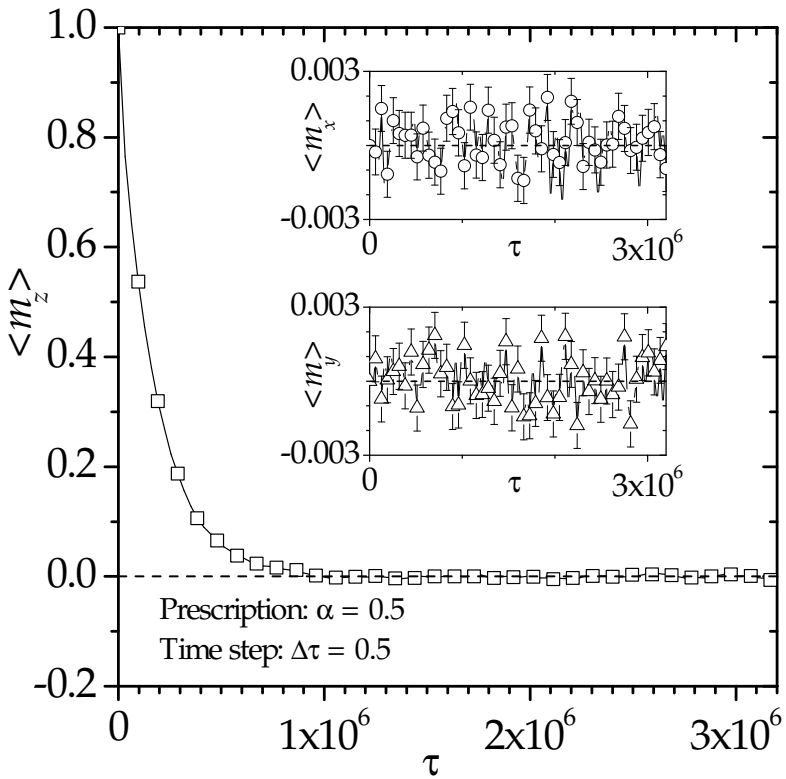
Magnetisation dynamics

Typical trajectories of the three magnetisation components



Magnetisation dynamics

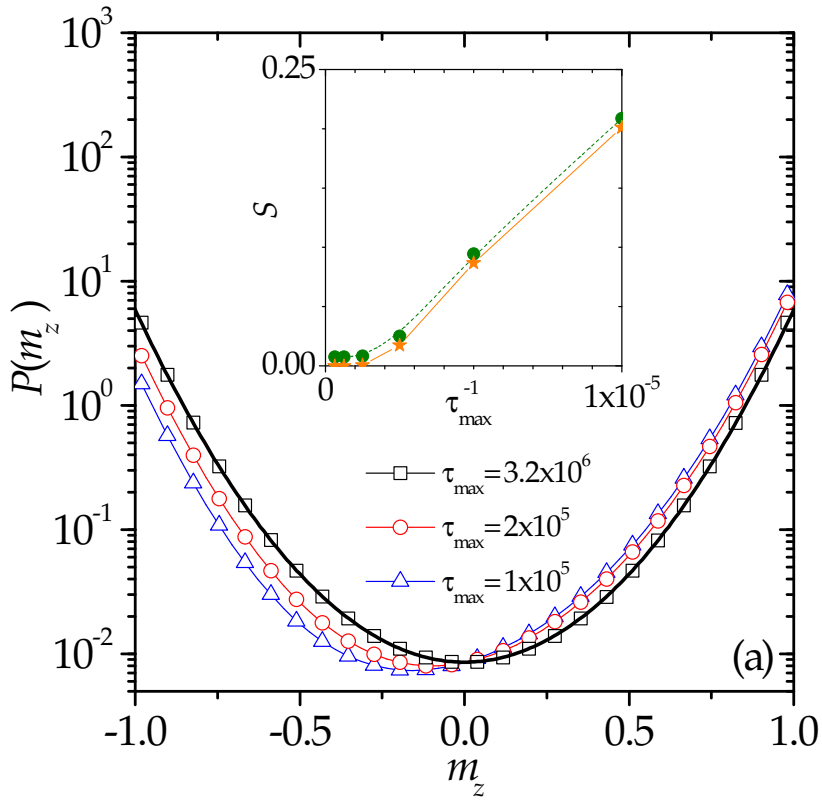
Decay of the averaged m_z component



Stratonovich scheme

Magnetisation dynamics

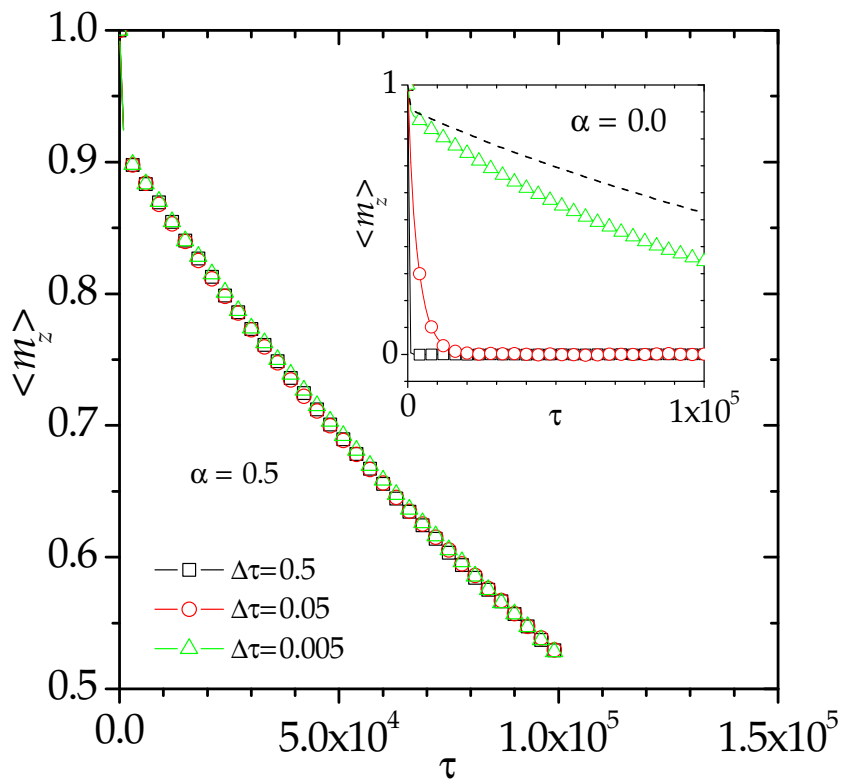
Distribution of the m_z component



Stratonovich scheme, comparison to the analytic form (solid line)

