Stage de M1 au LPTHE

Analysis of Coupled Langevin Equations:
Application to Magneto-Mechanical Systems

M1 Physique fondamentale et Application

Sebastian H. Castedo

Encadrante:
Leticia F. Cugliandolo

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Contents

1 Introduction

I have undertaken a 9 week internship at the High Energy and Theoretical Physics Laboratory (LPTHE) a joint research unit of Sorbonne University (Pierre and Marie Curie Campus) and the Institute of Physics (INP) of the National Center of Scientific Research (CNRS). LPTHE is composed of 19 CNRS researchers and 10 teaching researchers divided into 4 groups: Mathematical Physics, Strings Branes & Fields, Particle Physics & Cosmology and Condensed Matter & Statistical Physics where I conducted my Internship. My supervisor for this internship was Leticia F. Cugliandolo a professor and researcher at Sorbonne University. I conducted my work on site at LPTHE for the duration of my internship hosted in an office shared with other students. During my time in the lab I attended various seminars given by LPTHE and visiting researchers on topics in and around my subject matter which I found very engaging. I also participated in Monday tea break discussions and student talks hosted by the doctoral students at my laboratory.

My internship was focused on stochastic processes and more specifically a coupled magneto-mechanical system. I had not yet covered this subject in my studies and so the first part of my internship was composed of self-studying the techniques needed to tackle the set system. This included learning about the Langevin and the Fokker-Planck equations, stochastic calculus and path integrals. In addition, I numerically integrated and simulated several model stochastic systems to learn about different numerical methods and to check that my analytical derivations were correct.

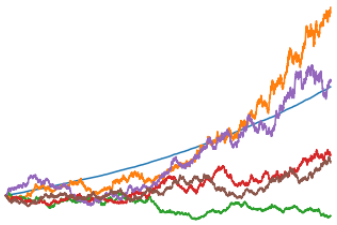


Figure 1: Illustration of standard Brownian motion

2 Topic

Physics can be said to be the study of interacting entities. Studying macroscopic phenomena using physics can be difficult however, as we need to be able to take into account an unimaginable number of said entities. The beauty of physics lies in the fact that one usually does not need more than a few variables guided by simple laws to be able to effectively describe such systems. In most macroscopic phenomenological models, one can easily integrate away an enormous number of degrees of freedom to leave a simple deterministic description. However, in some cases, one needs to more carefully take into account microscopic descriptions in order to effectively describe the system. These microscopic effects are usually felt are as noises in the macroscopic domain arising from thermal or quantum fluctuations. These systems have come to be called Stochastic Processes.
Historically, this domain was born through the attempt to explain Brownian motion Fig.1, the random jittery motion experienced by a particle when placed in a liquid. This effect was first explained by Einstein in his seminal 1905 paper [1] and later by Langevin in 1908 [2]. Usefully, one can use techniques from Brownian motion to describe many different noisy systems. One such system is the dynamic processional motion of the magnetisation $\boldsymbol{M}$ in a ferromagnet.

2.1 Magnetism

The ability to control magnetic materials is at the centre of information technologies today, and the search for smaller, more efficient, storage devices has spurred both fundamental and applied investigations into this subject. The design of such materials relies on a thorough understanding how magnetisation is affected by external magnetic fields. Until now, most research has centred around spins placed on fixed lattices, but recent advancements in smart devices has spurred investigation into magneto-mechanical materials which can serve as efficient actuators and sensors [3]. These materials are highly complex due to the interaction between the different degrees of freedom.
Magneto-mechanical effects can include applying stress to a material which cause the magnetic moments to rotate thus changing the overall magnetisation of the material and an applied field causing the rotation of magnetic moments which causes a strain in the material. In addition to magneto-mechanical effects one has to take into account dissipation and thermal fluctuations for sufficiently fine ferromagnetic particles [4]. Such fluctuations are well described by following Langevin's approach to Brownian motion where the spin system is connected to a thermal bath in a canonical way. Accurate numerical simulations of these effects are essential to test the underlying assumptions of theories and to interpret and predict experimental observations.

2.2 Landau-Lifshitz-Gilbert Equation

The standard Langevin equation describes well the dynamical degrees of freedom for such a system. For the magnetic degrees of freedom, the time evolution of the magnetisation is explained phenomenologically by the Landau-Lifshitz-Gilbert (LLG) equation (eq.4). To allow the equation to also describe ferromagnetic nano-particles, thermal fluctuations were introduced by Brown [4]. This was done by including an additional random magnetic field dependant on the temperature in a similar way to the Langevin equation. Even though the interaction between spins is due to the overlap of the electronic wave-functions, for most relevant cases, the macroscopic object can be modelled classically. Explicit analytical solutions to the stochastic LLG (sLLG) equation are only available in a few select cases and for most applied use cases numerical integration of this equation is required.

