Stochastic Spin Dynamics & Langevin-Landau-Gilbert Simulations

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Summary

Here I discuss the dynamics of microscopic systems, primarily for spin models, in thermal equilibrium, where the temperature causes random forces or torques, which are in competition with a damping force. This includes summarizing Langevin dynamics and finding methods for integrating the Landau-Gilbert equation of micromagnetics in time, with damping & temperature. The goal is to understand how to set the random forces according to a selected temperature that is desired.

1 Spin Dynamics at Zero Temperature

I start with a spin model for spin degrees of freedom $\mathbf{S}_i$ (localized atomic angular momenta) at zero temperature, that could have some damping included. Index i labels the spins or the sites where they are located. There is some kind of effective magnetic field $\mathbf{B}_i$ that acts on each spin, and the spins themselves belong to an object that also has magnetic moment $\vec{\mu}_i$ and a rotational inertia I_i (taken as a scalar).

1.1 Spin dynamics

The ratio of magnetic moment to angular momentum is the gyromagnetic ratio γ. Review this for a classical charged particle (mass m, charge q) that is making a circular orbit of radius r at frequency f. The orbital angular momentum is $L = mvr = m(2\pi rf)r$ while the magnetic dipole moment is $\mu = iA = i\pi r^2 = qf\pi r^2$. Then the classical gyromagnetic ratio for an orbiting electron is

$$\gamma = \frac{\mu}{L} = \frac{qf\pi r^2}{m(2\pi rf)r} = \frac{q}{2m}, \qquad \vec{\mu}_i = \gamma \mathbf{L}. \tag{1.1}$$

Due to quantum effects, this result is approximately doubled for a quantum electron, when instead applied to its spin angular momentum. Also for real electrons it is negative, due to the negative electron charge, and has a value about $\gamma_e \approx -1.76 \times 10^{11}$ $(\mathrm{Ts})^{-1}$. Mostly I will not care about the particular value, but need to be aware that μ is obtained from S by including a factor of γ. Also, I will not care about any distinction between orbital and spin angular momentum. I will call it all, spin. Then generally one assumes the relation,

$$\vec{\mu}_i = \gamma \mathbf{S}_i. \tag{1.2}$$

Consider just one spin and its dynamics. The local magnetic field determines an energy or Hamiltonian H for this one spin, which is just a scalar product of its magnetic moment with the field,

$$H = -\vec{\mu} \cdot \mathbf{B} = -\gamma \mathbf{S} \cdot \mathbf{B} \tag{1.3}$$

For the moment, the index i is suppressed. There would be a term like this for each particle. The dynamics is governed by the usual Newton's second law for rotation, that the time rate of change of angular momentum is equal to the torque. But the torque on the magnetic dipole is its cross product

with the magnetic field. Then the equation of motion for the dynamics can be written either for $\mathbf{S}$ or for $\vec{\mu}$:

$$\frac{d\mathbf{S}}{dt} = \vec{\mu} \times \mathbf{B} = \gamma \mathbf{S} \times \mathbf{B}, \qquad \frac{d\vec{\mu}}{dt} = \gamma \vec{\mu} \times \mathbf{B}. \tag{1.4}$$

The effective field $\mathbf{F}$ that enters is a gradient of the Hamiltonian w.r.t. that dynamic variable,

$$\mathbf{F} = \gamma \mathbf{B} = -\frac{\delta H}{\delta \mathbf{S}} \tag{1.5}$$

Written this way, one sees that γ effectively drops out of the mathematical problem. Returning to the problem with many spins, each one has an equation of motion determined by

$$\frac{d\mathbf{S}_i}{dt} = \mathbf{S}_i \times \mathbf{F}_i, \qquad \mathbf{F}_i = -\frac{\delta H}{\delta \mathbf{S}_i}. \tag{1.6}$$

Alternatively, γ can be scaled out by changing to a different time variable, $t' = \gamma t$. Then the equations of motion are

$$\frac{d\mathbf{S}_i}{dt'} = \mathbf{S}_i \times \mathbf{B}_i, \qquad \mathbf{B}_i = -\frac{1}{\gamma}\frac{\delta H}{\delta \mathbf{S}_i}. \tag{1.7}$$

But in this approach the gyromagnetic ratio still appears.

So generally I'll use the dynamics the first way, whose Cartesian components are

$$\begin{aligned} \dot{S}_x &= S_y F_z - S_z F_y \\ \dot{S}_y &= S_z F_x - S_x F_z \\ \dot{S}_z &= S_x F_y - S_y F_x \end{aligned} \tag{1.8}$$

To completely specify the problem, the "force" components must be given, which depend on the type of model being considered. Below we try a few simple cases.

1.2 Damping

The equations can be damped (energy non-conserving) by adding a term whose torque has a component along the effective fields. There are two ways to do this that are essentially equivalent, up to a rescaling of the time variable. The vector $\mathbf{S} \times \mathbf{F}$ is perpendicular to both $\mathbf{S}$ and $\mathbf{F}$. Then $(\mathbf{S} \times \mathbf{F}) \times \mathbf{S}$ can be seen to have a positive component along $\mathbf{F}$. To get a torque along $\mathbf{F}$, a term $+\alpha(\mathbf{S} \times \mathbf{F}) \times \mathbf{S}$ or $+\alpha' \dot{\mathbf{S}} \times \mathbf{S}$. Here the dot is used to denote the time derivative and α and α' determine the strength of damping. In the first way, the dynamics of a single spin follows

$$\dot{\mathbf{S}} = \mathbf{S} \times \mathbf{F} + \alpha(\mathbf{S} \times \mathbf{F}) \times \mathbf{S}, \tag{1.9}$$

and in the second way the dynamics is

$$\dot{\mathbf{S}} = \mathbf{S} \times \mathbf{F} + \alpha'(\dot{\mathbf{S}} \times \mathbf{S}). \tag{1.10}$$

To show these are related, substitute this last equation into itself for the damping term,

$$\dot{\mathbf{S}} = \mathbf{S} \times \mathbf{F} + \alpha' \left[\mathbf{S} \times \mathbf{F} + \alpha'(\dot{\mathbf{S}} \times \mathbf{S}) \right] \times \mathbf{S} \tag{1.11}$$

Expand out the last double cross product:

$$(\dot{\mathbf{S}} \times \mathbf{S}) \times \mathbf{S} = (\dot{\mathbf{S}} \cdot \mathbf{S})\mathbf{S} - S^2 \dot{\mathbf{S}} = -S^2 \dot{\mathbf{S}} \tag{1.12}$$

The term $(\dot{\mathbf{S}} \cdot \mathbf{S}) = 0$ as can be verified from the equation of motion, which guarantees a conserved spin length. Now the equation above is

$$\begin{aligned} \dot{\mathbf{S}} &= \mathbf{S} \times \mathbf{F} + \alpha' \left[(\mathbf{S} \times \mathbf{F}) \times \mathbf{S} + \alpha'(-S^2 \dot{\mathbf{S}}) \right] \\ (1 + \alpha'^2 S^2)\dot{\mathbf{S}} &= \mathbf{S} \times \mathbf{F} + \alpha'(\mathbf{S} \times \mathbf{F}) \times \mathbf{S} \end{aligned} \tag{1.13}$$

Then one can see that this is almost the same as the first damping, (1.9), except for a rescaling of the time due to the factor on the LHS. At small damping parameter, this will not make any real difference. At large parameter, this second form of damping is "slower", because it results in smaller net time derivative of the spin. It also slows down the original torque effect (1st term on RHS).

1.2.1 A single spin in a fixed field: no damping

Suppose there is a spin precessing in a fixed magnetic field, but with the first kind of damping turned on. Starting from a given initial state $\mathbf{S}(0)$, what is the time evolution?

The field $\mathbf{F} = \gamma\mathbf{B}$ is constant in time. Try solving first without damping and then seeing how to correct for it. The homogenous solution at $\alpha = 0$ satisfies

$$\dot{\mathbf{S}} = \mathbf{S} \times \mathbf{F}. \tag{1.14}$$

Assume without loss of generality that the field direction defines the $\hat{z}$-axis, $\mathbf{F} = F\hat{z}$. Then the components of the spin satisfy simple precessional equations,

$$\dot{S}_x = S_y F, \qquad \dot{S}_y = -S_x F, \qquad \dot{S}_z = 0. \tag{1.15}$$

A harmonic solution exists with frequency $\omega = F$, since $\ddot{S}_x = -F^2 S_x$ and $\ddot{S}_y = -F^2 S_y$, and it follows

$$S_x = a\cos\omega t + b\sin\omega t, \qquad S_y = \frac{1}{F}\dot{S}_x = -a\sin\omega t + b\cos\omega t. \tag{1.16}$$

The coefficients are set easily by the spin direction at time $t = 0$, such that $a = S_x(0)$ and $b = S_y(0)$. The z-component does not change. Then the full solution without damping is

$$\begin{aligned} S_x(t) &= +S_x(0)\cos\omega t + S_y(0)\sin\omega t, \qquad \omega = F = \gamma B, \\ S_y(t) &= -S_x(0)\sin\omega t + S_y(0)\cos\omega t \\ S_z(t) &= +S_z(0) \end{aligned} \tag{1.17}$$

This is just a continous rotation of the original xy components. It can also be written with a rotation matrix,

$$\begin{pmatrix} S_x(t) \\ S_y(t) \\ S_z(t) \end{pmatrix} = \begin{pmatrix} \cos\omega t & \sin\omega t & 0 \\ -\sin\omega t & \cos\omega t & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} S_x(0) \\ S_y(0) \\ S_z(0) \end{pmatrix}. \tag{1.18}$$

For positive $\omega = \gamma B$, the rotation is in the negative (left hand or clockwise) sense around the z-axis. Electrons would precess opposite to this, due to their negative charge.

1.2.2 A single spin in a fixed field: with damping

Next, what if the damping is included? The equation of motion becomes

$$\dot{\mathbf{S}} = \mathbf{S} \times \mathbf{F} + \alpha\left[S^2\mathbf{F} - (\mathbf{S}\cdot\mathbf{F})\mathbf{S}\right] \tag{1.19}$$

The extra "force" due to the damping term pushes the spin towards the magnetic field direction. The first term here is along $\mathbf{F}$ and does not affect the x and y components. Now in terms of components the equations are

$$\begin{aligned} \dot{S}_x &= S_y F - \alpha(S_z F)S_x, \\ \dot{S}_y &= -S_x F - \alpha(S_z F)S_y, \\ \dot{S}_z &= \alpha S^2 F - \alpha(S_z F)S_z. \end{aligned} \tag{1.20}$$

It is lucky that the z component equation is separated from the other two. Then it can be solved first although it is nonlinear. It separates as

$$\begin{aligned} \text{use } S_z = S\tanh\theta \;\rightarrow \int_{S_z(0)}^{S_z(t)} \frac{dS_z}{S^2 - S_z^2} &= \int_0^t \alpha F \; dt, \\ \frac{1}{S}\left[\tanh^{-1}\frac{S_z(t)}{S} - \tanh^{-1}\frac{S_z(0)}{S}\right] &= \alpha F t \end{aligned} \tag{1.21}$$

The solution is

$$S_z(t) = S\tanh\left[\tanh^{-1}\left(\frac{S_z(0)}{S}\right) + \alpha F S t\right] \tag{1.22}$$

It is interesting that the spin very slows goes towards the applied field. In the limit of inifinite time the hyperbolic tangent goes to 1 and thus $S_z \to S$, as it should. It might be better, though, to have done the integration by partial fractions and get logarithms (or use the log expression for the inverse hyperbolic tangent). Had I done it that way, one gets,

$$\frac{1}{2S}\left[\ln\left|\frac{S+S_z(t)}{S-S_z(t)}\right| - \ln\left|\frac{S+S_z(0)}{S-S_z(0)}\right|\right] = \alpha F t \tag{1.23}$$

Some rearragnements will give the solution. First do the obvious,

$$\ln\left|\frac{S+S_z(t)}{S-S_z(t)}\cdot\frac{S-S_z(0)}{S+S_z(0)}\right| = 2S\alpha F t. \tag{1.24}$$

With some obvious identifications, this is in the same form as

$$\frac{S+z}{S-z}A = e^\beta \quad \text{or} \quad (S+z)A = (S-z)e^\beta, \quad \Rightarrow \quad z = S\frac{e^\beta - A}{e^\beta + A} \tag{1.25}$$

Translating back to the physical variables, with a time scale defined as $\tau = [\alpha S F]^{-1}$, this gives

$$S_z(t) = S\,\frac{e^{2t/\tau} - \frac{S-S_z(0)}{S+S_z(0)}}{e^{2t/\tau} + \frac{S-S_z(0)}{S+S_z(0)}} = S\,\frac{[S+S_z(0)]e^{2t/\tau} - [S-S_z(0)]}{[S+S_z(0)]e^{2t/\tau} + [S-S_z(0)]} \tag{1.26}$$

This algebra basically did the sum inside the inverse tangent of the other expression. No matter what the initial condition, the spin will head towards the final state of $S_z(\infty) = S$.