Magnetisation dynamics

Decay of the m_z component

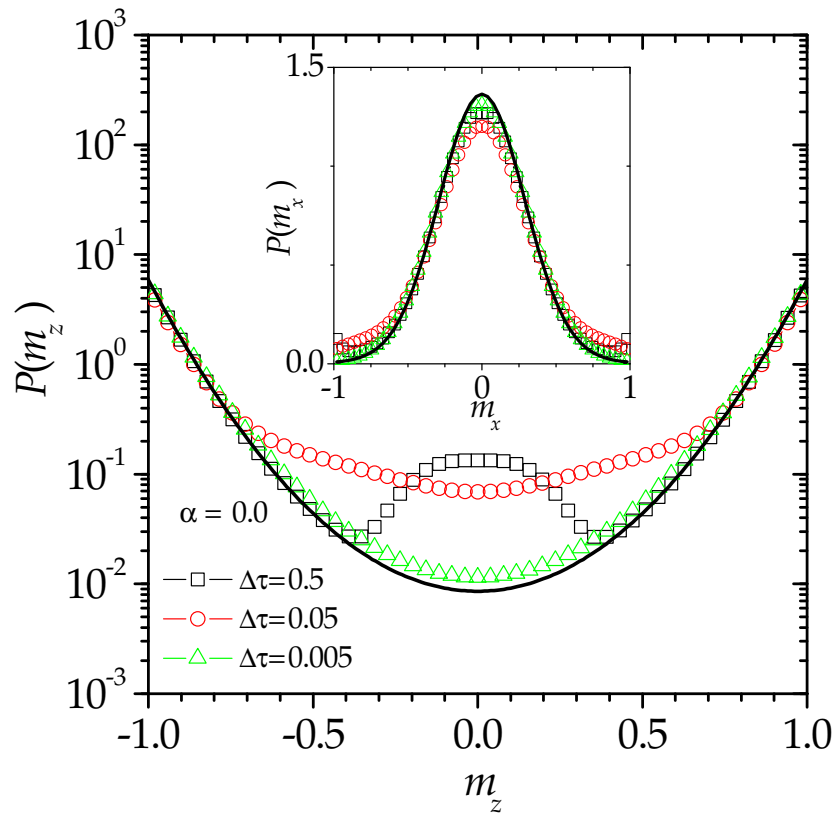


Dependence on $\Delta\tau$; $\alpha = 1/2$ (main) and $\alpha = 0$ (inset)

cfr. **Kloeden & Platen** *Numerical solutions of stochastic differential equations*

Magnetisation dynamics

Distribution of the m_z component, Itō scheme



For $\alpha = 0$, $\Delta\tau = 0.05$ is needed to get close to the equilibrium pdf.

