Comportement en temps long d'une nano–particule

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Plan

The physical problem I

- Model the evolution of a ferro–magnet submitted to an external field b.
- Consider a single magnetic moment μ with values on $\mathcal{S}(\mathbb{R}^3)$

$$\frac{d\mu}{dt} = -\mu \wedge b - \alpha \mu \wedge (\mu \wedge b),$$

  where $\alpha > 0$ and $\mu_0 \in \mathcal{S}(\mathbb{R}^3)$.
- μ satisfies two major physical properties
  i. for all $t \geq 0$, $|\mu_t| = 1$,
  ii. for all $t \geq 0$, $\frac{d}{dt}(\mu_t \cdot b) = \alpha(|b|^2 - (\mu \cdot b)^2) \geq 0$.

The physical problem II

A few observations

- The system has two equilibrium positions $\pm b$.
- It is impossible to escape from $-b$ which is yet an unstable position for the system.
- No hysteresis phenomena.

Our goals

- Find a modelisation of thermal effects by introducing a stochastic perturbation in the model (ie. by adding some white noise to the field b)
- Highlight hysteresis phenomena for the stochastic model

Plan

The model I

From the previous remarks, we are tempted to consider the following dynamics for the process μ with values in $\mathbb{R}^3$ for the process μ with values in $\mathbb{R}^3$

$$d\mu_t = -\mu_t \wedge (b\ dt + \varepsilon\ dW_t) - \alpha\mu_t \wedge (\mu_t \wedge (b\ dt + \varepsilon\ dW_t))$$

where W is a 3-dimensional Brownian motion.
But

$$d|\mu_t|^2 = \sum_{i=1}^{3} d\left\langle \mu^i, \mu^i \right\rangle_t = 2\varepsilon^2(\alpha^2 + 1) > 0$$

This violates with the fundamental physical property $|\mu_t| = 1$.

The model II

Hence, we consider the pair of processes (Y, μ)

$$\begin{cases} dY_t & = -\mu_t \wedge (b\, dt + \varepsilon\, dW_t) - \alpha \mu_t \wedge \mu_t \wedge (b\, dt + \varepsilon\, dW_t) \\ \mu_t & = \frac{Y_t}{|Y_t|} \\ Y_0 & = y \in \mathcal{S}(\mathbb{R}^3). \end{cases} \qquad (1)$$

Assume this system has a solution, then

$$d\,|Y_t|^2 = 2\varepsilon^2(\alpha^2 + 1)dt.$$

$|Y_t|$ is deterministic and hence μ solves an autonomous SDE which enables to prove the existence and uniqueness of a pair (Y, μ) solving (1).

The model III

The most important quantity for understanding the behaviour of μ is the angle between μ and b, which is characterized by $(\mu \cdot b)$.
We define $h(t) = |Y_t|$

$$h(t) = \sqrt{2\varepsilon^2(\alpha^2 + 1)t + 1}.$$

We can establish the following SDE for $\mu_t \cdot b$

$$\begin{aligned} d(\mu_t \cdot b) = &-(\mu_t \cdot b)\frac{h'(t)}{h(t)}dt + \frac{\alpha}{h(t)}\left|\mu_t \wedge b\right|^2 dt \\ &+ \frac{\varepsilon}{h(t)}\big(\mu_t \wedge b - \alpha((\mu_t \cdot b)\mu_t - b)\big) \cdot dW_t \end{aligned}$$

Particular case $\alpha = 0$

$$d(\mu_t \cdot b) = -(\mu_t \cdot b)\frac{h'(t)}{h(t)}dt + \frac{\varepsilon}{h(t)}(\mu_t \wedge b) \cdot dW_t$$

$e(t) = \mathbb{E}(\mu_t \cdot b)$ solves the ODE

$$e'(t) = -\frac{h'(t)}{h(t)}e(t).$$

Hence,

$$e(t) = \frac{e(0)}{h(t)} \xrightarrow[t \longrightarrow \infty]{} 0$$

In the following, $\alpha > 0$.