Now that produces a considerable perturbation to the other components. They require the extra factor dependent on $\alpha F S_z(t)$. Before trying to integrate them, one can see a (non)-conservation law for the spin length. Multiplying each by the component and adding, there results,

$$\frac{d}{dt}(S_x^2 + S_y^2) = 2S_x\dot{S}_x + 2S_y\dot{S}_y = -2\alpha F S_z(t)(S_x^2 + S_y^2). \tag{1.27}$$

If I let the squared sum be called $w = S_x^2 + S_y^2$, then this in an ODE for $w(t)$:

$$\frac{dw}{dt} = -2\alpha F S_z\, w, \qquad \Rightarrow \qquad \int_{w(0)}^{w(t)}\frac{dw}{w} = -\int_0^t dt\; 2\alpha F S_z(t) \tag{1.28}$$

The RHS involves the time integral of S_z. Using the first form for the S_z solution, one can integrate the hyperbolic tangent very easily, with $b = \alpha F S$,

$$\int dt\;\tanh(a+bt) = \frac{1}{b}\int dx\;\frac{\sinh x}{\cosh x} = \frac{1}{b}\ln\cosh(a+bt). \tag{1.29}$$

Applied here this gives

$$\ln\frac{w(t)}{w(0)} = -\frac{2\alpha F S}{\alpha F S}\ln\frac{\cosh[\tanh^{-1}\frac{S_z(0)}{S} + \alpha F S t]}{\cosh[\tanh^{-1}\frac{S_z(0)}{S}]} \tag{1.30}$$

Then the in-plane spin length behaves as

$$w(t) = w(0)\frac{\cosh^2[\tanh^{-1}\frac{S_z(0)}{S}]}{\cosh^2[\tanh^{-1}\frac{S_z(0)}{S} + \alpha F S t]} \tag{1.31}$$

One can see it goes to zero at large times, as it should, when the spin converges towards the direction of the field $\mathbf{F}$, with a time scale $\tau = (\alpha F S)^{-1}$. Further, this realy will not contain more information than we already have, because $w = S^2 - S_z^2$ should hold.

To check that, it may help to simplify this expression. The numerator can be simplified by using $1 - \tanh^2 x = \operatorname{sech}^2 x$, so that with $x = \tanh^{-1} \frac{S_z(0)}{S}$,

$$\cosh^2 \left[\tanh^{-1} \frac{S_z(0)}{S} \right] = \frac{1}{\operatorname{sech}^2 x} = \frac{1}{1 - \tanh^2 x} = \frac{1}{1 - (S_z(0)/S)^2} = \frac{S^2}{S^2 - S_z^2(0)} \tag{1.32}$$

The denominator has a sum of two angles in the argument. With $e^x = \cosh x + \sinh x$ and $e^{-x} = \cosh x - \sinh x$, the rule for addition is

$$\begin{aligned} \cosh(x+y) &= \frac{e^{x+y} + e^{-x-y}}{2} \\ &= \frac{1}{2} \left[(\cosh x + \sinh x)(\cosh y + \sinh y) + (\cosh x - \sinh x)(\cosh y - \sinh y) \right] \\ &= \cosh x \cosh y + \sinh x \sinh y. \end{aligned} \tag{1.33}$$

Here let $y = \alpha F S t$, then together with $\tanh x = \frac{S_z(0)}{S}$, one can use

$$\cosh x = \frac{1}{\operatorname{sech} x} = \frac{1}{\sqrt{1 - \tanh^2 x}} = \frac{S}{\sqrt{S^2 - S_z^2(0)}}, \tag{1.34}$$

$$\sinh x = \sqrt{\cosh^2 x - 1} = \frac{S_z(0)}{\sqrt{S^2 - S_z^2(0)}}. \tag{1.35}$$

Inserting these gives

$$\cosh(x+y) = \frac{S \cosh y + S_z(0) \sinh y}{\sqrt{S^2 - S_z^2(0)}} \tag{1.36}$$

Squaring gives

$$\cosh^2(x+y) = \frac{(S \cosh y + S_z(0) \sinh y)^2}{S^2 - S_z^2(0)} \tag{1.37}$$

Then putting things together, with $w(0) = S^2 - S_z^2(0)$, the in-plane squared spin length is expressed

$$w(t) = \frac{S^2 (S^2 - S_z^2(0))}{(S \cosh y + S_z(0) \sinh y)^2} \tag{1.38}$$

If all is correct, the identity $w(t) + S_z^2(t) = S^2$ must hold. Try the following:

$$\begin{aligned} S^2 - w(t) &= S^2 \left\{ 1 - \frac{(S^2 - S_z^2(0))}{(S \cosh y + S_z(0) \sinh y)^2} \right\} \\ &= S^2 \left\{ \frac{(S \cosh y + S_z(0) \sinh y)^2 - (S^2 - S_z^2(0))}{(S \cosh y + S_z(0) \sinh y)^2} \right\} \\ &= S^2 \left\{ \frac{(S \sinh y + S_z(0) \cosh y)^2}{(S \cosh y + S_z(0) \sinh y)^2} \right\} \end{aligned} \tag{1.39}$$

Compare the expression for $S_z(t)$, writing its factors in terms of $y = t/\tau$.

$$\begin{aligned} S_z(t) &= S \frac{[S + S_z(0)](\cosh y + \sinh y) - [S - S_z(0)](\cosh y - \sinh y)}{[S + S_z(0)](\cosh y + \sinh y) + [S - S_z(0)](\cosh y - \sinh y)} \\ &= S \frac{S \sinh y + S_z(0) \cosh y}{S \cosh y + S_z(0) \sinh y} \end{aligned} \tag{1.40}$$

One can see the the relation $w(t) + S_z^2(t) = S^2$ does indeed hold!

1.2.3 A single damped spin in a fixed field: the in-plane motion

Now to get the in-plane motion, look again at the differential equations (1.20). They have another obvious symmetry that allows one to cancel out the damping terms for the xy motion. Do the following combination:

$$S_y\dot{S}_x - S_x\dot{S}_y = F(S_x^2+S_y^2), \quad \text{or} \quad \frac{S_y\dot{S}_x - S_x\dot{S}_y}{S_x^2+S_y^2} = F. \tag{1.41}$$

But this combination of derivatives is related to the derivative of the in-plane angle, i.e., check the algebra,

$$\phi = \tan^{-1}\left(\frac{S_y}{S_x}\right), \qquad \dot{\phi} = \frac{1}{1+\left(\frac{S_y}{S_x}\right)^2}\frac{S_x\dot{S}_y - S_y\dot{S}_x}{S_x^2} = \frac{S_x\dot{S}_y - S_y\dot{S}_x}{S_x^2+S_y^2}. \tag{1.42}$$

So the motion in-plane is very simple, and surprisingly, unaffected by the damping:

$$\dot{\phi} = \frac{S_x\dot{S}_y - S_y\dot{S}_x}{S_x^2+S_y^2} = -F, \quad \Longrightarrow \quad \phi(t) = -\omega t + \phi_0, \quad \omega = F. \tag{1.43}$$

So we can summarize the total motion, which is described by giving $S_z(t)$ and $\phi(t)$. There is a uniform precession around the z-axis at frequency $\omega = F = \gamma B$, while the S_z component slowly goes towards it maximum value of S.

$$S_z(t) = S\,\frac{S\sinh\alpha S\omega t + S_z(0)\cosh\alpha S\omega t}{S\cosh\alpha S\omega t + S_z(0)\sinh\alpha S\omega t}, \qquad \phi(t) = -\omega t + \phi_0, \quad \omega = \gamma B. \tag{1.44}$$

The S_z equation may also be expressed in terms of the polar angle between the spin and the applied field, $\theta(t)$, by

$$\cos\theta(t) = \frac{S_z(t)}{S} = \frac{\sinh\alpha S\omega t + \cos\theta_0\cosh\alpha S\omega t}{\cosh\alpha S\omega t + \cos\theta_0\sinh\alpha S\omega t} \tag{1.45}$$

1.3 Easy-plane spins & planar rotor dynamics, undamped

The rotor model is an approximate model for spins that can only move within the XY plane. They are assumed to have zero z components (2D spins). This model is simple for adding the random forces due to temperature, hence it is good to start with it and then see the modifications that will be needed for a 3D spin model.

To get to the rotor model, start from the easy plane model. It will help first to look at the equations of motion in in-plane angle ϕ and out of plane component S_z, as we saw that was useful above. With $\phi = \tan^{-1}\left(\frac{S_y}{S_x}\right)$, its dynamics is expressed as

$$\dot{\phi} = \frac{S_x\dot{S}_y - S_y\dot{S}_x}{S_x^2+S_y^2} = \frac{S_x(S_zF_x - S_xF_z) - S_y(S_yF_z - S_zF_y)}{S_x^2+S_y^2} \tag{1.46}$$

Then this must be solved together with the out of plane motion,

$$\dot{\phi} = S_z\left(\frac{S_xF_x + S_yF_y}{S_x^2+S_y^2}\right) - F_z, \tag{1.47}$$

$$\dot{S}_z = S_xF_y - S_yF_x. \tag{1.48}$$

It is typical to write this completely using spherical coordinates for the spins,

$$\mathbf{S} = S(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \tag{1.49}$$

Then the dynamic equations are generally, for any model,

$$\dot{\phi} = \frac{S_z}{\sqrt{S^2-S_z^2}}\left(F_x\cos\phi + F_y\sin\phi\right) - F_z, \tag{1.50}$$

$$\dot{S}_z = \sqrt{S^2-S_z^2}\left(F_y\cos\phi - F_x\sin\phi\right). \tag{1.51}$$

Now look at the easy-plane Heisenberg model, where the exchange Hamiltonian involves only nearest neighbor interactions with ferromagnetic exchange J, and $\lambda < 1$ is the anisotropy parameter,

$$H = -J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z) \tag{1.52}$$

The forces on site i come from sums over its nearest neighbors,

$$F_i^x = J \sum_{\langle j \rangle} S_j^x, \quad F_i^y = J \sum_{\langle j \rangle} S_j^y, \quad F_i^z = J\lambda \sum_{\langle j \rangle} S_j^z. \tag{1.53}$$