Conclusions

Numerics

- All discretisation schemes converge to Gibbs-Boltzmann equilibrium

$$P(\mathbf{M}) = Z^{-1} e^{-\beta V U(\mathbf{M})}$$

  once the correct drift term has been added.

- The magnetisation modulus is conserved by the numerical integration with no need for artificial rescaling.

- The Stratonovich convention is the most efficient one in the sense that one can use larger values of $\Delta\tau$ and stay close to the continuous time limit.

  We will study the dependence of the algorithms' precision, for different α, in the future

Plan

- Macromagnetism: the stochastic Landau-Lifshitz-Gilbert-Brown (sLLGB) equation (precession, dissipation, noise and torque).
- Discretisation schemes for multiplicative white noise (Markov) stochastic differential equations. Asymptotic measure and drift term.
- Back to the sLLGB equation, analytic approach:
  drift term & functional formalism in Cartesian and spherical coordinates ; exact results.
- Back to the sLLGB equation, numerical simulations:
  analysis of a benchmark.
- Future work.

Related & future work

Some projects *en route*

Analytics : Dean-Kawasaki stochastic equation for the spatial magnetisation density of magnetic moments in pair interaction and controlled by the sLLGB microscopic equation.

LFC, Déjardin, Lozano & van Wijland, arXiv:1412.6497

Numerics : spin-torque effect, experimentally relevant situations.

Better understanding of the algorithms' precision.

Romá, LFC & Lozano

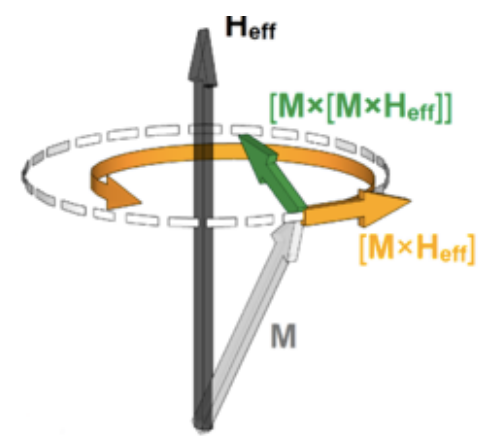
Dissipative effects

Landau-Lifshitz & Gilbert equations

$$\boxed{\mathrm{d}_t\mathbf{M} = -\frac{\gamma_0}{1+\eta^2\gamma_0^2}\,\mathbf{M}\wedge\left[\mathbf{H}_{\mathrm{eff}} + \frac{\eta\gamma_0}{M_s}\,(\mathbf{M}\wedge\mathbf{H}_{\mathrm{eff}})\right]}$$

Landau & Lifshitz 35

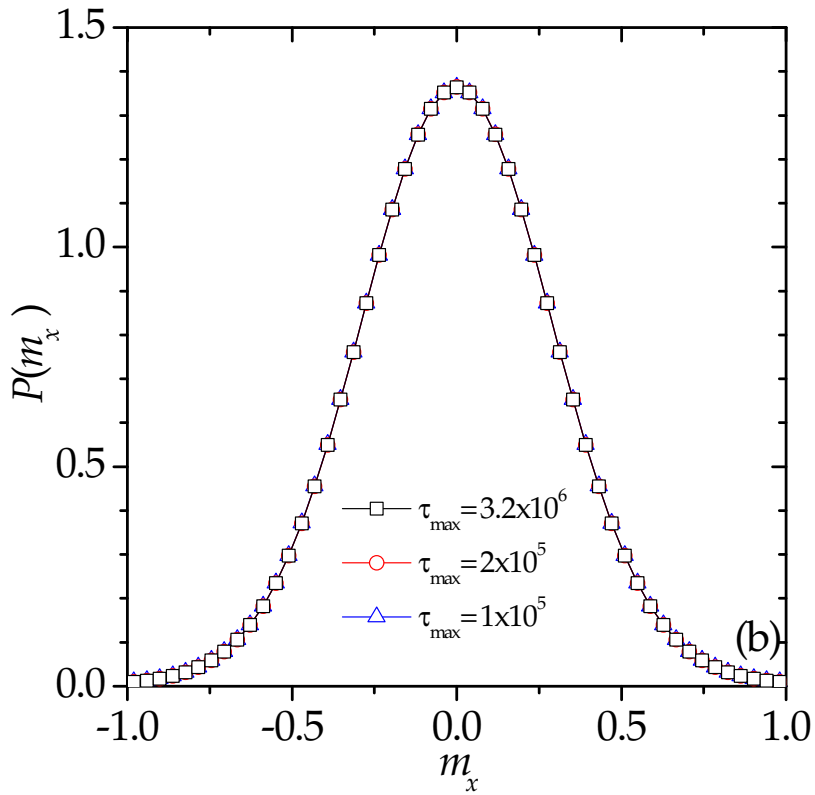
2nd terms in RHS: dissipative mechanisms slow down the precession and push $\mathbf{M}$ towards $\mathbf{H}_{\mathrm{eff}}$ with $2\mathbf{M}\cdot\mathrm{d}_t\mathbf{M} = \mathrm{d}_t|\mathbf{M}|^2 = 0$ and $\mathrm{d}_t(\mathbf{M}\cdot\mathbf{H}_{\mathrm{eff}}) > 0$



