Comportement en temps long d’une nano-particule

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Plan

1. Introduction

2. The stochastic nano particule
   - Modelisation
   - Long time behaviour

3. Hysteresis phenomenon
The physical problem I

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

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

where $\alpha > 0$ and $\mu_0 \in S(\mathbb{R}^3)$.
- $\mu$ 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
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The model I

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

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

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

Hence, we consider the pair of processes \((Y, \mu)\)

\[
\begin{aligned}
    dY_t &= -\mu_t \land (b \, dt + \varepsilon \, dW_t) - \alpha \mu_t \land \mu_t \land (b \, dt + \varepsilon \, dW_t) \\
    \mu_t &= \frac{Y_t}{|Y_t|} \\
    Y_0 &= y \in S(\mathbb{R}^3).
\end{aligned}
\] (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 \(\mu\) solves an autonomous SDE which enables to prove the existence and uniqueness of a pair \((Y, \mu)\) solving (1).
The model III

The most important quantity for understanding the behaviour of $\mu$ is the angle between $\mu$ 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 $\mu_t \cdot b$

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

$$+ \frac{2\varepsilon}{h(t)} (\mu_t \wedge b - \alpha((\mu_t \cdot b)\mu_t - b)) \cdot dW_t$$
Particular case $\alpha = 0$

\[ d(\mu_t \cdot b) = - (\mu_t \cdot b) \frac{h'(t)}{h(t)} dt + \frac{\varepsilon}{h(t)} (\mu_t \land b) \cdot dW_t \]

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

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

Hence,

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

In the following, $\alpha > 0$. 
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A few highlights on $\mu \cdot b$

\[
d(\mu_t \cdot b) = -(\mu_t \cdot b) \frac{h'(t)}{h(t)} dt + \frac{\alpha}{h(t)} |\mu_t \wedge b|^2 dt
\]

\[
+ \frac{\varepsilon}{h(t)} (\mu_t \wedge b - \alpha((\mu_t \cdot b)\mu_t - b)) \cdot dW_t
\]

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

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

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

Theorem

\[
\lim_{t \to \infty} \mu_t \cdot b = |b| \text{ a.s.}
\]
Northern polar caps are recurrent I

Since

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

and

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

it suffices to show that \( P(\tilde{\tau}_s < \infty, \mu_s \cdot b < \eta) = P(\mu_s \cdot b < \eta) \).

Let \( A_s = \{\mu_s \cdot b < \eta\} \).

Integrating and applying the stopping theorem to \( d(\mu_t \cdot b) \) gives

\[
E(\mu_t \wedge (s+\tilde{\tau}_s) \cdot b 1_{\{A_s\}}) - E(\mu_s \cdot b 1_{\{A_s\}}) = \\
E \left[ \int_s^t \left( -\left( \mu_u \cdot b \right) \frac{h'(u)}{h(u)} + \frac{\alpha}{h(u)} |\mu_u \wedge b|^2 \right) 1_{\{u \leq s+\tilde{\tau}_s\}} du 1_{\{A_s\}} \right].
\]
Northern polar caps are recurrrent 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 recurrent III

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

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

\[
\geq \min(|b|, \alpha |b|^2) \frac{1}{2} \frac{h'(u)}{h(u)}.
\]

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 \( A_s \cap \{ u \leq s + \tilde{\tau}_s \} \),

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

which is non integrable and where \( c > 0 \) depends on \( \eta \).
Northern polar caps are recurrent IV

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

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

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

otherwise \( \mathbb{E} (\mu_{t \wedge \tilde{\tau}_s} \cdot b 1_{\{A_s\}}) \xrightarrow{t \to \infty} \infty \) which would contradict the boundedness of the process \( \mu \).

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

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

- This is the set of paths staying a small cap near the northern pole.
- For $t \geq s$, $A^{t_0}_t \subset A^{t_0}_s$.
- From the a.s. convergence,

$$\forall 0 < \delta < 1, \exists t_0 \text{ s.t. } \forall t \geq t_0, \mathbb{P}(A^{t_0}_t) \geq 1 - \delta.$$ 

We only study the convergence rate along these paths.
Convergence rate II

**Theorem**

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

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

$$\frac{\varepsilon^2(1 + \alpha^2)(1 - \delta)}{2\alpha} \leq \liminf_{t \to \infty} E\left(h(t)(|b| - \mu_t \cdot b)1_{\{A^C_t\}}\right).$$

**Remark** : $\eta$ and $\delta$ should be thought of as small quantities, hence there is very little space left between the upper and lower bounds.

*It suggests that the limit of $\frac{2\alpha \sqrt{2}}{\varepsilon \sqrt{(1+\alpha^2)}} \sqrt{t} E(|b| - \mu_t \cdot b)$ 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 $\bar{\eta} > 0$, $\mathbb{P}(t^\beta(|b| - \mu_t \cdot b) \geq \bar{\eta}) \to 0$.

2. For all $t \geq t_0$ and all $0 < \bar{\eta} < \eta$, we have

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

$$b_t^n = (1 - 2t \eta) \ b \quad \forall t \leq 1/\eta$$

The pair of processes $(Y, \mu)$ are now defined by

$$
\begin{align*}
\left\{ 
  dY_t^n &= -\mu_t^n \wedge (b_t^n \ dt + \varepsilon \ dW_t) - \alpha \mu_t^n \wedge \mu_t^n \wedge (b_t^n \ dt + \varepsilon \ dW_t) \\
  \mu_t^n &= \frac{Y_t^n}{|Y_t^n|} \\
  Y_0^n &= b
\end{align*}
$$

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

$$b(t) = b_{t/\eta}^n, \quad Z_t = Y_{t/\eta}^n, \quad \lambda_t = \mu_{t/\eta}^n.$$
Model for highlighting hysteresis II

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

$$dZ_t = -\lambda_t \wedge \left( b_t \frac{1}{\eta} dt + \varepsilon \frac{1}{\sqrt{\eta}} dW_t \right) - \alpha \lambda_t \wedge \lambda_t \wedge \left( b_t \frac{1}{\eta} dt + \varepsilon \frac{1}{\sqrt{\eta}} dW_t \right)$$

We know that $\left( \sqrt{\eta} W_{t/\eta} \right)$ 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 phenomenon

**Theorem**

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

This means that on average the path of \( \lambda^\eta \cdot b \) is strictly 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 $\mu_t \cdot b$ and the green curve is $1/h^\eta(t)$. 
**Figure**: Zoom of the previous Figure around $t = 1/2$. The blue curve is the evolution of $\mu_t \cdot b$ and the green curve is $1/h^n(t)$. 
Conclusion

- The stochastic perturbation enabled to model thermal effects: the only stable position is $+b$, and for any $\mu_0$, $\mu$ 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 $\eta$, ie. for a slowly varying external field.
- No true CLT, even tough simulations tend to show one.