Then a little algebra for the in-plane component gives

$$\begin{aligned}
\dot{\phi}_i &= \frac{S_i^z}{\sqrt{S^2 - (S_i^z)^2}} \; J \sum_{\langle j \rangle} \left(S_j^x \cos\phi_i + S_j^y \sin\phi_i \right) - J\lambda \sum_{\langle j \rangle} S_j^z \\
&= J \sum_{\langle j \rangle} \left\{ S_i^z \sqrt{\frac{S^2 - (S_j^z)^2}{S^2 - (S_i^z)^2}} (\cos\phi_j \cos\phi_i + \sin\phi_j \sin\phi_i) - \lambda S_j^z \right\} \\
&= J \sum_{\langle j \rangle} \left\{ S_i^z \sqrt{\frac{S^2 - (S_j^z)^2}{S^2 - (S_i^z)^2}} \cos(\phi_i - \phi_j) - \lambda S_j^z \right\}
\end{aligned} \tag{1.54}$$

Some other algebra for the out of plane component,

$$\begin{aligned}
\dot{S}_i^z &= \sqrt{S^2 - (S_i^z)^2} \; J \sum_{\langle j \rangle} (S_j^y \cos\phi_i - S_j^x \sin\phi_i) \\
&= J \sqrt{S^2 - (S_i^z)^2} \; \sum_{\langle j \rangle} \sqrt{S^2 - (S_j^z)^2} \; (\sin\phi_j \cos\phi_i - \cos\phi_j \sin\phi_i) \\
&= -J \sqrt{S^2 - (S_i^z)^2} \; \sum_{\langle j \rangle} \sqrt{S^2 - (S_j^z)^2} \; \sin(\phi_i - \phi_j)
\end{aligned} \tag{1.55}$$

1.3.1 XY model

These last are the exact equations for the easy-plane model. But now make the approximation that the z-components are small, $S_i^z \ll S$. Then square root factors simplify and the approximate equations for the easy-plane model are

$$\dot{\phi}_i \approx J \sum_{\langle j \rangle} \left\{ S_i^z \cos(\phi_i - \phi_j) - \lambda S_j^z \right\}, \tag{1.56}$$

$$\dot{S}_i^z \approx -JS^2 \sum_{\langle j \rangle} \sin(\phi_i - \phi_j). \tag{1.57}$$

Now in the limit of $\lambda = 0$, the model is the XY model and the spins mostly stay near the xy plane, with small out of plane deviations. Thus it is reasonable to suppose that the differences $\phi_i - \phi_j$ and the components S_i^z are of similar orders of smallness. If the equations are further approximated, to the leading order, there results only

$$\dot{\phi}_i \approx JS_i^z \sum_{\langle j \rangle} 1 \approx n_i J S_i^z, \tag{1.58}$$

$$\dot{S}_i^z \approx -JS^2 \sum_{\langle j \rangle} \sin(\phi_i - \phi_j). \tag{1.59}$$

The factor n_i is the number of nearest neighbors that site i has; for a square lattice it is $n_i = 4$, except at the boundary of the system, where it is smaller. The sum over the sines cannot be so approximated or there would be no dynamics left. This is the approximate dynamics for the XY model (3D spins with strong planar anisotropy).

1.3.2 Planar rotor model

Now the XY model can be contrasted to the planar rotor model, which has 2D rotating masses with angular momentum only around the z-axis, L_i, rotational inertia I, and kinetic energy $L_i^2/2I$, coupled in a fashion similar to that for the XY model. Their dynamics is described by the orientation in the xy plane, ϕ_i, of each rod or rotator. As each moves, it has an angular velocity $\omega_i = \dot{\phi}_i$. One can start from its Lagrangian, which includes the potential like that in the XY model, which tends to align the rotors when the parameter $K > 0$ here,

$$\mathcal{L} = T - V = \sum_i \frac{1}{2} I \dot{\phi}_i^2 - (-K) \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) \tag{1.60}$$

The momentum conjugate to the angles is the angular mometum component,

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{\phi}_i} = I \dot{\phi}_i = I \omega_i = L_i. \tag{1.61}$$

The Lagrange equations of motion are simple, based on

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}_i} \right) - \frac{\partial \mathcal{L}}{\partial \phi_i} = 0 \tag{1.62}$$

This gives

$$\frac{d}{dt}(I\omega_i) = \frac{\partial \mathcal{L}}{\partial \phi_i} = \frac{\partial}{\partial \phi_i} K \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) = -K \sum_{\langle j \rangle} \sin(\phi_i - \phi_j), \tag{1.63}$$

or a single second order differential equation,

$$I \ddot{\phi}_i = -K \sum_{\langle j \rangle} \sin(\phi_i - \phi_j). \tag{1.64}$$

The dynamics can also be considered as coupled first order equations for (ϕ_i, ω_i).

$$\dot{\phi}_i = \omega_i, \tag{1.65}$$

$$\dot{\omega}_i = -\frac{K}{I} \sum_{\langle j \rangle} \sin(\phi_i - \phi_j). \tag{1.66}$$

This is mathematically the same as the XY model (when all n_i are the same). The parameters and the interpretations of the variables in the two models are different, however. To make the XY model equations match this, one could define a new variable there, $\omega_i = n_i J S_i^z$. This makes the first equation for the XY dynamics the same as the rotor, $\dot{\phi}_i = \omega_i$. Then the second equation becomes

$$n_i J \dot{S}_i = \dot{\omega}_i = -n_i (JS)^2 \sum_{\langle j \rangle} \sin(\phi_i - \phi_j). \tag{1.67}$$

One sees that the XY model will be equivalent to the rotor model if the parameters are matched as follows, using site-dependent rotational indertia,

$$n_i (JS)^2 = \frac{K}{I_i} \quad \Longrightarrow \quad I_i = \frac{K}{n_i (JS)^2} \tag{1.68}$$

The latter form indicates the rotor inertias needed to match the two models' dynamics. Further, if one is solving the rotor model but imagining that it represents an XY model, then the amount of out of plane spin motion associated with the rotor's velocity is given by the mapping,

$$S_i^z = \frac{\omega_i}{n_i J}. \tag{1.69}$$

Faster moving rotors correspond to spins tilting more so out of the xy plane. In the model on a square lattice, most of the $n_i = 4$, within the interior ofthe lattice.

1.3.3 Planar rotor in Cartesian components

One can associate a planar spin for the rotor model $\mathbf{S}_i = S(\cos\phi_i, \sin\phi_i)$. Then their dynamics is simple,

$$\dot{S}_i^x = -S\dot{\phi}_i \sin\phi_i, \qquad \dot{S}_i^y = +S\dot{\phi}_i \cos\phi_i. \tag{1.70}$$

or summarize this as

$$\begin{aligned} \dot{S}_i^x &= -\omega_i S_i^y \\ \dot{S}_i^y &= +\omega_i S_i^x. \end{aligned} \tag{1.71}$$

If ω_i were constant, it is uniform precessional motion. But ω_i changes with time, according to the applied torque,

$$\dot{\omega}_i = -\frac{K}{IS^2}\sum_{\langle j\rangle} S^2(\sin\phi_i^y \cos\phi_j - \cos\phi_i \sin\phi_j) = -\frac{K}{IS^2}\sum_{\langle j\rangle}(S_i^y S_j^x - S_i^x S_j^y) \tag{1.72}$$

or more simply,

$$\dot{\omega}_i = \frac{K}{IS^2}\sum_{\langle j\rangle}(S_i^x S_j^y - S_i^y S_j^x) \tag{1.73}$$

If one is doing numerical integration of these equations, this form is good due to the lack of trigonometric evaluations. The only problem, perhaps, is that now the problem is overspecified, having three components, S_i^x, S_i^y, ω_i, when two are sufficient. The numerical integration needs to be stable enough to preserve the spin length. One sees from the three dynamic equations an effective force on each spin,

$$F_i^x = \frac{K}{IS^2}\sum_{\langle j\rangle} S_j^x, \qquad F_i^y = \frac{K}{IS^2}\sum_{\langle j\rangle} S_j^y, \qquad F_i^z = -\omega_i \tag{1.74}$$

The functions that change $L_i = I\omega_i$ are torques. Thus one might also write these torques as the basic mechanical torques, which are the conservative part of the dynamics,

$$(\tau_m)_i = \frac{K}{S^2}\sum_{\langle j\rangle}(S_i^x S_j^y - S_i^y S_j^x) \tag{1.75}$$

The dynamics can also have other torques, $\tau_{\rm damping}$ due to viscous damping and $\tau_{\rm random}$ due to random forces associated with the temperature. Then one will want to consider the dynamics due to all of these torques acting together,

$$I\dot{\omega}_i = (\tau_m)_i + (\tau_{\rm damping})_i + (\tau_{\rm random})_i \tag{1.76}$$

That is the overall goal in this project, especially for models more general than the planar rotor model. But the rotor model is good for understanding the initial analysis.

2 Stochastics: Thermal fluctuations in the planar rotor model

In thermal equilibrium, the dynamics still goes on, but a system is continuously kicked by things outside of it, that are in a temperature bath. Einstein and others (Langevin, Markov, etc.) considered this problem of Brownian motion over a hundred years ago, to prove the existence of atoms. The atoms (or molecules) are bumping larger particles and sharing their energy, at the same time, the particles' motion is slowed down by the surounding fluid. Thus, a particle is exposed to damping and to random forces. We can suppose a similar effect takes place in the rotor or other magnetic system, although now there are viscous damping torques and random torques. The basic question, is how to describe the thermal fluctuations, the distribution of random torques, and the dynamics of the rotors (or magnetic dipoles) in their presence.

To begin, look at the dynamics of a free rotor, one not interacting with neighboring rotors. It is assumed to be exposed to a heat bath that acts on it with random and viscous torques. There is no usual mechanical torque. Still, the rotor will move around and its direction will follow some kind of random walk. We want to consider first the correlations and fluctuations in its angular speed, $\omega(t)$.

2.1 Langevin equation for a rotor

The equations of motion for this one rotor are

$$\dot{\phi} = \omega, \qquad I\ddot{\phi} = I\dot{\omega} = \tau(t) - \alpha I\omega \tag{2.1}$$

Here α is a damping constant with inverse time units, and $\tau(t)$ is the random or fluctuating torque, and $-\alpha I\omega$ is the viscous torque. This is known as the Langevin equation, especially if we had included a usual deterministic mechanical torque. Look at how to solve for the velocity $\omega(t)$, based on some rather simple assumptions about the random torque. For one we suppose the random torque depends on the temperature, and should be stronger with higher temperature. But that is quantified later. For another, it is supposed that the fluctuating torque at one time is completely unrelated to its value at an earlier time. That is the stochastic assumption. One can think there are many solutions for the velocity, starting from some initial value–we need to do an averaging procedure over all of the possible solutions, which correspond to different histories of the fluctuating torque.