2.3 LAMMPS equations

LAMMPS is a molecular dynamics package that can be used to simulate magnetic nano-particles that have coupled dynamics and spins. The differential equations used in this package are variations of Lagrangian and sLLG equations and are presented in a paper by Tranchida et al. [5] (eq.19). Recently, a team in Argentina (F. Roma, E. Bringa and G. dos Santos) have been using LAMMPS to simulate various systems but found certain anomalous results when using a high damping constant in the equations. Most spin-lattice dynamics packages, including LAMMPS, depend on a spin temperature independent of damping, however, the Argentinian team discovered that the equilibrium results (e.g. average magnetisation) at temperature T depend on the value of the spin damping (whose dynamics is modelled by Tranchida's sLLG) with a pre-factor that tends to one for small damping. The package works approximately well for low damping but there are several cases where it is useful to have a higher value than assumed in the approximation e.g. for atomistic spin dynamics and micro-magnetism where artificially high damping (even as high as 100) allows the magnetisation to reach a steady state more quickly and thus decreases the computational cost. Initial investigations from F. Roma pointed to the fact that the error came from the equations laid out by Tranchida in [5]. The sLLG equation used is slightly different to the one defined by Brown (eq.4) as it does not couple a noise term to the dissipative part of the equation which we predict is the cause of adverse effects.

The task for this project is then stated as follows: after getting comfortable with topics in stochastic processes and corresponding analytical and numerical methods I will derive the Langevin equations given by Tranchida [5] using a concrete model for the environment giving rise to dissipations and noise. Then, I will obtain the corresponding Fokker-Planck equations and check whether the Boltzmann measure is a solution to the steady state equation [6].

3 Methods

In this investigation I have had to develop my understanding of Langevin equations and how to derive the corresponding Fokker-Planck equation. I have also learned how to numerically integrate these equations and the following section outlines these analytical and numerical techniques.

3.1 Langevin Equation

In the Langevin description of stochastic processes, the focus is on the movement of a single particle as opposed to finding a differential equation for the whole system. For Brownian motion, the simplest

stochastic system, starting from Newton's Second Law of Motion $\vec{F} = m\ddot{\vec{x}}$, we first account for the friction experienced by the particle due to the viscosity of the surrounding medium by separating out a drag term:

$$m\ddot{\vec{x}} = -\gamma\dot{\vec{x}} + \vec{F}, \tag{1}$$

where γ is the coefficient of friction. If one knows the force, $\vec{F}$, acting on this particle, its motion can be described by a completely deterministic equation. However, in order to explain the jittery motion, we have to accept that we can never truly know the value of $\vec{F}$ as it is itself random. Langevin's solution was to split the force into a deterministic background potential (V) and a random force term (ξ). The resulting equation is known as the *Langevin Equation*: [2]

$$m\ddot{\vec{x}} = -\gamma\dot{\vec{x}} - \nabla V + \vec{\xi}(t)\,. \tag{2}$$

Note that we do not know the exact value of $\vec{\xi}(t)$ at any time and it is because of this that we call it a *stochastic* differential equation. However, it is possible to deduce certain characteristics of this term. One usually defines $\vec{\xi}(t)$ according to a specific prescription which in our case is Gaussian White Noise (GWN) which is valid whenever the environment relaxes back down to equilibrium much faster than the system. The average and variance of GWN (1st and 2nd moments) are defined as [7]

$$\begin{aligned} \langle\vec{\xi}(t)\rangle &= 0 \\ \langle\vec{\xi_i}(t)\vec{\xi_j}(t')\rangle &= 2D\,\delta_{ij}\delta(t'-t), \end{aligned} \tag{3}$$

where D is the fluctuation-dissipation relation derived by Einstein as $D = \gamma\, k_b T$. These equations allow us to accurately describe the phenomenon of Brownian Motion but more importantly for us, it gives us the necessary formalism to be able to model other, more pertinent systems. The main Langevin equation in our investigation is the stochastic Landau-Lifshitz-Gilbert (sLLG) equation which is given by Brown [4] as :

$$\frac{d\boldsymbol{M}}{dt} = -\frac{\gamma_0}{1+\gamma_0^2\eta^2}\boldsymbol{M}\times\left[(\boldsymbol{H}+\boldsymbol{\zeta}) + \frac{\eta\gamma_0}{M_s}\,\boldsymbol{M}\times(\boldsymbol{H}+\boldsymbol{\zeta})\right] \tag{4}$$

where $\boldsymbol{H}$ is the local magnetic field, $\times$ is the cross product, $\boldsymbol{\zeta}$ is the Gaussian white noise term defined by eq. (3) and $\gamma_0 = \gamma\mu_0$ is the product of gyromagnetic ratio relating the magnetisation to the angular momentum and the vacuum permeability constant. η is a damping constant taking into account several dissipative mechanisms (spin-orbit coupling, magnon-phonon, magnon-impurity, etc.). M_s is the saturation magnetisation and the fluctuation-dissipation relation D [8] is given as

$$D = \frac{\eta\, k_B T}{M_s}. \tag{5}$$

The first term in the rhs of eq (4) describes the magnetisation precession around the local effective magnetic field H, while the second term is a phenomenological description of the dissipative mechanisms, introduced by Gilbert, which slow down this precession and push $\boldsymbol{M}$ towards the magnetic field $\boldsymbol{H}$ while keeping the modulus M_s fixed.