Plan

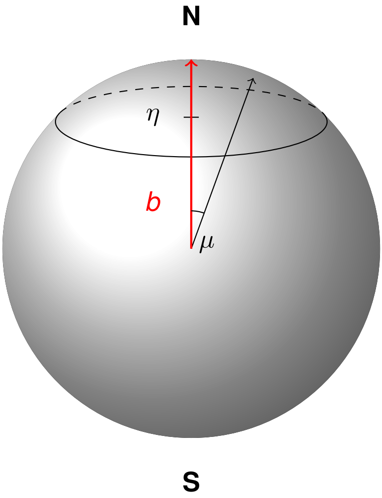
A few highlights on $\mu \cdot b$

$$d(\mu_t \cdot b) = -(\mu_t \cdot b)\frac{h'(t)}{h(t)}dt + \frac{\alpha}{h(t)}\left|\mu_t \wedge b\right|^2 dt + \frac{\varepsilon}{h(t)}\big(\mu_t \wedge b - \alpha((\mu_t \cdot b)\mu_t - b)\big) \cdot dW_t$$

- When μ_t is close to $\pm b$, the "dW_t" terms vanish.
- When μ_t is close to $-b$, $d(\mu_t \cdot b) \approx |b|\frac{h'(t)}{h(t)}dt$.
- When μ_t is close to b, $d(\mu_t \cdot b) \approx -|b|\frac{h'(t)}{h(t)}dt$.
- When taking $\mathbb{E}$, the "dW_t" terms vanish

$$\mathbb{E}(\mu_t \cdot b) - \mathbb{E}(\mu_s \cdot b) = \mathbb{E}\int_s^t \left(-(\mu_u \cdot b)\frac{h'(u)}{h(u)} + \frac{\alpha}{h(u)}\left|\mu_u \wedge b\right|^2\right) du$$

Almost sure convergence I



Almost sure convergence

For $0 < \delta < \eta < |b|$,

$$\tilde{\tau}_s = \inf\{t \geq 0 : \ \mu_{t+s} \cdot b \geq \eta\}$$
$$\tau_s = \inf\{t \geq 0; \ \mu_{s+\tilde{\tau}_s+t} \cdot b \leq \eta - \delta\}$$

Proposition

- *Nothern polar caps are recurrent.*
  For all $0 < \eta < |b|$ *and* $s > 0$, $\mathbb{P}(\tilde{\tau}_s < \infty) = 1$.
- *For all* $t > 0$, $\lim_{s \to \infty} \mathbb{P}(\tau_s \leq t) = 0$, *ie. the family* $(\tau_s)_s$ *tends to infinity in probability.*

Theorem

$\lim_{t \longrightarrow \infty} \mu_t \cdot b = |b|$ *a.s.*

Northern polar caps are reccurent I

Since

$$\mathbb{P}(\tilde{\tau}_s < \infty) = \mathbb{P}(\tilde{\tau}_s < \infty,\ \mu_s \cdot b < \eta) + \mathbb{P}(\tilde{\tau}_s < \infty,\ \mu_s \cdot b \geq \eta),$$

and

$$\mathbb{P}(\tilde{\tau}_s < \infty,\ \mu_s \cdot b \geq \eta) = \mathbb{P}(\mu_s \cdot b \geq \eta),$$

it suffices to show that $\mathbb{P}(\tilde{\tau}_s < \infty,\ \mu_s \cdot b < \eta) = \mathbb{P}(\mu_s \cdot b < \eta)$.
Let $A_s = \{\mu_s \cdot b < \eta\}$.
Integrating and applying the stopping theorem to $d(\mu_t \cdot b)$ gives

$$\mathbb{E}(\mu_{t\wedge(s+\tilde{\tau}_s)} \cdot b\mathbf{1}_{\{A_s\}}) - \mathbb{E}(\mu_s \cdot b\mathbf{1}_{\{A_s\}}) =$$
$$\mathbb{E}\left[\int_s^t \left(-(\mu_u \cdot b)\frac{h'(u)}{h(u)} + \frac{\alpha}{h(u)}\left|\mu_u \wedge b\right|^2\right)\mathbf{1}_{\{u\leq s+\tilde{\tau}_s\}} du \mathbf{1}_{\{A_s\}}\right].$$