Can write a formal solution to (2.1) by combining its homogenous solution for no fluctuating torque, with the particular solution when the torque is present. The homogeneous equation is

$$\dot{\omega} = -\alpha\omega \tag{2.2}$$

and its solution, starting from initial velocity ω_0, is

$$\omega(t) = \omega_0 e^{-\alpha t} \tag{2.3}$$

When the fluctuating torque is included, add some function $g(t)$ to get the total solution. Let $\omega(t) = \omega_0 e^{-\alpha t} + g(t)$. Now one has

$$\dot{\omega}(t) = -\alpha\omega_0 e^{-\alpha t} + \dot{g} \tag{2.4}$$

and substituted into the dynamics this gives

$$I(\dot{\omega} + \alpha\omega) = I(\dot{g} + \alpha g) = \tau(t). \tag{2.5}$$

This is the same as the orginal equation, so we gained little. Now try to solve by an ansatz,

$$g(t) = e^{-\alpha t} f(t), \qquad \dot{g} = -\alpha e^{-\alpha t} f + e^{-\alpha t}\dot{f}. \tag{2.6}$$

Then the ODE becomes

$$Ie^{-\alpha t}\dot{f} = \tau(t), \qquad \Rightarrow \quad I\dot{f} = e^{\alpha t}\tau(t). \tag{2.7}$$

This can be formally integrated,

$$f(t) = f(0) + \frac{1}{I}\int_0^t dt'\ e^{\alpha t'}\tau(t') \tag{2.8}$$

$$g(t) = e^{-\alpha t} f(t) = e^{-\alpha t} f(0) + \frac{1}{I}\int_0^t dt'\ e^{-\alpha(t-t')}\tau(t') \tag{2.9}$$

If one uses the boundary condition, $f(0) = \omega_0$, the correct homogeneous solution is recovered. So the formal solution for the velocity, with an arbitrary torque function is

$$\omega(t) = \omega_0 e^{-\alpha t} + \frac{1}{I}\int_0^t dt'\ e^{-\alpha(t-t')}\tau(t') \tag{2.10}$$

2.2 Planar rotator velocity autocorrelation function

Now although the torques are not known, a velocity autocorrelation function can be found. The idea is that this rotor starts with initial speed ω_0 and then gets slowed down and affected by the random torques. But we don't know them exactly, however, we can get the average over all possible $\tau(t)$ (with some reasonable assumptions about their distribution). One has to assume that the averaged torque is zero, however, that does not mean that its effects are zero.

The velocity autocorrelation function is $\langle\omega(t)\omega(t)\rangle$. For large times it should converge towards a value expected from equipartition, because it is related to the averaged kinetic energy,

$$\frac{1}{2}I\ \langle\omega(t)\omega(t)\rangle \longrightarrow \frac{1}{2}k_BT \tag{2.11}$$

where k_B is Boltzmann's constant and T is absolute temperature.

Using the solution found above, one has,

$$\begin{aligned}\langle\omega(t)\omega(t)\rangle &= \left\langle e^{-2\alpha t}\left[\omega_0+\frac{1}{I}\int_0^t dt'\ e^{\alpha t'}\tau(t')\right]\left[\omega_0+\frac{1}{I}\int_0^t dt''\ e^{\alpha t''}\tau(t'')\right]\right\rangle \\ &= e^{-2\alpha t}\left\{\omega_0^2+2\frac{\omega_0}{I}\int_0^t dt'\ e^{\alpha t'}\langle\tau(t')\rangle\right. \\ &\quad \left.+\frac{1}{I^2}\int_0^t dt'\ e^{\alpha t'}\int_0^t dt''\ e^{\alpha t''}\langle\tau(t')\tau(t'')\rangle\right\}\end{aligned} \tag{2.12}$$

The brackets show the averaging over the torque functions. But we assume there is no bias in these functions, that they have an average effect of zero on the velocity. So the first average is

$$\langle\tau(t')\rangle = 0. \tag{2.13}$$

The second average involves the product of a torque function, at two different times, averaged over all the possible torque functions. They are assumed to be completely independent, and stochastic, which means that the average gives zero unless the times are the same. So we take

$$\langle\tau(t')\tau(t'')\rangle = A\,\delta(t'-t''). \tag{2.14}$$

The normalization constant A will determined by equipartition. With that, one can continue to evaluate the resulting integral. It is

$$\begin{aligned}a &= \int_0^t dt'\ e^{\alpha t'}\int_0^t dt''\ e^{\alpha t''}A\,\delta(t'-t'') \\ &= A\int_0^t dt'\ e^{\alpha t'}e^{\alpha t'} = A\frac{1}{2\alpha}\left(e^{2\alpha t}-1\right).\end{aligned} \tag{2.15}$$

Finally this gives the autocorrelation function,

$$\langle\omega(t)\omega(t)\rangle = \omega_0^2e^{-2\alpha t}+\frac{A}{2\alpha I^2}\left(1-e^{-2\alpha t}\right) \tag{2.16}$$

To determine the constant, match the value as $t\to\infty$ with that required by equipartition in thermal equilibrium (this is amazing that this works!)

$$\langle\omega(t)\omega(t)\rangle_{t\to\infty} = \frac{A}{2\alpha I^2} = \frac{k_BT}{I} \qquad \Rightarrow \qquad A = 2\alpha I k_BT. \tag{2.17}$$

That means the correlation of the torques had to follow the requirement,

$$\boxed{\langle\tau(t')\tau(t'')\rangle = 2\alpha I k_BT\ \delta(t'-t'').} \tag{2.18}$$

This is refered to as the fluctuation-dissipation theorem, since it relates the strength of the torque fluctuations to the strength of the damping (or dissipation). The final velocity autocorrelation is forced to be very simple,

$$\langle\omega(t)\omega(t)\rangle = \omega_0^2e^{-2\alpha t}+\frac{k_BT}{I}\left(1-e^{-2\alpha t}\right). \tag{2.19}$$

2.3 Planar rotor diffusion

With a little more work, even the averaged position of the rotor can be determined, by integrating the other differential equation, $\dot{\phi} = \omega$, in an average sense. This is

$$\begin{aligned}\phi(t) &= \phi_0 + \int_0^t dt' \left[\omega_0 e^{-\alpha t'} + \frac{1}{I}\int_0^{t'} dt''\ e^{-\alpha(t'-t'')}\tau(t'')\right] \\ &= \phi_0 + \frac{\omega_0}{\alpha}\left(1 - e^{-\alpha t}\right) + \frac{1}{I}\int_0^t dt'\ \int_0^{t'} dt''\ e^{-\alpha(t'-t'')}\tau(t''). \end{aligned} \tag{2.20}$$

Of course, that depends on the choice of $\tau(t)$ and so it has an infinite number of possible trajectories. Instead, look at the mean-squared displacement from the starting point, as appropriate for a random walk. This is averaged over the torque functions,

$$\begin{aligned}\langle(\phi(t) - \phi_0)^2\rangle &= \frac{\omega_0^2}{\alpha^2}\left(1 - e^{-\alpha t}\right)^2 \\ &+ \frac{1}{I^2}\left\langle \int_0^t dt_1\ \int_0^{t_1} dt_2\ e^{-\alpha(t_1-t_2)}\tau(t_2)\int_0^t dt_3\ \int_0^{t_3} dt_4\ e^{-\alpha(t_3-t_4)}\tau(t_4)\right\rangle \end{aligned} \tag{2.21}$$

I already dropped the cross term, and now one can use the correlation function,

$$\langle\tau(t_2)\tau(t_4)\rangle = A\ \delta(t_2 - t_4) \tag{2.22}$$

But care is needed in the application of this! Use it to do the integration over t_4 first. The delta function picks out the point $t_4 = t_2$, but only if t_2 is inside the range of integration. That constraint is that $t_2 < t_3$ for a nonzero result. So the integration over only t_4 gives

$$\int_0^{t_3} dt_4\ e^{-\alpha(t_3-t_4)} A\ \delta(t_2 - t_4) = \begin{cases} 0 & \text{if } t_2 > t_3 \\ Ae^{-\alpha(t_3-t_2)} & \text{if } t_2 < t_3 \end{cases} \tag{2.23}$$

Next the integration over t_3 can be performed, but since it requires $t_3 > t_2$, the limits are modified to

$$\int_0^t dt_3 \to \int_{t_2}^t dt_3. \tag{2.24}$$

With that, there results

$$\int_{t_2}^t dt_3\ Ae^{-\alpha(t_3-t_2)} = \frac{-A}{\alpha}\left(e^{-\alpha(t-t_2)} - 1\right). \tag{2.25}$$

The rest of the integrations are straightforward, with the integration over t_2:

$$\begin{aligned} a &= \int_0^{t_1} dt_2\ e^{-\alpha(t_1-t_2)}\frac{-A}{\alpha}\left(e^{-\alpha(t-t_2)} - 1\right) \\ &= -\frac{A}{\alpha}e^{-\alpha t_1}\int_0^{t_1} dt_2\left(e^{-\alpha(t-2t_2)} - e^{\alpha t_2}\right) \\ &= -\frac{A}{\alpha}e^{-\alpha t_1}\left[\frac{1}{2\alpha}\left(e^{-\alpha(t-2t_1)} - e^{-\alpha t}\right) - \frac{1}{\alpha}\left(e^{\alpha t_1} - 1\right)\right] \\ &= -\frac{A}{\alpha^2}\left[\frac{1}{2}\left(e^{-\alpha(t-t_1)} - e^{-\alpha(t+t_1)}\right) - \left(1 - e^{-\alpha t_1}\right)\right] \end{aligned} \tag{2.26}$$

Finally there is the integration over t_1:

$$\begin{aligned} b &= -\frac{A}{\alpha^2}\int_0^t dt_1\ \left[\frac{e^{-\alpha t}}{2}\left(e^{\alpha t_1} - e^{-\alpha t_1}\right) - \left(1 - e^{-\alpha t_1}\right)\right] \\ &= -\frac{A}{\alpha^2}\left[\frac{1}{2\alpha}e^{-\alpha t}\left(e^{\alpha t} - 1 + e^{-\alpha t} - 1\right) - t - \frac{1}{\alpha}\left(e^{-\alpha t} - 1\right)\right] \\ &= \frac{A}{\alpha^3}\left(\alpha t - \frac{3}{2} + 2e^{-\alpha t} - \frac{1}{2}e^{-2\alpha t}\right) \end{aligned} \tag{2.27}$$

So the mean-squared displacement is found as

$$\langle(\phi(t)-\phi_0)^2\rangle = \frac{\omega_0^2}{\alpha^2}\left(1-e^{-\alpha t}\right)^2 + \frac{2k_BT}{I\alpha^2}\left(\alpha t - \frac{3}{2} + 2e^{-\alpha t} - \frac{1}{2}e^{-2\alpha t}\right). \tag{2.28}$$

One can look at the short time and long time behaviors. For short times, there is

$$\begin{aligned}\langle(\phi(t)-\phi_0)^2\rangle &\approx \frac{\omega_0^2}{\alpha^2}\left[1-(1-\alpha t)\right]^2 + \frac{2k_BT}{I\alpha^2}\left[\alpha t - \frac{3}{2} + 2(1-\alpha t+\frac{\alpha^2t^2}{2}) - \frac{1}{2}(1-2\alpha t+\frac{4\alpha^2t^2}{2})\right] \\ &= \omega_0^2t^2 + \frac{2k_BT}{I\alpha^2}\left[\alpha^2t^2-\alpha^2t^2\right] \approx \omega_0^2t^2. \end{aligned} \tag{2.29}$$

Curiously, all of the constant terms and terms linear in t cancel out, and so do the temperature dependent terms in t^2. The net result is very simple and shows a ballistic result (motion at constant speed). Compare at long times, where these is a diffusion,

$$\langle(\phi(t)-\phi_0)^2\rangle \approx \frac{\omega_0^2}{\alpha^2} + \frac{2k_BT}{I\alpha^2}\left(\alpha t - \frac{3}{2}\right) = \frac{1}{\alpha^2}\left(\omega_0^2 - \frac{3k_BT}{I}\right) + \frac{2k_BT}{I\alpha}t \approx \frac{2k_BT}{I\alpha}t \tag{2.30}$$

At very long times the linear term dominates and the constant term does not matter. Then the root-mean-squared displacement is

$$\sqrt{\langle(\phi(t)-\phi_0)^2\rangle} \approx \sqrt{\frac{2k_BT}{I\alpha}t} = \sqrt{2Dt}, \tag{2.31}$$

where the difusion constant here is

$$D = \frac{k_BT}{I\alpha} \tag{2.32}$$

One might think that the angular displacement has a limit, not going beyond 2π, however, this mathematics is such that if the walker goes beyond 2π, the angle is continued into the next branch, is moving towards 4π, etc.