3.2 Fokker Planck equation

The Fokker-Planck equation takes a slightly different approach to the Langevin equation. It is a deterministic partial differential equation that models the evolution of the probability that the particle will be in a certain state at a certain time [9]. It is a useful formalism to prove that a certain Langevin equation

with Gaussian White Noise takes the system to equilibrium at the working temperature.
We start from the Chapman-Kolmogorov equation [7]

$$P(\vec{y}, t+\Delta t) = \int d\vec{y}_0 \; P(\vec{y}, t+\Delta t|\vec{y}_0, t) P(\vec{y}_0, t) \tag{6}$$

where $P(\vec{y}, t+\Delta t|\vec{y}_0, t)$ is the conditional probability of finding $\vec{y}$ at time $t+\Delta t$ given that the system was in the state $\vec{y}_0$ at time t. We obtain the Fokker-Planck description from the Langevin one by defining the conditional probabilities and using the definition of $P(\vec{y}, t)$ via the Dirac delta

Typo: should have been t+\Delta t

$$P(\vec{y}, t+\Delta t|\vec{y}_0, t) = \langle \delta(\vec{y} - \vec{y}_\xi(t)) \rangle \tag{7}$$

where $\vec{y}_{\xi,\zeta}(t+\Delta t)$ is the solution to the Langevin equation evaluated at time $t+\Delta t$, with initial condition $\vec{y}(t) = \vec{y}_0$, which clearly depends on the noises. We now expand around $\vec{y}_\xi(t) \sim \vec{y}_0$ since the time increment (Δt) and $\vec{y}$ increment ($\Delta \vec{y}$) are small. Using $\vec{y} = \vec{y}_0 + \Delta\vec{y}$,

$$\begin{aligned} &P(\vec{y}, t+\Delta t|\vec{y}_0, t) = \\ &\quad \delta(\vec{y} - \vec{y}_0) - \partial_\alpha \left(\delta(\vec{y} - \vec{y}_0)\langle \Delta y_\alpha \rangle\right) + \frac{1}{2}\partial_\alpha\partial_\beta \left(\delta(\vec{y} - \vec{y}_0)\langle \Delta y_\alpha \Delta y_\beta \rangle\right) + \mathcal{O}(\Delta t^2). \end{aligned} \tag{8}$$

Combining the three previous equations one gets

$$P(\vec{y}, t+\Delta t) = P(\vec{y}, t) - \partial_\alpha \left(\langle \Delta \vec{y}_\alpha \rangle P(\vec{y}, t)\right) + \frac{1}{2}\partial_\alpha\partial_\beta \left(\langle \Delta y_\alpha \Delta y_\beta \rangle P(\vec{y}, t)\right) + \mathcal{O}(\Delta t^2)\,. \tag{9}$$

Taking the limit for the differential of P,

$$\partial_t P(\vec{y}, t) = \lim_{\Delta t \to 0} \frac{P(\vec{y}, t+\Delta t) - P(\vec{y}, t)}{\Delta t}\,,$$

eliminates any terms higher than Δt in the rhs of (9). The Fokker-Planck equation thus must have the structure

$$\partial_t P(\vec{y}, t) = -\partial_\alpha \left[\frac{\langle \Delta y_\alpha \rangle}{\Delta t} P(\vec{y}, t)\right] + \frac{1}{2}\partial_\alpha\partial_\beta \left[\frac{\langle \Delta y_\alpha \Delta y_\beta \rangle}{\Delta t} P(\vec{y}, t)\right]\,. \tag{10}$$

3.3 Stochastic Calculus

The way in which a stochastic differential equation is integrated or evaluated is important. Consider a first order stochastic differential equation of the form

$$d_t x(t) = f(x(t)) + g(x(t))\xi(t) \tag{11}$$

where ξ is a Gaussian White Noise process satisfying eq.3 and f & g are the drift and diffusion terms respectively. The fact that ξ has infinite variance means the integral is ill defined and thus we need to give the product $g(x(t))\xi(t)$ a microscopic meaning. Integrating this equation, we introduce the Wiener process W as $\xi(t) = dW(t)/dt$, giving

$$x(t) = \int f(x(t))dt + \int g(x(t))dW(t). \tag{12}$$

A Wiener process, unfortunately, is nowhere differentiable and thus we must define the factor $g(t)$, sampling the function in the Riemann sum in different places. We discretise the time, and select the α covariant notation seen in [8]:

$$g(\bar{x}) = g\left(\alpha x(t_{n+1}) + (1-\alpha)x(t_n)\right), \tag{13}$$

for which there are two popular schemes: Itô, where $\alpha = 1$, and Stratonovich, where $\alpha = 1/2$ [10]. Itô samples the function at the beginning of the sub-interval and Stratonovich samples it with the mean of its value at both ends of the sub-intervals. Itô calculus is more efficient computationally because it is based on the Taylor expansion and random quantities become independent however in our case we will stick to mostly using Stratonovich as it conserves the modulus of the magnetisation in the sLLG equation that we will be studying (eq.4) [8].

3.4 Numerical Methods

In order to numerically integrate the Langevin equation, we discretise the time, $t_k = \epsilon k$, where ϵ is the time step and k is an integer, reaching a compromise between the result being accurate enough and the time interval being long enough.
When discretising the Langevin equation in order to numerically integrate it the stochastic field can be described using the definition of a Wiener Process [7]:

$$\xi\,\Delta\tau = \Delta W_i = \omega_i\sqrt{2D_s\Delta t}, \tag{14}$$

where ω_i is a random normally distributed value with 0 mean and unit variance and D_s is the fluctuation-dissipation relation. For Langevin equations with multiplicative noise, one has to choose an integration prescription as explained in section 3.3 which will depend on the type of system that you are modelling. The numerical algorithm that will be used will be Heun's Method [11] which is described in the following way: First, an initial estimation step is made of the Euler method:

$$\tilde{x}(t+\Delta t) = x(x(t),t,\xi) + \dot{x}(x(t),t,\xi)\Delta t \tag{15}$$

Then the next step is calculated using the trapezoidal rule

$$x(t+\Delta t) = x(t) + \frac{1}{2}\left[\dot{x}(x(t),t,\xi) + \dot{x}(\tilde{x}(t+\Delta t),t,\xi)\right]\Delta t \tag{16}$$

4 Analysis and Results

4.1 Study of Tranchida's Equations

Federico: this is the important section

In this section I will take Tranchida's Langevin equations [5], derive the corresponding Fokker-Planck equation and prove that the steady state solution doesn't go to equilibrium.