Northern polar caps are reccurent II

We always have $|\mu_u \cdot b| \leq |b|$.
Let $u \leq s + \tilde{\tau}_s$.
On the set $\{0 < \mu_u \cdot b < \eta\}$, we have $|\mu_u \wedge b|^2 \geq |b|^2 - \eta^2$. Thus,

$$-(\mu_u \cdot b)\frac{h'(u)}{h(u)} + \frac{\alpha}{h(u)} |\mu_u \wedge b|^2 \geq -|b| \frac{h'(u)}{h(u)} + \alpha \frac{|b|^2 - \eta^2}{h(u)}.$$

There exists $U > s$ (non random) such that for all $u \geq U$,

$$-|b| \frac{h'(u)}{h(u)} + \alpha \frac{|b|^2 - \eta^2}{h(u)} \geq \alpha \frac{|b|^2 - \eta^2}{2h(u)}.$$

Northern polar caps are reccurent III

On the set $\{\mu_u \cdot b \leq 0\}$ we have

$$-(\mu_u \cdot b)\frac{h'(u)}{h(u)} + \frac{\alpha}{h(u)}\left|\mu_u \wedge b\right|^2 \geq (-(\mu_u \cdot b) + \alpha\left|\mu_u \wedge b\right|^2)\frac{h'(u)}{h(u)}$$
$$\geq \min(|b|, \alpha\,|b|^2)\frac{1}{2}\frac{h'(u)}{h(u)}.$$

The last inequality comes from the fact that if $\pi/2 \leq x \leq 3\pi/2$, we have either $-\cos(x) \geq \sqrt{2}/2$ or $|\sin(x)| \geq \sqrt{2}/2$.

Therefore, there exists $\bar{U} \geq U$ (non random), such that for all $u \geq \bar{U}$, on the event $A_s \cap \{u \leq s + \tilde{\tau}_s\}$,

$$-(\mu_u \cdot b)\frac{h'(u)}{h(u)} + \frac{\alpha}{h(u)}\left|\mu_u \wedge b\right|^2 \geq c\frac{h'(u)}{h(u)}$$

which is non integrable and where $c > 0$ depends on η.

Northern polar caps are reccurent IV

$$
\begin{aligned}
\mathbb{E}(\mu_{t\wedge\tilde{\tau}_s} \cdot b\mathbf{1}_{\{A_s\}}) - \mathbb{E}(\mu_s \cdot b\mathbf{1}_{\{A_s\}}) \geq \\
\mathbb{E}\left(\int_s^{\bar{U}} \left(-(\mu_u \cdot b)\frac{h'(u)}{h(u)} + \alpha\frac{|\mu_u \wedge b|^2}{h(u)}\right)\mathbf{1}_{\{u \leq s+\tilde{\tau}_s, A_s\}} du\right) \\
+ \int_{\bar{U}}^t c\frac{h'(u)}{h(u)}\mathbb{P}(u \leq \tilde{s} + \tau_s,\ A_s) du
\end{aligned}
$$

As $c\frac{h'(u)}{h(u)} > 0$ is non integrable, we must have

$$
\lim_{u\longrightarrow\infty} \mathbb{P}(u \leq s + \tilde{\tau}_s,\ A_s) = 0,
$$

otherwise $\mathbb{E}(\mu_{t\wedge\tilde{\tau}_s} \cdot b\mathbf{1}_{\{A_s\}}) \xrightarrow[t\longrightarrow\infty]{} \infty$ which would contradict the boundedness of the process μ.

Thus, $\mathbb{P}(s + \tilde{\tau}_s < \infty,\ A_s) = \lim_{u\to\infty} \mathbb{P}(s + \tilde{\tau}_s < u,\ A_s) = \mathbb{P}(A_s)$.