3 Numerical solutions of the Langevin equation

The main difficulty for numerical integrations of the differential equation is the task of producing random torques with the correct distribution. Towards that end, first look at how this is done for a mass experiences forces (instead of torques), as would take place for a usual Brownian particle in 1D. After that, I'll translate to the appropriate quantities for the rotor problem, since they are mathematically equivalent.

The Langevin equation for a mass m with position $r(t)$ and velocity $v(t)$, experiencing determinisitic or conservative forces $F(t)$, random forces $F_s(t)$ and a viscous drag force scaled by coefficeint α is

$$ma = F_{\rm net} \quad\Rightarrow\quad m\dot{v} = F(t) - \alpha m v + F_s(t), \qquad \dot{r} = v. \tag{3.1}$$

The deterministic mechanical force $F(t)$ could be due to some potential. Sometimes it is better to use forces $F(t)$ and $F_s(t)$ scaled as force per unit mass, $f(t) = F(t)/m$ and $f_s(t) = F_s(t)/m$, then the mass drops out and we want to solve the simplified version,

$$\dot{v} = f(t) - \alpha v + f_s(t), \qquad \dot{r} = v. \tag{3.2}$$

The forces F_s are stochastic. With the translations between the rotor model and the moving particle model, of $\omega \leftrightarrow v$ and $I \leftrightarrow m$ and $\tau \leftrightarrow F$, one can see that their correlations must satisfy the fluctuation-dissipation theorem,

$$\langle F_s(t')F_s(t'')\rangle = 2\alpha m k_BT\ \delta(t'-t''). \tag{3.3}$$

In terms of the force per mass, this is changed to

$$\langle f_s(t')f_s(t'')\rangle = \frac{2\alpha k_B T}{m}\ \delta(t'-t''). \tag{3.4}$$

Recalling that the brackets imply an average all all possible force functions, we also assume there is no directional bias to the averaged force,

$$\langle f_s(t')\rangle = 0. \tag{3.5}$$

3.1 Langevin Euler method

Now for the simplest integration method, which is the Euler method, look at the approximation to the ODE with a time step Δt. The derivatives w.r.t. time are approximated as

$$\dot{v}(t) \approx \frac{v(t+\Delta t)-v(t)}{\Delta t}, \qquad \dot{r}(t) \approx \frac{r(t+\Delta t)-r(t)}{\Delta t}. \tag{3.6}$$

The velocity equation (for this free particle without a potential) can be integrated independently of the position equation. Or one could always add the potential force to $f_s(t)$. Either way, the time evolution for one time step of a usual Euler method is

$$v(t+\Delta t) = v(t) + \dot{v}\Delta t = v(t) + f(t)\Delta t - \alpha v(t)\Delta t + f_s(t)\Delta t, \qquad r(t+\Delta t) = r(t) + v(t)\Delta t. \tag{3.7}$$

But this does not apply well here, because the force $f_s(t)$ is rapidly varying. Instead, one needs to integrate the ODE over the time step, and account for the variations in the force. So with an integral approach,

$$\int_t^{t+\Delta t} dt'\ \dot{v}(t') = \int_t^{t+\Delta t} dt'\ [f(t') - \alpha v(t') + f_s(t')] \tag{3.8}$$

The LHS gives the change in velocity. The second term on RHS can be approximated various ways, but the simplest is to suppose $v(t')$ is a constant there (the value at one of the end points), or the average of the endpoints. The fluctuating force term is zero, if averaged over many sample functions. But that does not mean a particular value or sample of this integral is zero. One assumes there is some distribution to the value of the integral, whose average is zero. Denote the integral as the "stochastic acceleration" $a(\Delta t)$ that it caused during Δt (recall that f is force per mass, so this is really acceleration times Δt):

$$a(\Delta t) = \int_t^{t+\Delta t} dt'\ f_s(t'), \qquad \text{with} \quad \langle a(\Delta t)\rangle = 0. \tag{3.9}$$

Although the average is zero, there is some width to the distribution. One can determine the squared variance, which is nonzero,

$$\begin{aligned}\sigma_a^2 &= \langle a^2(\Delta t)\rangle = \left\langle \int_t^{t+\Delta t} dt'\ f_s(t') \int_t^{t+\Delta t} dt''\ f_s(t'') \right\rangle = \int_t^{t+\Delta t} dt'\ \int_t^{t+\Delta t} dt''\ \langle f_s(t')f_s(t'')\rangle \\ &= \int_t^{t+\Delta t} dt'\ \int_t^{t+\Delta t} dt''\ \frac{2\alpha k_B T}{m}\delta(t'-t'') = \int_t^{t+\Delta t} dt'\ \frac{2\alpha k_B T}{m} = \frac{2\alpha k_B T}{m}\Delta t \end{aligned} \tag{3.10}$$

That's surprising one can find this out with so little information about the forces. This is only based on the behavior the forces must have for establishing thermal equilibrium. Then going back to the integrated equation of motion, it can be expressed using the simplest approximation for the damping and conservative force terms,

$$v(t+\Delta t) = v(t) + f(t)\Delta t - \alpha v(t)\Delta t + a(\Delta t) \tag{3.11}$$

To do this updating numerically, it means that $a(\Delta t)$ is replaced by a random number, whose average is zero and whose variance is that determined in (3.10). In computation, random number generators return a value w with zero mean and typically, a unit variance. Then it means here we should do

$$v(t+\Delta t) = v(t) + f(t)\Delta t - \alpha v(t)\Delta t + \sigma_a(\Delta t)w \tag{3.12}$$

$$r(t+\Delta t) = r(t) + v(t)\Delta t \tag{3.13}$$

or, the random acceleration term is

$$a(\Delta t) = \sigma_a(\Delta t)w = \left[\frac{2\alpha k_B T}{m}\Delta t\right]^{1/2} w. \tag{3.14}$$

It is a curious result. The random acceleration increases with the square root of the time step. But this reflects the fact that during the time step, it is as if the particle is experiencing a small random walk. How much it gets pushed has a diffusive behavior.

One then supposes that this same random acceleration term is included even if there is also a potential force present. The two act together to determine the net dynamics.

If instead the planar rotor model is being solved numerically by this scheme, the change is quite simple, translating the variables, a single step is

$$\omega(t+\Delta t) = \omega(t) + \tau(t)\Delta t - \alpha\omega(t)\Delta t + \sigma_a(\Delta t)w \tag{3.15}$$

$$\phi(t+\Delta t) = \phi(t) + \omega(t)\Delta t \tag{3.16}$$

The deterministic torque per unit inertia is $\tau(t)$ and the random torque per unit inertia is the last term, which is a random angular acceleration,

$$a(\Delta t) = \sigma_a(\Delta t)w = \left[\frac{2\alpha k_B T}{I}\Delta t\right]^{1/2} w. \tag{3.17}$$

A note about the random numbers. If the random number generator is Gaussian, it will give a unit variance, and the procedure above makes sense. Alternatively, one could use a random number x uniformly distributed from -0.5 to +0.5, as Loft and de Grand did in 1987. Then you need to fix your random numbers so that they have the desired variance. For uniform randoms x from -0.5 to +0.5, their squared variance is

$$\sigma_x^2 = \int_{-0.5}^{+0.5} dx\; x^2 P(x) = \int_{-0.5}^{+0.5} dx\; x^2 = 2\frac{0.5^3}{3} = \frac{1}{12}. \tag{3.18}$$

Then to get the desired accelerations, one must scale them up by $\sqrt{12}$ to get a unit variance, and apply them as $w = x\sqrt{12}$, or

$$a(\Delta t) = \sigma_a(\Delta t)w = \left[\frac{24\alpha k_B T}{m}\Delta t\right]^{1/2} x. \tag{3.19}$$

Thus the explanation of the mysterious factor of 24 in the Loft and de Grand paper!

This scheme is not going to be very accurate, for the position it is first order accurate in the time step. One can improve it by going to a second order or possibly higher order scheme. There are different ways to do that, discussed next.

3.2 Verlet algorithm, without stochastic forces

For reference, the Verlet algorithm is mentioned here because it is a well-known 2nd order method and could be useful for pointing out how to be adapted for stochastic forces.

Verlet is based on finite difference expressions for the position of a particle at closely spaced times. The basic expansion in a Taylor series for position advancing forward in time is

$$r(t+\Delta t) = r(t) + \Delta t\, v(t) + \frac{1}{2!}\Delta t^2 v'(t) + \frac{1}{3!}\Delta t^3 v''(t) + \frac{1}{4!}\Delta t^4 v'''(t) + ... \tag{3.20}$$

One can do the same for the velocity,

$$v(t+\Delta t) = v(t) + \Delta t\, v'(t) + \frac{1}{2!}\Delta t^2 v''(t) + \frac{1}{3!}\Delta t^3 v'''(t) + \frac{1}{4!}\Delta t^4 v^{(4)}(t) + ... \tag{3.21}$$

and the position can be run backward in time too,

$$r(t-\Delta t) = r(t) - \Delta t\, v(t) + \frac{1}{2!}\Delta t^2 v'(t) - \frac{1}{3!}\Delta t^3 v''(t) + \frac{1}{4!}\Delta t^4 v'''(t) + ... \tag{3.22}$$

If the forward and backward position equations are added, the odd powers of time step cancel out,

$$r(t+\Delta t) + r(t-\Delta t) = 2r(t) + \Delta t^2 v'(t) + \frac{2}{4!}\Delta t^4 v'''(t) + ... \tag{3.23}$$

and there results a three-point iteration for the position,

$$r(t+\Delta t) = -r(t-\Delta t) + 2r(t) + \Delta t^2\, f(t) + \frac{1}{12}\Delta t^4 v'''(t) + ... \tag{3.24}$$

The error depends on Δt^4, so this equation is accurate to third order, by itself. Note that it could be useful computationally to write it as giving the changes in position, viz.,

$$[r(t+\Delta t) - r(t)] = [r(t) - r(t-\Delta t)] + \Delta t^2\, f(t) + \mathcal{O}(\Delta t^4) \tag{3.25}$$

The velocity must be updated too. Taking the difference of the forward and backward position equations gives

$$r(t+\Delta t) - r(t-\Delta t) = 2\Delta t\, v(t) + \frac{2}{3!}\Delta t^3 v''(t) + ... \tag{3.26}$$

and rewriting to give the velocity from the two points,

$$v(t) = \frac{1}{2\Delta t}\left[r(t+\Delta t) - r(t-\Delta t)\right] - \frac{1}{3!}\Delta t^2 v''(t) + ... \tag{3.27}$$

This is only accurate to first order in the time step, which demonstrates that the velocity will always be more difficult to obtain, and at least one order less accurate than the position. Probably it has some advantage over the Euler method, although their errors for the velocity are similar. The main advantage here is that the position should be much more accurate than in the Euler method. This can also be written as a sum of changes in position. Let the times be denoted with an index n, where $t = t_n = n\Delta t$, and $r_n = r(t_n)$, $v_n = v(t_n)$, etc. Then the Verlet algorithm can be summarized in this index notation as

$$r_{n+1} = -r_{n-1} + 2r_n + \Delta t^2\, f_n + \mathcal{O}(\Delta t^4) \tag{3.28}$$

$$v_n = \frac{1}{2\Delta t}\left[r_{n+1} - r_{n-1}\right] + \mathcal{O}(\Delta t^2) \tag{3.29}$$

The algorithm can also be written in terms of position changes. The change in position at the nth time step can be expressed as

$$\Delta r_{n+1} \equiv r(t+\Delta t) - r(t) = r_{n+1} - r_n \tag{3.30}$$

Then the Verlet algorithm can be summarized as

$$\Delta r_{n+1} = \Delta r_n + \Delta t^2\, f_n + \mathcal{O}(\Delta t^4) \tag{3.31}$$

$$v_n = \frac{1}{2\Delta t}\left[\Delta r_{n+1} + \Delta r_n\right] + \mathcal{O}(\Delta t^2) \tag{3.32}$$

The accuracy quoted assumes the forces depend only on position, but we have a velocity dependent damping force, so I think the accuracy depends on how that is implemented.