4.1.1 Langevin set of equations

We take a set of $i = 1, \ldots, N$ particles at positions $\vec{r}^{\,i} = (r_1^i, \ldots, r_d^i)$ with magnetic moments $\boldsymbol{s^i}$. The magnetic moments are normalised such that $|\boldsymbol{s}^i|^2 = s_s^2$ for each particle.

The interactions, as defined by Tranchida are quantified by the energy function $\mathcal{H}_{sl}$. It reads

$$\mathcal{H}_{sl} = -\mu_B\mu_0\sum_{i=0}^{N} g^i\boldsymbol{s^i}\cdot H_{ext} - \underset{\text{1/2}}{\sum_{i,j,i\neq j}^{N}} J(r_{ij})\;\boldsymbol{s^i}\cdot\boldsymbol{s^j} + \sum_{i=1}^{N}\frac{|\boldsymbol{p}^i|^2}{2m^i} + \underset{\text{1/2}}{\sum_{i,j=1}^{N}} V(r_{ij}) \tag{17}$$

where μ_0 is the vacuum permeability, μ_B is the Bohr magneton, g_i is the Landé g-factor, m is the mass of the particle and $V(r_{ij})$ is the mechanical pair-potential term. The sub-index a runs from one to three,

the dimension of space and the number of components of the magnetic moment as well. $J(r_{ij})$ is the coupling strength and depends on the distance between the particles

$$r_{ij} = |\vec{r}^{\,i} - \vec{r}^{\,j}| = \left[\sum_{b=1}^{d} (r_b^i - r_b^j)^2\right]^{1/2} . \tag{18}$$

The first term in eq.17 is the interaction energy due to an external magnetic uniform field H_{ext}. We set this field to 0 in our equations. The Langevin equations are given as

$$\begin{aligned} d_t r_a^i &= \frac{p_a^i}{m^i} , \\ d_t p_a^i &= \sum_{j(\neq i)}^{N} \left[-\frac{dV(r_{ij})}{dr_{ij}} + \frac{dJ(r_{ij})}{dr_{ij}} s^i \cdot s^j \right] - \frac{\gamma_L}{m^i} p_a^i + \xi(t)_a^i , \\ d_t s_a^i &= g_{ab}^i \, h_{eff,b}^* \; + f_{ab} \, \zeta_b , \end{aligned} \tag{19}$$

Typo

r_i r_i

We note that Tranchida does not add a noise to h_eff in the first term in the rhs

$h_{eff}^* = -\frac{1}{\hbar}\frac{\partial \mathcal{H}}{\partial \vec{s}_i}$ a spin force and γ_L is a damping parameter. Summation over repeated $b = 1, 2, 3$ indices is assumed; not over the particle indices, which we wrote explicitly when needed. We have used the notation of Aron et al. [8] where

$$\begin{aligned} g_{ab} &= \frac{1}{1+\eta_0^2}(\epsilon_{abc} s_c + \eta_0 (s_s^2 \delta_{ab} - s_a s_b) \\ f_{ab} &= \frac{1}{1+\eta_0^2}(\epsilon_{abc} s_c) \end{aligned} \tag{20}$$

\eta_0 = \eta \gamma_0

and η_0 is a transverse damping constant. In the following, we evaluate the stochastic integrals according to the Stratonovich formalism to conserve the modulus of the magnetisation as explained in section 3.3. The noises $\vec{\xi}^i$ and $\vec{\zeta}^i$ are independent, and white with zero mean and correlations are defined in [5] as

$$\langle \xi_a^i(t) \xi_b^j(t') \rangle = D_L \delta_{ab} \delta^{ij} \delta(t-t') , \qquad \langle \zeta_a^i(t) \zeta_b^j(t') \rangle = 2 D_s \delta_{ab} \delta^{ij} \delta(t-t') . \tag{21}$$

There is no cross correlation between $\vec{\xi}^i$ and $\vec{\zeta}^i$. In the following we note $\langle \dots \rangle$ the average over both noises. Tranchida defines the fluctuation dissipation relations as

$$D_s = \frac{2\pi\eta_0 k_B T}{\hbar}, \tag{22}$$

$$D_L = \gamma k_B T. \tag{23}$$

The aim is to find whether the values of D_L and D_s given by Tranchida take the system to thermal equilibrium.