Proof : take the scalar product with $\mathbf{H}_{\mathrm{eff}}$ and use $(\mathbf{M}\cdot\mathbf{H}_{\mathrm{eff}})^2 < M_s^2 H_{\mathrm{eff}}^2$

Magnetisation dynamics

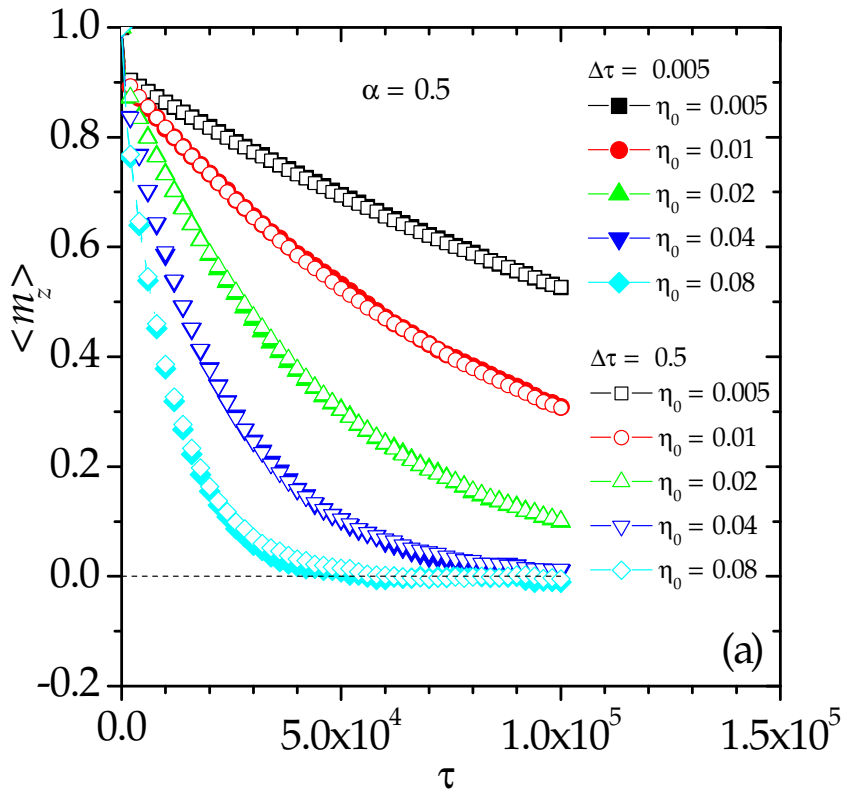
Distribution of the m_x component



Stratonovich scheme, Gaussian pdf

Magnetisation dynamics

Decay of the average m_z component

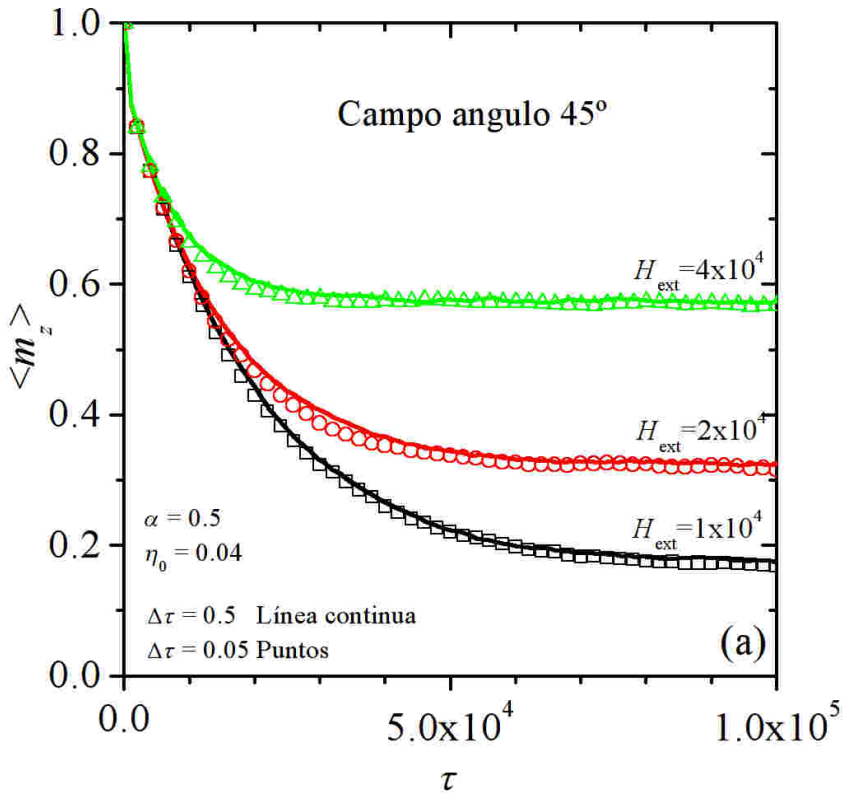


Stratonovich scheme

dependence on the friction coefficient η_0 and the time-step $\Delta\tau$