Another problem with the Verlet algorithm, is that the force in the position update is implemented by multiplying by Δt^2. This is a small parameter and could lead to imprecision (when added to the other larger terms). However, I don't honestly see the real difficulty with that, except perhaps due to numerical round off in a low precision computer (too few significant digits). All in all, the Verlet algorithm will be accurate to second order in the time step for the position variable, because that is limited by the velocity precision.

3.3 Velocity-Verlet algorithm, without stochastic forces

This is a slight modification of the Verlet algorithm, it is hard to see why it is any better or worse, and is said to be algebraically equivalent to the Verlet algorithm. The main difference, is that the force appears both in the position update and in the velocity update. Perhaps that lends it a better symmetry.

The first is the position update, which is the same as the forward time step expansion used to derive Verlet, with the force (per mass) substituted for $v'(t)$,

$$r(t+\Delta t) = r(t) + \Delta t\, v(t) + \frac{1}{2!}\Delta t^2 f(t) + \frac{1}{3!}\Delta t^3 v''(t) + ... \tag{3.33}$$

For the velocity updating, however, first consider this expression shifted forward one stime step, that is,

$$r(t+2\Delta t) = r(t+\Delta t) + \Delta t\, v(t+\Delta t) + \frac{1}{2!}\Delta t^2 f(t+\Delta t) + \frac{1}{3!}\Delta t^3 v''(t+\Delta t) + ... \tag{3.34}$$

Now we already know a way to get the velocity at time $t+\Delta t$, which is the difference,

$$v(t+\Delta t) = \frac{1}{2\Delta t}\left[r(t+2\Delta t) - r(t)\right] - \frac{1}{3!}\Delta t^2 v''(t+\Delta t) + ... \tag{3.35}$$

Substituting the expression for $r(t+2\Delta t)$, one has,

$$\begin{aligned} v(t+\Delta t) &= \frac{1}{2\Delta t}\left\{ r(t+\Delta t) + \Delta t\, v(t+\Delta t) + \frac{1}{2!}\Delta t^2 f(t+\Delta t) \right. \\ &+ \left. \frac{1}{3!}\Delta t^3 v''(t+\Delta t) - r(t) \right\} - \frac{1}{3!}\Delta t^2 v''(t+\Delta t) + ... \end{aligned} \tag{3.36}$$

The difference $r(t+\Delta t) - r(t)$ is obtained from (3.33), so this is

$$\begin{aligned} v(t+\Delta t) &= \frac{1}{2\Delta t}\left\{ \Delta t\, v(t) + \frac{1}{2!}\Delta t^2 f(t) + \frac{1}{3!}\Delta t^3 v''(t) + \Delta t\, v(t+\Delta t) + \frac{1}{2!}\Delta t^2 f(t+\Delta t) \right\} \\ &+ -\frac{1}{12}\Delta t^2 v''(t+\Delta t) + ... \\ &= \frac{1}{2\Delta t}\left\{ v(t) + v(t+\Delta t) + \frac{\Delta t}{2}\left[f(t) + f(t+\Delta t)\right] \right\} \\ &+ \frac{\Delta t^2}{12}\left(v''(t) - v''(t+\Delta t)\right) + ... \end{aligned} \tag{3.37}$$

Rearranging the new velocity to the LHS only, there results the velocity updatng, that uses the force averaged over the end points,

$$v(t+\Delta t) = v(t) + \frac{\Delta t}{2}\left[f(t) + f(t+\Delta t)\right] + \frac{\Delta t^2}{3!}\left(v''(t) - v''(t+\Delta t)\right) + ... \tag{3.38}$$

The last term is the error, so the step is accurate to first order in the time step. Again adopting the index notation with $t_n = n\Delta t$ and $r_n = r(t_n)$, etc., the Velocity-Verlet algorithm can be summarized as

$$r_{n+1} = r_n + \Delta t\, v_n + \frac{1}{2}\Delta t^2\, f_n + \mathcal{O}(\Delta t^3) \tag{3.39}$$

$$v_{n+1} = v_n + \frac{1}{2}\Delta t\left[f_n + f_{n+1}\right] + \mathcal{O}(\Delta t^2) \tag{3.40}$$

In terms of the position, the velocity-Verlet is accurate to second order in the time step. One advantage of this scheme it that it appears more symmetrical between the position and velocity updating, as the force appears in both of them.

3.4 The velocity dependent damping force

When the velocity dependent damping force is used, the above schemes should probably be modified, because they really were designed for forces that depend on position.

Look at the Verlet scheme discussion, with $f(t) \to f(t) - \alpha v(t)$, to include the damping explicitly. Then $f(t)$ contains only the conservative forces. Then for the $v(t)$ here, use the two-point symmetric formula. With that, the position updating becomes

$$\begin{aligned} r(t+\Delta t) &= -r(t-\Delta t) + 2r(t) + \Delta t^2 f(t) \\ &- \alpha \Delta t^2 \left\{ \frac{1}{2\Delta t} \left[r(t+\Delta t) - r(t-\Delta t) \right] - \frac{1}{3!} \Delta t^2 v''(t) \right\} + \frac{1}{12} \Delta t^4 v'''(t) + ... \end{aligned} \tag{3.41}$$

This can be cleaned up a bit,

$$\begin{aligned} \left(1 + \alpha \frac{\Delta t}{2} \right) r(t+\Delta t) &= -\left(1 - \alpha \frac{\Delta t}{2} \right) r(t-\Delta t) + 2r(t) + \Delta t^2 f(t) \\ &+ \frac{1}{3!} \Delta t^4 \left(\alpha v''(t) + \frac{1}{2} v'''(t) \right) + ... \end{aligned} \tag{3.42}$$

That keeps the error term as Δt^4, which is good. The bad part is the extra calculations, however, this may be more stable than implementing $v(t)$ numerically, I think. For the Verlet algorithm, there is going to be no change in the velocity update. Then Verlet with explicit damping looks like:

$$\left(1 + \alpha \frac{\Delta t}{2} \right) r_{n+1} = -\left(1 - \alpha \frac{\Delta t}{2} \right) r_{n-1} + 2r_n + \Delta t^2 f_n + \mathcal{O}(\Delta t^4) \tag{3.43}$$

$$v_n = \frac{1}{2\Delta t} \left[r_{n+1} - r_{n-1} \right] + \mathcal{O}(\Delta t^2) \tag{3.44}$$

Try the same correction for velocity-Verlet. The position updating will have a similar change,

$$r_{n+1} = r_n + \Delta t \, v_n + \frac{1}{2} \Delta t^2 f_n - \alpha \frac{1}{2} \Delta t^2 \frac{1}{2\Delta t} \left[r_{n+1} - r_{n-1} \right] + \mathcal{O}(\Delta t^3) \tag{3.45}$$

This is going to require knowledge of a previous position, however, so it should probably be abandoned. In this equation, instead the damping could be simply expressed with $-\alpha v_n$ on the RHS, then,

$$r_{n+1} = r_n + \Delta t \left(1 - \alpha \frac{\Delta t}{2} \right) v_n + \frac{1}{2} \Delta t^2 f_n + \mathcal{O}(\Delta t^3) \tag{3.46}$$

The damping slows down the ballistic jump of the particle. But this change in the algorithm is no different than having the damping as a part of the forces. The same type of change can be tried for the velocity update,

$$v_{n+1} = v_n + \frac{1}{2} \Delta t \left[f_n + f_{n+1} - \alpha (v_n + v_{n+1}) \right] + \mathcal{O}(\Delta t^2) \tag{3.47}$$

Here, the presence of v_{n+1} on the RHS does modify the algorithm and will make it more stable. In fact, it is hard to define the algorithm without doing this. The result is the velocity update for velocity-Verlet with explicit damping,

$$\left(1 + \alpha \frac{\Delta t}{2} \right) v_{n+1} = \left(1 - \alpha \frac{\Delta t}{2} \right) v_n + \frac{1}{2} \Delta t \left[f_n + f_{n+1} \right] + \mathcal{O}(\Delta t^2) \tag{3.48}$$

3.5 Numerical stability with or without explicit damping?

Look at the Verlet scheme for position update, Eq. (3.28). If the damping is part of the implied force f_n, you wouldn't be able to use $f_n = -\alpha v_n$ in numerical implementation, because only v_{n-1}

is known when the position update is applied. Suppose you were doing a simulation with only the damping force and doing $f_n = -\alpha v_{n-1}$, is it a stable iteration? The position update with this "old" velocity give a discrete equation,

$$\begin{aligned} r_{n+1} &= -r_{n-1} + 2r_n + \Delta t^2(-\alpha v_{n-1}) \\ &= -r_{n-1} + 2r_n - \alpha\Delta t^2 \frac{1}{2\Delta t}\left(r_n - r_{n-2}\right) \\ &= -r_{n-1} + 2r_n - \beta\left(r_n - r_{n-2}\right), \qquad \beta = \frac{\alpha\Delta t}{2}. \end{aligned} \tag{3.49}$$

One can try a solution like $r_n = a^n$ to see if this is stable. Unfortunately it gives a third order algebraic equation, not sure is the roots can be easily extracted. The equation becomes

$$\begin{aligned} a^{n+1} &= -a^{n-1} + (2-\beta)a^n + \beta a^{n-2} \\ 0 &= -a^3 + (2-\beta)a^2 - a + \beta \end{aligned} \tag{3.50}$$

Forget that for now...

Instead, what if the damping is included as in the explicit method? Check the stability there when there is only the damping force:

$$\begin{aligned} (1+\beta)r_{n+1} &= -(1-\beta)r_{n-1} + 2r_n, \qquad \text{put} \quad r_n = a^n \\ 0 &= (1+\beta)a^2 - 2a + (1-\beta) \\ a &= \frac{1}{2(1+\beta)}\left[2 \pm \sqrt{4 - 4(1+\beta)(1-\beta)}\right] \end{aligned} \tag{3.51}$$

The roots reduce to

$$a = \frac{1}{(1+\beta)}\left[1 \pm \sqrt{\beta^2}\right] = \begin{cases} 1 & \text{(positive square root)} \\ \frac{1-\beta}{1+\beta} & \text{(negative square root)} \end{cases} \tag{3.52}$$

I think this is unstable. The unit root it OK, because it leads to a constant position, which is what to expect from viscous damping. But the root less than 1 will lead to $r_n \to 0$ for large n, which means the particle is artificially pulled to the origin. That does not make physical sense, so probably this scheme is not good. Thus, the Verlet algorithm appears to be problematic as far as including the damping.