4.1.2 Deriving the Fokker-Planck Equation

Using eq.10, we now need to calculate the averages $\langle \Delta y_\alpha \rangle$ and $\langle \Delta y_\alpha \Delta y_\beta \rangle$ to leading order in Δt using the Langevin eq. (19) which read in discrete time:

$$\begin{aligned} \Delta r_a^i &\equiv r_a^i(t+\Delta t) - r_a^i(t) = \frac{p_a^i}{m^i} \, \Delta t , \\ \Delta s_a^i &\equiv s_a^i(t+\Delta t) - s_a^i(t) = g_{ab}^i \, h_{eff,b}^{i*} \, \Delta t \; + f_{ab}^i \, \zeta_b^i \, \Delta t , \\ \Delta p_a^i &\equiv p_a^i(t+\Delta t) - p_a^i(t) = \sum_{j(\neq i)}^{N} \left[-\frac{dV(r_{ij})}{dr_{ij}} + \frac{dJ(r_{ij})}{dr_{ij}} \vec{s}^{\,i} \cdot \vec{s}^{\,j} \right] \Delta t - \frac{\gamma_L}{m^i} p_a^i \Delta t + \xi(t)_a^i \Delta t . \end{aligned} \tag{24}$$

Note the typos signalled above

All variables in the right-hand-side (rhs), and in particular $\vec{s}$ in g and r in J, are evaluated at the mid-point $\vec{y}_{\rm mp} = [\vec{y}(t)+\vec{y}(t+\Delta t)]/2$ since we chose to work with the Stratonovich prescription as explained in section 3.3. When working at $\mathcal{O}(\Delta t)$ we will be able to, in some cases, replace this mid-point by the initial one $\vec{y}_0$ in the interval $[t, t+\Delta t]$.
The averages of the position component increments are

$$\begin{aligned}\langle \Delta r_a^i \rangle &= \langle p_a^i \frac{\Delta t}{m^i} \rangle \\ &= \frac{p_a^i}{m^i}\Delta t + \mathcal{O}(\Delta t^2)\end{aligned} \tag{25}$$

The average of the product of two position increments is

$$\langle \Delta r_a^i \ \Delta r_b^j \rangle = \mathcal{O}(\Delta t^2) \tag{26}$$

The averages of the momentum component increments are

$$\begin{aligned}\langle \Delta p_a^i \rangle &= \langle \sum_{j(\neq i)}^{N} \left[-\frac{dV(r_{ij})}{dr_{ij}} + \frac{dJ(r_{ij})}{dr_{ij}} \vec{s}^{\,i} \cdot \vec{s}^{\,j} \right] \Delta t - \frac{\gamma_L}{m^i} p_a^i \Delta t \rangle \\ &= \sum_{j(\neq i)}^{N} \left[-\frac{dV(r_{ij})}{dr_{ij}} + \frac{dJ(r_{ij})}{dr_{ij}} s^i \cdot s^j \right] \Delta t - \frac{\gamma_L}{m^i} p_a^i \Delta t + \mathcal{O}(\Delta t^{3/2})\end{aligned} \tag{27}$$

The average of the product of two momentum increments is

$$\langle \Delta p_a^i \ \Delta p_b^j \rangle = D_L \delta_{ab} \delta^{ij} \Delta t + \mathcal{O}(\Delta t^{3/2}) \tag{28}$$

The averages of the magnetisation component increments are

$$\begin{aligned}\langle \Delta s_a^i \rangle &= \langle g_{ab}\ h^*_{eff,b}\ \Delta t \ + f_{ab}\ \zeta_b\ \Delta t \rangle \\ &= g_{ab} h^*_{eff,b} \Delta t + \langle f_{ab} [\vec{s} + \frac{\Delta \vec{s}}{2}] \zeta_b \Delta t \rangle \\ &= g_{ab} h^*_{eff,b} \Delta t + \langle f_{ab} \zeta_b \Delta t \rangle + \langle \frac{\Delta f_{cd}}{2} \partial_c f_{ab} \zeta_d \zeta_b \Delta t^2 \rangle \\ &= g_{ab} h^*_{eff,b} \Delta t + D_s \delta_{bd} f_{cd} \partial_c f_{ab}\ \Delta t + \mathcal{O}(\Delta t^{3/2}) \\ &= \frac{2 g_{ab}}{\hbar} \sum_{i,j,i\neq j}^{N} J(r_{ij}) s_b^j\ \Delta t - 2 D_s \frac{s_a^i}{(1+\eta_0^2)^2}\ \Delta t + \mathcal{O}(\Delta t^{3/2})\end{aligned} \tag{29}$$

typo in sum

where $h^*_{eff,b} = -\partial_{Sb}\mathcal{H}/\hbar$
The average of the product of two magnetisation increments is

$$\begin{aligned}\langle \Delta s_a^i \ \Delta s_b^j \rangle &= f_{ad}^i\ \xi_d\ \Delta t\ f_{bc}^j\ \xi_c\ \Delta t + \mathcal{O}(\Delta t^{3/2}) \\ &= \frac{2}{(1+\eta_0^2)^2} D_s \left(s_s^2 \delta_{ab} - s_a^i s_b^i \right) \Delta t + \mathcal{O}(\Delta t^{3/2})\end{aligned} \tag{30}$$

The averages over the cross products are all sub-leading since $\vec{\xi}$, $\vec{\zeta}$ are not correlated.