Convergence rate I

Sofar, we have not been able to prove a CLT but…
Let $\eta > 0$ (small) be fixed. For any fixed $t_0 > 0$, we introduce

$$A_t^{t_0} = \left\{ \sup_{t_0 \le u \le t} |b| - \mu_u \cdot b < \eta \right\}.$$

- This is the set of paths staying a small cap near the northern pole.
- For $t \ge s$, $A_t^{t_0} \subset A_s^{t_0}$.
- From the a.s. convergence,
  $\forall 0 < \delta < 1$, $\exists t_0$ s.t. $\forall t \ge t_0$, $\mathbb{P}(A_t^{t_0}) \ge 1 - \delta$.

We only study the convergence rate along these paths.

Convergence rate II

Theorem

For $0 < \eta < 2|b|$ *and* $0 < \delta < 1$

$$\mathbb{E}\left(h(t)(|b| - \mu_t \cdot b)\mathbf{1}_{\{A_t^{t_0}\}}\right) \leq \frac{\varepsilon^2(1+\alpha^2)}{\alpha(2-\eta/|b|)} \quad \forall t \geq t_0,$$

$$\frac{\varepsilon^2(1+\alpha^2)(1-\delta)}{2\alpha} \leq \liminf_{t \longrightarrow \infty} \mathbb{E}\left(h(t)(|b| - \mu_t \cdot b)\mathbf{1}_{\{A_t^{t_0}\}}\right).$$

Remark : η and δ should be thought of as small quantities, hence there is very little space left between the upper and lower bounds. *It suggests that that the limit of* $\frac{2\alpha\sqrt{2}}{\varepsilon\sqrt{(1+\alpha^2)}}\sqrt{t}\,\mathbb{E}(|b| - \mu_t.b)$ *when* $t \to \infty$ *should be equal to one.*

Convergence rate III

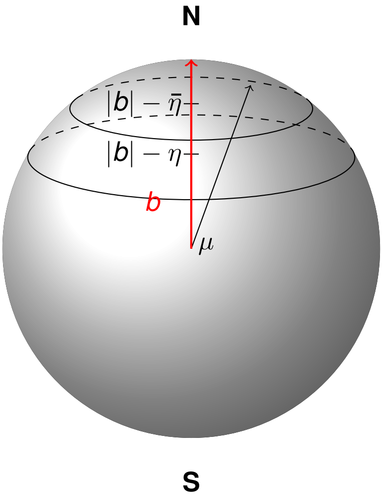
Theorem

The following results hold

1. *For all* $0 < \beta < 1/2$ *and* $\bar{\eta} > 0$, $\mathbb{P}(t^\beta(|b| - \mu_t \cdot b) \geq \bar{\eta}) \longrightarrow 0$.
2. *For all* $t \geq t_0$ *and all* $0 < \bar{\eta} < \eta$, *we have*

$$\mathbb{P}(|b| - \mu_t \cdot b \geq \bar{\eta}; \sup_{t_0 \leq u \leq t} |b| - \mu_u \cdot b < \eta) \leq \frac{\varepsilon^2(1+\alpha^2)}{\alpha(2 - \eta/|b|)\bar{\eta}} \quad \frac{1}{h(t)}.$$

Convergence rate IV



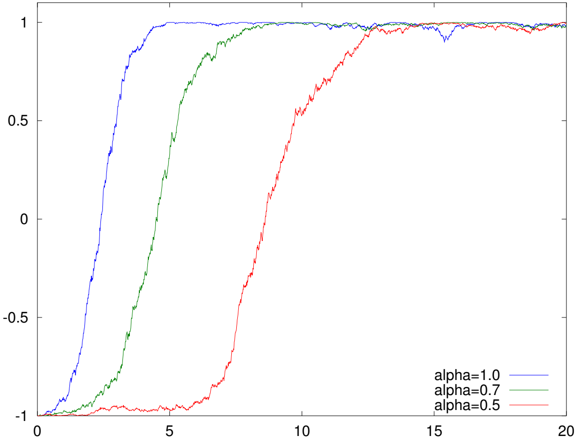


FIGURE : Almost sure convergence of $\mu_t \cdot b$ with $\mu_0 = -b$, $|b| = 1$, $\varepsilon = 0.1$.