What about the velocity-Verlet with damping? Let me just check the explicit damping, since it is the only thing that really makes sense anyway. Here one only needs to look at the velocity updatng, which is essentially decoupled from the position updating. With only damping, one has (again with $\beta = \frac{\alpha\Delta t}{2}$)

$$(1+\beta)v_{n+1} = (1-\beta)v_n \tag{3.53}$$

Upon iteration starting from v_o, this obviously leads to a solution,

$$v_n = \left(\frac{1-\beta}{1+\beta}\right)^n v_o. \tag{3.54}$$

This closely approximates the correct exponential solution, and if we let the total time of integration $t = n\Delta t$ be fixed and the number of steps very large, there results:

$$v_n = \left(\frac{1-\frac{\alpha t}{2n}}{1+\frac{\alpha t}{2n}}\right)^n v_o \to \frac{e^{-\alpha t/2}}{e^{\alpha t/2}} v_0 = e^{-\alpha t} v_o. \tag{3.55}$$

It is indeed the correct solution for a particle only affected by the damping force. Then this is an obvious advantage of using the velocity-Verlet instead of the just-Verlet algorithm! In addition, the position now will be determined by the velocity and should be stable, with r_n going to a constant at large n, as it should.

OK, that was a summary of the Verlet type algorithms for molecular dynamics. The question now, of course, is whether is it easy to modify them to include the stochastic forces. Next I suggest some ideas towards that end, that should be methods with second order accuracy in the position. Following that, I recall another scheme that includes stochastic forces, and is indeed second order for the position.

3.6 Developing Langevin second order methods?

One needs better approximations than first order, that include the stochastic forces correctly. The Verlet algorithm and the velocity-Verlet algorithms, discussed in the previous sections do not have stochastic forces. Still, the way to proceed is by integrating the ODE, not by finite difference expressions alone. Thus is seems a little difficult to derive anything by comparison with the derivations of Verlet and velocity-Verlet.

Here are some ideas about integrating numerically, however, this is not at all Verlet or velocity-Verlet, but some of my own ideas on how to proceed.

Consider the basic ODE as having both stochastic forces $f_s(t)$ and all other deterministic mechanical forces contained in $f(t)$ (per unit mass). Thus, $f(t)$ includes the damping and any forces due to a potential, such as any conservative forces. The dynamics is assumed to follow from

$$\dot{v} = f(t) + f_s(t), \qquad \dot{r} = v(t). \tag{3.56}$$

Now the velocity equation can be integrated, twice, to get the position. For simplicity of notation, the starting time is $t = 0$ and the final time of one time step is $t = \Delta t$. But first we integrate to some arbitrary time inside that interval:

$$v(t) - v(0) = \int_0^t dt' \ \dot{v} = \int_0^t dt' \ \ [f(t') + f_s(t')] \tag{3.57}$$

Now integrate again, this time, to the end of the interval.

$$\int_0^{\Delta t} dt \ \ [v(t) - v(0)] = \int_0^{\Delta t} dt \ \int_0^t dt' \ \ [f(t') + f_s(t')] \tag{3.58}$$

The LHS can be integrated exactly because $v = \dot{r}$. That gives

$$\int_0^{\Delta t} dt \ \ [v(t) - v(0)] = r(\Delta t) - r(0) - v(0)\Delta t. \tag{3.59}$$

The RHS of (3.58) needs some approximation for the integration of the deterministic mechanical forces. Consider first the simplest, which is to say that that force is a constant during the time step. Then that term gives

$$\int_0^{\Delta t} dt \ \int_0^t dt' \ f(t') \approx \frac{1}{2}(\Delta t)^2 f(0) \tag{3.60}$$

Obviously this might be improved somewhat, by using the average of the force at beginning and ends of the interval, *if that can be known numerically.* Or alternatively, using the force at the middle of the interval, again with the same caveat. The stochastic force integral is more interesting, and I give it some name,

$$s = s(\Delta t) \equiv \int_0^{\Delta t} dt \ \int_0^t dt' \ f_s(t') \tag{3.61}$$

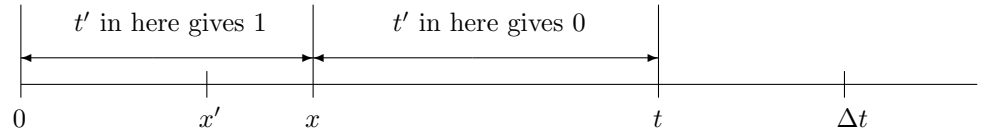
Dimensionally, s is force per mass times time squared, or length. It corresponds to the displacement caused by the stochastic force during Δt. Now, s must be averaged over all stochastic force functions. But that average is zero as long as the force has no net bias in one direction. Still there is some width to its distribution. We can try to find the squared variance of s.

$$\begin{aligned}
\sigma_s^2 &= \langle s^2 \rangle = \left\langle \int_0^{\Delta t} dt \int_0^t dt' \ f_s(t') \int_0^{\Delta t} dx \int_0^x dx' \ f_s(x') \right\rangle \\
&= \int_0^{\Delta t} dt \int_0^t dt' \int_0^{\Delta t} dx \int_0^x dx' \ \langle f_s(t') f_s(x') \rangle \\
&= \int_0^{\Delta t} dt \int_0^t dt' \int_0^{\Delta t} dx \int_0^x dx' \ \frac{2\alpha k_B T}{m} \ \delta(t' - x') \\
&= \frac{2\alpha k_B T}{m} \int_0^{\Delta t} dt \int_0^{\Delta t} dx \int_0^t dt' \int_0^x dx' \ \delta(t' - x')
\end{aligned} \tag{3.62}$$

Now, this integral takes some special care. Consider especially the integrations over x' and t', and the value of

$$Z = \int_0^t dt' \int_0^x dx' \; \delta(t' - x') \tag{3.63}$$

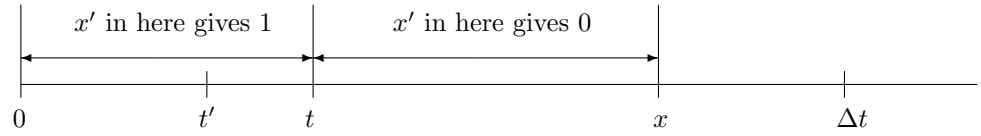
For the integration over x', a nonzero result requires t' between 0 and x. Here is a diagram of the times, supposing that $x < t$. It shows the results of the integration over x':



Then for this case, the following integration over t' gives

$$Z = \int_0^t dt' \; H(x - t') = x, \qquad \text{for } x < t. \tag{3.64}$$

The other possible case is that $t < x$, then the diagram for the integration over t' with the values of that integration shown is



Then for this case, the following integration over x' gives

$$Z = \int_0^t dx' \; H(t - x') = t, \qquad \text{for } t < x. \tag{3.65}$$

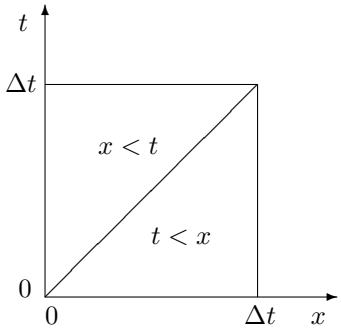
So the general result for Z is

$$Z = \int_0^t dt' \int_0^x dx' \; \delta(t' - x') = \begin{cases} x & \text{if } x < t \\ t & \text{if } t < x \end{cases} = \min(x, t). \tag{3.66}$$

That allows for the remainder of the integration to be done,

$$J = \int_0^{\Delta t} dt \int_0^{\Delta t} dx \; \min(x, t) \tag{3.67}$$

This integration is within a unit square of the xt plane. Half of the result comes from the lower triangle where $t < x$ and the other half comes from the upper triangle where $x < t$. So we can integrate just one of these triangles and then double that. Doubling the $t < x$ region, the integral is



$$\begin{aligned} J &= 2 \int_0^{\Delta t} dx \int_0^x dt \; t \\ &= 2 \int_0^{\Delta t} dx \; \frac{1}{2} x^2 = \frac{1}{3} (\Delta t)^3. \end{aligned}$$

Then the result for the squared variance of s is

$$\sigma_s^2 = \left(\frac{2 \alpha k_B T}{m} \right) \cdot \frac{1}{3} (\Delta t)^3$$

That is an interesting dependence on the size of the time step. So now to apply this to the numerical integration of the ODE, assume again there is a random number generator giving a distribution of numbers w with zero mean and unit variance. We use that to generate the random displacements s by

$$s = \sigma_s \cdot w = \left[\left(\frac{2\alpha k_B T}{m} \right) \cdot \frac{1}{3} (\Delta t)^3 \right]^{1/2} w. \tag{3.68}$$

Putting together all the contributions to the displacement, the twice-integrated Langevin equation is now approximated as

$$r(\Delta t) - r(0) - v(0)\Delta t = \frac{1}{2}(\Delta t)^2 f(0) + \sigma_s \cdot w. \tag{3.69}$$

Then the actual update of the particle takes place as follows:

$$r(\Delta t) = r(0) + v(0)\Delta t + \frac{1}{2}(\Delta t)^2 f(0) + \sigma_s \cdot w. \tag{3.70}$$

I believe this is a good method, but perhaps it is difficult to decide the order of the errors. However, the difference terms are the same as in the velocity-Verlet method. So the error should probably be of the order of Δt^3, as it was in velocity-Verlet.[1]

Note, however, the somewhat annoying $v(0)$ factor can be removed, by combining this result with the same result for a step in the other direction,

$$r(-\Delta t) = r(0) - v(0)\Delta t + \frac{1}{2}(\Delta t)^2 f(0) + \sigma_s \cdot w'. \tag{3.71}$$

I reversed the time step, but must use a different random number in this other interval. One can think that the system starting at $t = 0$ was used for either of these expressions, and evolved either earlier or later in time by Δt. So the random forces will be different in either the backward or forward time evolutions. Then if they are added, these equations produce

$$r(\Delta t) + r(-\Delta t) = 2r(0) + (\Delta t)^2 f(0) + \sigma_s \cdot (w_1 + w_2). \tag{3.72}$$

where $w_1 = w'$ is the random number used in the negative time step and $w_2 = w$ is the random number in the positive time step. Then as an updating algorithm, one need to have r at two previous time steps to get the next one, i.e., shifting the time by t to an arbitrary one,

$$r(t + \Delta t) = -r(t - \Delta t) + 2r(t) + (\Delta t)^2 f(t) + \sigma_s \cdot (w_1 + w_2). \tag{3.73}$$

One can see that this is very similar to the position update for the Verlet algorithm, but with the addition of the stochastic displacement. Then it is a good bet that the error term here should be proportional to Δt^4 as in the Verlet scheme.

Keeping in mind that the random number w_1 took place and affected the system during the interval $[t - \Delta t : t]$, and the random number w_2 took place during the interval $[t : t + \Delta t]$, one needs to re-use the w_2 number again on the subsequent step. For that next step, one would generate another random number w_3, and apply the sum of $w_2 + w_3$, viz.,

$$r(t + 2\Delta t) = -r(t) + 2r(t + \Delta t) + (\Delta t)^2 f(t + \Delta t) + \sigma_s \cdot (w_2 + w_3). \tag{3.74}$$

and so on. I believe this is logically correct. I thought that the two randoms could be replaced by a single new random number with a $\sqrt{2}$ larger variance, but that could imply some inconsistent dynamics, if a very small w followed a larger one. In this proposed fashion, you still generate only one random number per step, but have to save and re-use the previous one.