Magnetisation dynamics

$\langle m_z \rangle$ **under an applied field** $H_{\text{ext}} \neq 0$

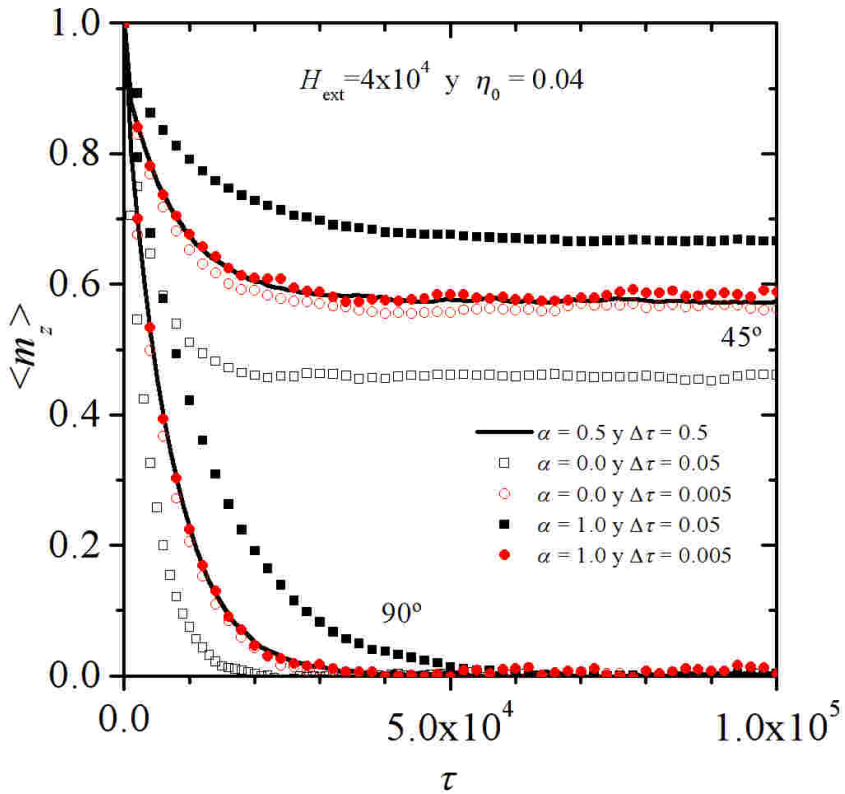


For $\alpha = 0.5$, little dependence on $\Delta\tau = 0.05$ vs $\Delta\tau = 0.5$

Note that a very large value $\Delta\tau = 0.5$ can be used.

Magnetisation dynamics

$\langle m_z \rangle$ **under an applied field** $H_{\rm ext} \neq 0$



Dependence on α cured by using smaller $\Delta\tau$:

poorer precision for $\alpha \neq 0.5$ confirmed.