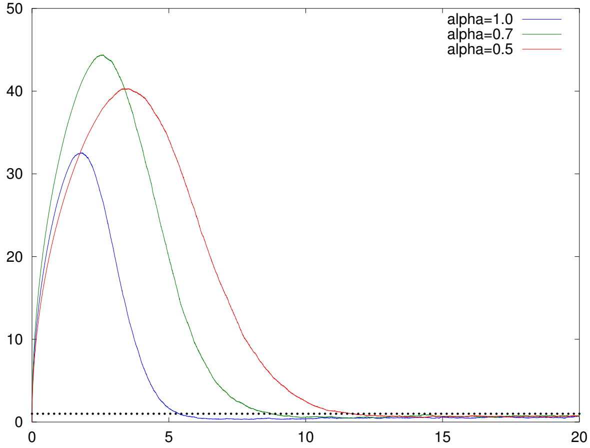


FIGURE : Convergence of $\frac{2\alpha\sqrt{2}}{\varepsilon\sqrt{(1+\alpha^2)}}\sqrt{t}\,\mathbb{E}(|b| - \mu_t.b)$ with $\mu_0 = -b$, $|b| = 1$ and $\varepsilon = 0.1$. The horizontal dashed line is at level one. The expectation is computed using a Monte–Carlo method with 100 samples.

Model for highlighting hysteresis I

Assume the magnetic field slowly varies between $+\boldsymbol{b}$ and $-\boldsymbol{b}$

$$b_t^\eta = (1 - 2t\,\eta)\,\boldsymbol{b} \quad \forall t \leq 1/\eta$$

The pair of processes (Y, μ) are now defined by

$$\begin{cases} dY_t^\eta & = -\mu_t^\eta \wedge (b_t^\eta\, dt + \varepsilon\, dW_t) - \alpha \mu_t^\eta \wedge \mu_t^\eta \wedge (b_t^\eta\, dt + \varepsilon\, dW_t) \\ \mu_t^\eta & = \frac{Y_t^\eta}{|Y_t^\eta|} \\ Y_0^\eta & = \boldsymbol{b} \end{cases}$$

In order to work on the interval $[0, 1]$, we introduce rescaled versions of both the external field and the magnetic moment defined for $t \in [0, 1]$.

$$b(t) = b^\eta_{t/\eta}, \qquad Z_t = Y^\eta_{t/\eta}, \qquad \lambda_t = \mu^\eta_{t/\eta}.$$

Model for highlighting hysteresis II

Using the time scale property of the stochastic integral, we can write

$$dZ_t = -\lambda_t \wedge \left(b_t \, \frac{1}{\eta} dt + \varepsilon \, dW_{t/\eta} \right) - \alpha \lambda_t \wedge \lambda_t \wedge \left(b_t \, \frac{1}{\eta} dt + \varepsilon \, dW_{t/\eta} \right)$$

We know that $(\sqrt{\eta} W_{t/\eta})$ is still a Brownian motion. So we get

$$\begin{cases} dZ_t & = -\lambda_t \wedge \left(b_t \, \frac{1}{\eta} dt + \varepsilon \, \frac{1}{\sqrt{\eta}} dW_t \right) - \alpha \lambda_t \wedge \lambda_t \wedge \left(b_t \, \frac{1}{\eta} dt + \varepsilon \frac{1}{\sqrt{\eta}} \, dW_t \right) \\ \lambda_t & = \frac{Y_t}{|Y_t|} \end{cases}$$

Hysteresis phynomenon

Theorem

$$\forall t \in [0, \frac{1}{2}],\ \mathbb{E}(\lambda_t^\eta \cdot \boldsymbol{b}) \geq \frac{1}{|Y_t|} \geq \frac{1}{\sqrt{1 + \frac{\varepsilon^2(1+\alpha^2)}{\eta}}}$$

This means that on average the path of $\lambda^\eta \cdot \boldsymbol{b}$ is striclty above 0 when the external b vanished.