We will now write eq.(10) in a more explicit form

$$\begin{aligned} P(\vec{y},t+\Delta t)-P(\vec{y},t) = &-\frac{\partial}{\partial r_a^i}\left[\langle\Delta r_a^i\rangle\, P\right]-\frac{\partial}{\partial p_a^i}\left[\langle\Delta p_a^i\rangle\, P\right]-\frac{\partial}{\partial s_a^i}\left[\langle\Delta s_a^i\rangle\, P\right] \\ &+\frac{1}{2}\frac{\partial}{\partial s_a^i}\frac{\partial}{\partial s_b^j}\left[\langle\Delta s_a^i\Delta s_b^j\rangle\, P\right] \\ &+\frac{1}{2}\frac{\partial}{\partial p_a^i}\frac{\partial}{\partial p_b^j}\left[\langle\Delta p_a^i\Delta p_b^j\rangle\, P\right]+\mathcal{O}(\Delta t^{3/2}) \end{aligned} \tag{31}$$

in which a sum over repeated indices (i,j,a,b) is assumed in the rhs. Replacing

$$\begin{aligned} \partial_t P(\vec{y},t) = &-\frac{\partial}{\partial r_a^i}\left[\frac{p_a^i}{m^i}\,P\right] \\ &-\frac{\partial}{\partial p_a^i}\left[\sum_{j(\neq i)}^{N}\left[-\frac{dV(r_{ij})}{dr_{ij}}+\frac{dJ(r_{ij})}{dr_{ij}}\vec{s}^{\,i}\cdot\vec{s}^{\,j}\right]P-\frac{\gamma_L}{m^i}p_a^i\,P\right] \\ &-\frac{\partial}{\partial s_a^i}\left[\frac{2g_{ab}}{\hbar}\sum_{i,j,i\neq j}^{N}J(r_{ij})s_b^j\,P-2D_s\frac{s_a^i}{(1+\eta_0^2)^2}\,P\right] \\ &+\frac{1}{2}\frac{\partial}{\partial p_a^i}\frac{\partial}{\partial p_b^j}\left[D_L\delta_{ab}\delta^{ij}\,P\right]+\frac{1}{2}\frac{\partial}{\partial s_a^i}\frac{\partial}{\partial s_b^j}\left[\frac{2D_s}{(1+\eta_0^2)^2}\left(s_s^2\delta_{ab}-s_a^i s_b^i\right)P\right] \end{aligned} \tag{32}$$

4.1.3 Stationary Solution

We will now check if $P=\mathcal{Z}^{-1}e^{-\beta\mathcal{H}}$ satisfies a stationary solution of the Fokker-Planck equation (32).

$$\begin{aligned} 0 = &-\sum_i^N\frac{p_a^i}{m^i}\frac{\partial P}{\partial r_a^i} \\ &-\sum_{j(\neq i)}^{N}\left[-\frac{dV(r_{ij})}{dr_{ij}}+\frac{dJ(r_{ij})}{dr_{ij}}\vec{s}^{\,i}\cdot\vec{s}^{\,j}\right]\frac{\partial P}{\partial p_a^i}+3\sum_i^N\frac{\gamma_L}{m^i}\,P+\sum_i^N\frac{\gamma_L}{m^i}p_a^i\frac{\partial P}{\partial p_a^i} \\ &+\sum_i^N\frac{4s_b^i\eta_0}{\hbar(1+\eta_0^2)}\sum_{i,j,i\neq j}^{N}J(r_{ij})s_b^j\,P-\frac{2g_{ab}}{\hbar}\sum_{i,j,i\neq j}^{N}J(r_{ij})s_b^j\frac{\partial P}{\partial s_a^i}+\frac{6D_s}{(1+\eta_0^2)^2}\,P+2D_s\sum_i^N\frac{s_a^i}{(1+\eta_0^2)^2}\,\frac{\partial P}{\partial s_a^i} \\ &+\frac{D_L}{2}\frac{\partial^2 P}{\partial {p_a^i}^2}+\frac{D_s}{(1+\eta_0)^2}\left[-6P-4s_a^i\frac{\partial P}{\partial s_a^i}+\left(s_s^2\delta_{ab}-s_a^i s_b^i\right)\frac{\partial P}{\partial s_a^i\partial s_b^i}\right] \end{aligned} \tag{33}$$

where $\partial_{Sa} g_{ab} = \frac{-2 s_b^i \eta_0}{1+\eta_0^2}$. Now calculating the probability derivatives remembering $\partial_x P = -\beta P \, \partial_x \mathcal{H}$

$$\frac{\partial}{\partial r_a^i} P = \left(\sum_{k \neq j} \frac{dJ(r_{kj})}{dr_a^i} \, \vec{s}^k \cdot \vec{s}^j - \sum_{i,j=1}^{n} \frac{dV(r_{ij})}{dr_a^i} \right) \beta \, P \tag{34}$$

$$\begin{aligned} \frac{\partial}{\partial s_a^i} P &= \sum_{k \neq j} J(r_{kj}) [\delta_{ab} \delta^{ik} s_b^j + \delta_{ab} \delta^{ij} s_b^k] \, \beta \, P \\ &= 2 \sum_{k(\neq i)} J(r_{ik}) s_a^k \, \beta \, P \end{aligned} \tag{35}$$

$$\frac{\partial^2 P}{\partial s_a^i \partial s_b^i} = 4\beta^2 \sum_{k \neq i}^{N} \left(J(r_{ik}) \right)^2 s_b^k s_a^k P \tag{36}$$

$$\frac{\partial}{\partial p_a^i} P = -\sum_{i}^{N} \frac{p_a^i}{m^i} \, \beta \, P \tag{37}$$

$$\frac{\partial^2}{\partial (p_a^i)^2} P = -\sum_{i}^{N} \frac{3}{m^i} \, \beta P + \left(\sum_{i}^{N} \frac{p_a^i}{m^i} \right)^2 \beta^2 \, P \tag{38}$$