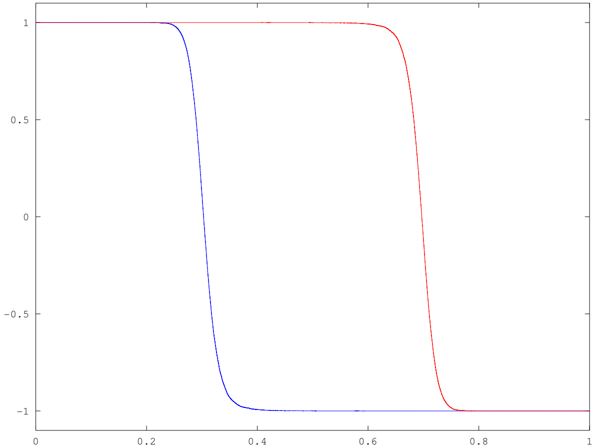


FIGURE : Pathwise hysteresis phenomena with $\alpha = 1$, $\varepsilon = 0.005$ and $\eta = 0.01$. The red curve is the forward path whereas the blue curve is the backward path.

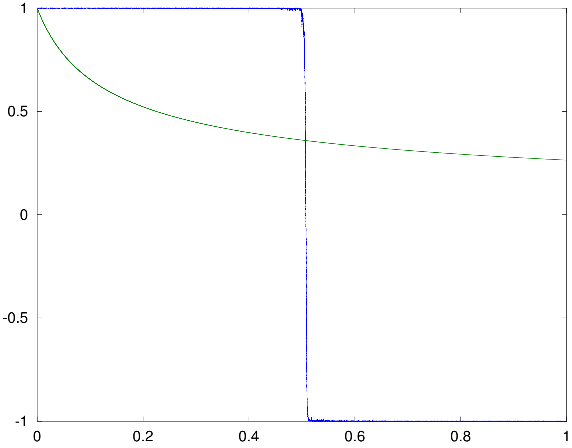


FIGURE : Pathwise hysteresis phenomena with $\alpha = 1$, $\varepsilon = 0.01$ and $\eta = 3.1E - 5$. The blue curve is the evolution of $\mu_t \cdot \boldsymbol{b}$ and the green curve is $1/h^\eta(t)$.

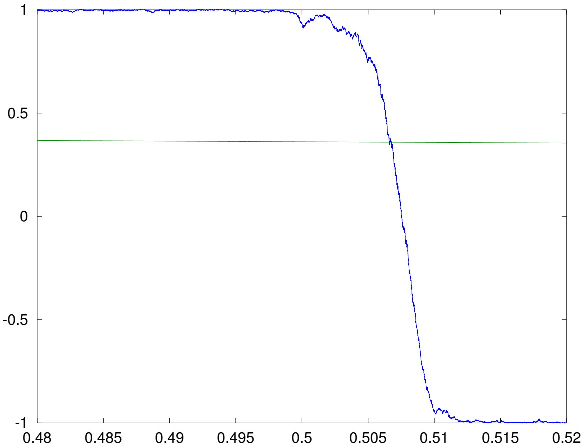


FIGURE : Zoom of th previous Figure around $t = 1/2$. The blue curve is the evolution of $\mu_t \cdot \boldsymbol{b}$ and the green curve is $1/h^\eta(t)$.

Conclusion

- The stochastic perturbation enabled to model thermal effects : the only stable position is $+b$, and for any μ_0, μ eventually stabilizes around $+b$.
- We managed to highlight hysteresis phenomena.
- The lower bound for the hysteresis phenomenon could be improved even though it is already very tight for small values of η, ie. for a slowly varying external field.
- No true CLT, even tough simulations tend to show one.