4.1.4 Dynamical terms

For the dynamical terms, replacing the probability derivatives gives:

$$\begin{aligned} 0 = &- \sum_{i}^{N} \frac{p_a^i}{m^i} \left(\sum_{k \neq j} \frac{\partial J(r_{kj})}{\partial r_a^i} \, \vec{s}^k \cdot \vec{s}^j - \sum_{i,j=1}^{n} \frac{\partial V(r_{ij})}{\partial r_a^i} \right) \beta \\ &+ \sum_{j(\neq i)}^{N} \left[-\frac{dV(r_{ij})}{dr_{ij}} + \frac{dJ(r_{ij})}{dr_{ij}} s_a^i \cdot s_a^j \right] \sum_{i}^{N} \frac{p_a^i}{m^i} \, \beta + 3 \sum_{i}^{N} \frac{\gamma_L}{m^i} - \gamma_L \beta \left(\sum_{i}^{N} \frac{p_a^i}{m^i} \right)^2 \\ &+ \frac{D_L}{2} \left[-\sum_{i}^{N} \frac{3}{m^i} \, \beta + \left(\sum_{i}^{N} \frac{p_a^i}{m^i} \right)^2 \beta^2 \right] \end{aligned} \tag{39}$$

The first line cancels out the first part of the second line leaving

$$\begin{aligned} 0 = &\, 3 \sum_{i}^{N} \frac{\gamma_L}{m^i} - \gamma_L \beta \left(\sum_{i}^{N} \frac{p_a^i}{m^i} \right)^2 \\ &+ \frac{D_L}{2} \left[-\sum_{i}^{N} \frac{3}{m^i} \, \beta + \left(\sum_{i}^{N} \frac{p_a^i}{m^i} \right)^2 \beta^2 \right], \end{aligned} \tag{40}$$

which gives the dynamical fluctuation-dissipation relation as

$$D_L = 2 \gamma_L k_B T \qquad \text{OK} \tag{41}$$

This is the exact same term as derived by Einstein and fits well in with our expectations. Tranchida's dynamic Langevin equation tends to equilibrium in the steady state. Note that there is a factor two difference between eq.41 and the D value below eq.3, this is due to the fact that Tranchida defined the correlations between the noises a factor of two from the standard definition.

He's calling "dynamic" the translastional part

4.1.5 Magnetic terms

The remaining magnetic terms are rearranged as

$$\begin{aligned}0 = &+\sum_{i}^{N}\frac{4s_b^i\eta_0}{\hbar(1+\eta_0^2)}\sum_{i,j,i\neq j}^{N}J(r_{ij})s_b^j - D_s\beta\sum_{i}^{N}\frac{4s_a^i}{(1+\eta_0^2)^2}\sum_{k(\neq i)}J(r_{ij})s_a^j\\ &+\frac{4\eta_0\beta}{\hbar(1+\eta_0^2)}\sum_{i,j,i\neq j}^{N}J(r_{ij})^2\left(s_s^2\delta_{ab}-s_a^is_b^i\right) - D_s\frac{4\beta^2}{(1+\eta_0^2)^2}\sum_{i}^{N}J(r_{ij})^2\left(s_s^2\delta_{ab}-s_a^is_b^i\right)\\ &+\frac{6D_s}{(1+\eta_0^2)^2}-\frac{6D_s}{(1+\eta_0^2)^2}\end{aligned} \tag{42}$$

This leaves the fluctuation-dissipation relation for the magnetic degree's of freedom as

$$D_s = \eta_0(1+\eta_0^2)k_BT/\hbar \tag{43}$$

Which is different to Tranchida's value for D_s (eq. 22) meaning that Tranchida's equations do not take the system to equilibrium. One can see that for small values of η_0, apart from some numerical prefactors, the two equations are equivalent. This is confirms the results from the numerical experiments conducted by the Argentinian team where equations in the LAMMPS package led to anomalous results when a high damping constant was applied.

4.1.6 Correct sLLG

Another issue noted is the fact that Tranchida's equations only couple the noise term to the magnetisation presession and not to the dissipative mechanisms as well like in the standard sLLG equation developed by Brown eq.4.
We re-did this derivation using the standard sLLG equation and found the fluctuation-dissipation relation to be $D_s \propto k_BT\eta_0$. This value is similar to the one proposed by Tranchida (eq.22) and thus it is likely that this is where their error came from.

4.2 Numerical Integration of Langevin Equations

To develop my proficiency in modelling stochastic systems both analytically and numerically, I numerically integrated the Langevin equation for Brownian motion in one dimension with no background potential ($\nabla V = 0$).
Starting off with the 2nd order eq.2, we turn it into two 1st order equations (where one is $v = dx/dt$) and discretise it to get

$$\begin{aligned}m\, d_tv(t) &= -\gamma v(t) + \xi(t)\\ v(t_{j+1}) &= v(t_j)e^{-\gamma\delta t/m} + \frac{e^{-\gamma\delta t/m}}{m}dw(t_j)\end{aligned} \tag{44}$$

where $dW(t)$ is a Wiener process as mentioned in section 3.4 with u_i a normally distributed value with 0 mean and unit variance. We evaluated this integral using Itô calculus but note that as the noise is additive in this equation, Itô and Stratonovich calculi are equivalent.

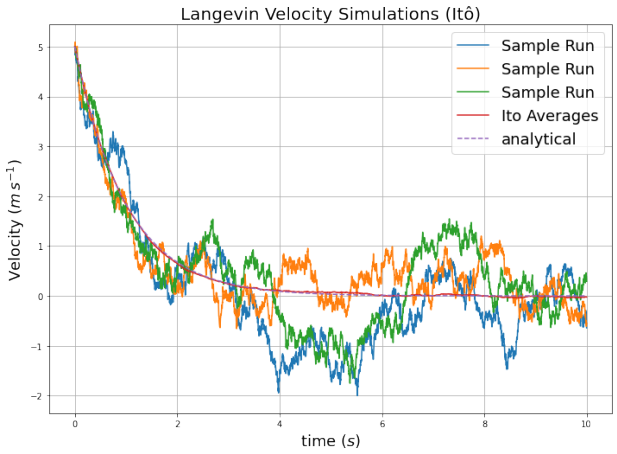
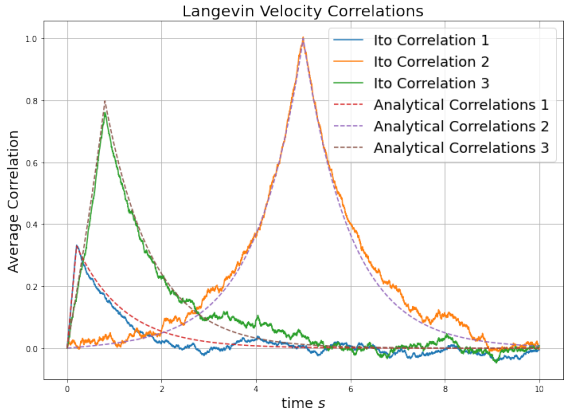
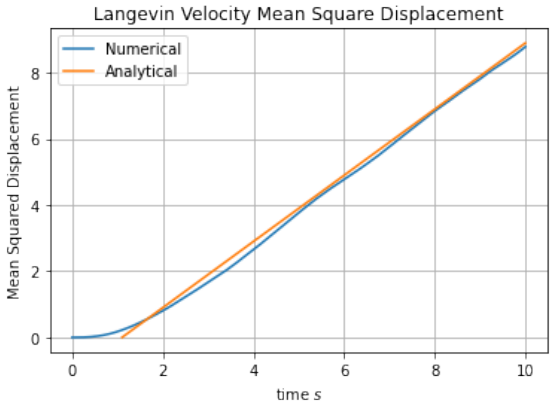


Figure 2: Plot showing the time evolution of the velocity of a particle undergoing Brownian Motion. Three sample runs are displayed including the velocity averaged over 100 runs and a derived analytical value



(a) Plot showing the averaged numerical and analytical values for the correlation between velocities at 3 different points



(b) Plot comparing the numerical and analytical values of the mean squared displacement of a Brownian system. $\bar{\alpha}$ was set to one

Figure 3

For the numerical simulation, we averaged over 1000 runs of the equation with a starting velocity of 5 and a time step of 0.02. We used the Heun method outlined in Section 3.4, and also investigated other implicit methods. Figure 2 shows three sample runs, the average and the expected analytical value following eq.44. As one can see the numerical and analytical values match up as expected.
Next, the correlation function is derived as

$$\langle v(t)v(t')\rangle = \frac{D\gamma}{m}\left(e^{|t-t'|} - e^{|t+t'|}\right) \tag{45}$$

which is used to see how likely it is that the particle has a a certain velocity at time t' given that it had a certain velocity at time t. The numerical simulation of the correlation between velocity is shown in

Figure 3b where we can see that the numerical and analytical values match up for 3 different compared velocities.
Finally, the mean square displacement is

$$\Delta^2(t) = \langle (x(t) - \langle x(t) \rangle)^2 \rangle = 2D\, t^{\bar{\alpha}} \tag{46}$$

which is used to see what kind of diffusion our system is undergoing for large t. If $\bar{\alpha} > 1$ it is undergoing superdiffusion and if $\bar{\alpha} < 1$ it is undergoing subdiffusion. Figure 3a shows the numerical simulation of this value and the analytical line is plotted with $\bar{\alpha} = 1$ which shows that this specific system is undergoing normal diffusion as expected.

5 Conclusion

Over the course of this internship I developed the analytical and numerical tools needed to study stochastic processes. I applied these techniques to a magneto-mechanical system and showed that a set of equations used in the LAMMPS molecular dynamics package [5] did not reach equilibrium for the steady state solution. The value for the dissipation-fluctuation relation stated in [5] came to be approximately correct for small damping values but for use cases with a higher damping constant we proposed an alternate value. Tranchida came to use a sLLG equation that was different to the standard definition, which is where we believe the error in their calculations came from.
I also performed numerical integrations of a few Langevin equations which provided a useful first task as it helped me get a better understanding of noisy systems. It also helped me in my analytical skills as it allowed me to verify my derivations for several systems. I also managed to perform some numerical simulations of Tranchida's equations showing them not to reach equilibrium. However, I did not have enough time to derive complete results and present them in this document. With more time I would have liked to finish off these numerical simulations and further explore the effect the damping values had on the system.
I wholeheartedly enjoyed my time at LPTHE. I would sincerely like to thank Leticia Cugliandolo for supervising me during this internship and supporting me throughout this process to ensure I could get the most out of this experience. I have learned an incredible amount during this internship, not only hard skills but also the value of collaboration and teamwork. I greatly enjoyed discussions with other interns and doctoral students alike and have made many friends who I will hope to continue to stay in contact with.

For the bibiography, I started with the paper by Aron [8] which provided a clear introduction into the subject matter. I then moved onto the paper by Tranchida [5] which formed a basis for most of my work. I expanded on these resources based on references found in these papers and searching through various archives like ArXiv.

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