[1] This is the error in the finite difference terms here that are identical to terms in the velocity-Verlet algorithm. There does not seem to be a simple error estimate for the stochastic term.

This algorithm, which might be called Langevin-Verlet [2], could be summarized for the arbitrary step n, where the times are $t_n = n\Delta t,\ n = 0, 1, 2, ...$ and the positions are $r_n = r(t_n)$, etc.,

$$\boxed{r_{n+1} = -r_{n-1} + 2r_n + (\Delta t)^2 f_n + \sigma_s \cdot (w_n + w_{n+1}).} \tag{3.75}$$

There is still the question of how to update the velocity, though. One idea is to take it as derived from the position, after the fact. But that doesn't work–you need to know $v(0)$ already to step forward. The difficulty also is to be sure an algorithm is accurate to 2nd order in the time step. Although what I have done to this point seems correct, it then runs into some questions about updating the velocity.

To get the velocity at time Δt correct to 2nd order in Δt, also requires a double step. The other ODE $\dot{r} = v$ does not depend on the forces. One can make Taylor expansions,

$$\begin{aligned} r(\Delta t) &\approx r(0) + v(0)\Delta t + \frac{1}{2!}\frac{dv}{dt}(\Delta t)^2 + \frac{1}{3!}\frac{d^2v}{dt^2}(\Delta t)^3 + ... \\ r(-\Delta t) &\approx r(0) - v(0)\Delta t + \frac{1}{2!}\frac{dv}{dt}(\Delta t)^2 - \frac{1}{3!}\frac{d^2v}{dt^2}(\Delta t)^3 + ... \end{aligned} \tag{3.76}$$

The difference will cancel the even powers of Δt, leading to a three-point 2nd order relation,

$$r(\Delta t) - r(-\Delta t) \approx 2v(0)\Delta t + \frac{2}{3!}\frac{d^2v}{dt^2}(\Delta t)^3 + ... \tag{3.77}$$

Then presumably this can always be used to get the velocity with an error proportional to $(\Delta t)^2$,

$$v(t) \approx \frac{1}{2\Delta t}\left[r(t + \Delta t) - r(t - \Delta t)\right] - \frac{1}{3!}\frac{d^2v}{dt^2}(\Delta t)^2 \tag{3.78}$$

Hence this gives v in the middle of an interval of $2\Delta t$. But it is clear this will work, except that the velocity will always be one step behind the position. That could possibly give difficulties in treating the damping term, where the force depends on velocity.

So to summarize this proposed Langevin-Verlet algorithm, the iteration is of

$$r_{n+1} = -r_{n-1} + 2r_n + (\Delta t)^2 f_n + \sigma_s \cdot (w_n + w_{n+1}). \tag{3.79}$$

$$v_n = \frac{1}{2\Delta t}\left[r_{n+1} - r_{n-1}\right] \tag{3.80}$$

As mentioned, this does not work well for the damping term, because to get that force, you need the velocity v_n, but it hasn't yet been calculated. One can include the damping directly into the first equation, as

$$f_n^{\rm damp} = -\alpha v_n = -\frac{\alpha}{2\Delta t}\left[r_{n+1} - r_{n-1}\right] \tag{3.81}$$

Then applying that in the first half-step, it becomes

$$\begin{aligned} r_{n+1} &= -r_{n-1} + 2r_n + (\Delta t)^2(f_n^{\rm damp} + f_n^c) + \sigma_s \cdot (w_n + w_{n+1}) \\ &= -r_{n-1} + 2r_n - (\Delta t)^2\frac{\alpha}{2\Delta t}\left[r_{n+1} - r_{n-1}\right] + (\Delta t)^2 f_n^c + \sigma_s \cdot (w_n + w_{n+1}) \end{aligned} \tag{3.82}$$

and this gives

$$\left(1 + \frac{\alpha}{2}\Delta t\right) r_{n+1} = -\left(1 - \frac{\alpha}{2}\Delta t\right) r_{n-1} + 2r_n + (\Delta t)^2 f_n^c + \sigma_s \cdot (w_n + w_{n+1}) \tag{3.83}$$

One can see this already reduces the effects of the conservative forces, f_n^c, and of the stochastic forces. However, based on the previous stability analysis, in the absence of conservative and stochastic forces, this scheme is unstable, causing the particle to tend to move to the origin, $r_n \to 0$ for large n. That is unfortunately a big problem with it.

[2] Without the stochastic term it is the Verlet algorithm.

Nevertheless, this method with including the damping explicitly into the algorithm is summarized as

$$\left(1+\frac{\alpha}{2}\Delta t\right) r_{n+1} = -\left(1-\frac{\alpha}{2}\Delta t\right) r_{n-1} + 2r_n + (\Delta t)^2 f_n^c + \sigma_s \cdot (w_n + w_{n+1}) \tag{3.84}$$

$$v_n = \frac{1}{2\Delta t}\left[r_{n+1} - r_{n-1}\right] \tag{3.85}$$

I do not think this method as been used by anyone, which makes sense due to its stability issue. Usually something simpler is taken. This is considered a "Verlet" algorithm, because there is no velocity explicitly in the iteration of the position.

3.6.1 A Langevin-Velocity-Verlet method?

One can try to do a different manipulation of the difference equations and get what could be called a "Langevin velocity-Verlet" algorithm. That would mean that the velocity does appear explicitly in the position updating, and the deterministic forces would appear in both the position and velocity updatings. Let's see if this works.

Start from the raw result for one time step, obtained from twice integrating Newton's law and using the index notation,

$$r_{n+1} = r_n + \Delta t\, v_n + \frac{1}{2}(\Delta t)^2 f_n + \sigma_s \cdot w_n. \tag{3.86}$$

Here w_n is the random number for this particular time interval Δt starting at t_n and ending at t_{n+1}. Earlier I said it was annoying that the velocity is present. Now in this case I don't mind! Instead of symmetrizing for $\pm\Delta t$, to get velocity-Verlet, a shift of the time $t \to t + \Delta t$ is considered, but still doing a forward time-evolution (the same steps as used for deriving standard velocity-Verlet):

$$r_{n+2} = r_{n+1} + \Delta t\, v_{n+1} + \frac{1}{2}(\Delta t)^2 f_{n+1} + \sigma_s \cdot w_{n+1}. \tag{3.87}$$

This is the evolution in the next time step, so there is a different random displacement term determined by w_{n+1}. Now use the symetric difference to get the velocity v_{n+1}, at the boundary of these two intervals,

$$v_{n+1} = \frac{1}{2\Delta t}(r_{n+2} - r_n) + \mathcal{O}(\Delta t^2) \tag{3.88}$$

Then using the position updates in this (first for r_{n+2}), one gets,

$$v_{n+1} = \frac{1}{2\Delta t}\left\{r_{n+1} - r_n + \Delta t\, v_{n+1} + \frac{1}{2}(\Delta t)^2 f_{n+1} + \sigma_s \cdot w_{n+1}\right\} + \mathcal{O}(\Delta t^2) \tag{3.89}$$

then with $r_{n+1} - r_n$ from (3.86),

$$v_{n+1} = \frac{1}{2\Delta t}\left\{\Delta t\, v_n + \frac{1}{2}(\Delta t)^2 f_n + \sigma_s \cdot w_n + \Delta t\, v_{n+1} + \frac{1}{2}(\Delta t)^2 f_{n+1} + \sigma_s \cdot w_{n+1}\right\} + \mathcal{O}(\Delta t^2) \tag{3.90}$$

Now moving both v_{n+1} to the LHS and arranging,

$$v_{n+1} = v_n + \frac{\Delta t}{2} \cdot (f_n + f_{n+1}) + \frac{\sigma_s}{\Delta t} \cdot (w_n + w_{n+1}) + \mathcal{O}(\Delta t^2) \tag{3.91}$$

This is clearly the stochastic generalization of the velocity-Verlet algorithm, when combined with (3.86). So these should be summarized together, which gives the **Langevin-velocity-Verlet** scheme,

$$r_{n+1} = r_n + \Delta t\, v_n + \frac{1}{2}(\Delta t)^2 f_n + \sigma_s \cdot w_n + \mathcal{O}(\Delta t^3) \tag{3.92}$$

$$v_{n+1} = v_n + \frac{\Delta t}{2} \cdot (f_n + f_{n+1}) + \frac{\sigma_s}{\Delta t} \cdot (w_n + w_{n+1}) + \mathcal{O}(\Delta t^2) \tag{3.93}$$

The same w_n should be used in both the position and velocity update, however, the velocity update requires the generation of the next random number w_{n+1}. Then that value w_{n+1} will itself go into the subsequent position update that gives r_{n+2}, and so on. It can be seen to be accurate to second order in the time step, for the position.

The time step divided into σ_s is interesting. This gives the constant,

$$\sigma_v \equiv \frac{\sigma_s}{\Delta t} = \left[\left(\frac{2\alpha k_B T}{m} \right) \cdot \frac{1}{3} \Delta t \right]^{1/2} = \frac{\sigma_a}{\sqrt{3}}. \tag{3.94}$$

Dimensionally, both σ_a and this new σ_v are velocities, while σ_s is displacement. So the variance in this stochastic change in velocity still depends on the square root of the time step. It would likely cause a usual diffusive (random walk) behavior of the velocity, which is what we want! Its strength should be correctly associated with the temperature. This Langevin-velocity-Verlet appears to be a good candidate for a useful integration scheme.

Finally, there is the one last slight modification if the damping force is included explicitly, which really needs to be the case for the velocity dependent force (otherwise, what to do with $-\alpha v_{n+1}$ that will appear on the RHS?). So including that, and using $\sigma_v = \sigma_s/\Delta t$ on the RHS of both updates, the LVV scheme can be summarized as

$$r_{n+1} = r_n + \Delta t \, (v_n + \frac{\Delta t}{2} \cdot f_n + \sigma_v \cdot w_n) + \mathcal{O}(\Delta t^3) \tag{3.95}$$

$$(1+\beta) v_{n+1} = (1-\beta) v_n + \frac{\Delta t}{2} \cdot (f_n + f_{n+1}) + \sigma_v \cdot (w_n + w_{n+1}) + \mathcal{O}(\Delta t^2) \tag{3.96}$$

where again, $\beta = \alpha \frac{\Delta t}{2}$ gives the scale of the damping. Written in this way the stochastic term is intriguing. It acts as a random velocity added to the current speed, for the position update. Then, that random velocity is combined with another one from the same distribution, and their net is used to change the particle velocity. As well, the same factor $\frac{\Delta t}{2} \cdot f_n + \sigma_v \cdot w_n$ is used in the position update and in the following velocity update. Another similar factor is generated to do the current velocity update *and* the next position update, and so on. It looks good and simple this way.

3.6.2 An out-of-phase (better) second order Langevin method

For the rotor.c magnet programs, I did a slight variation on the first order Euler method. It is actually a second order method for the position *and* the velocity, if the damping force is treated correctly.

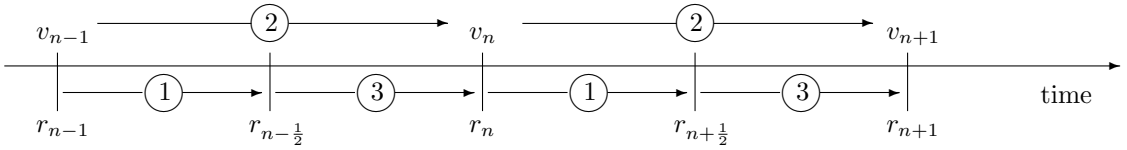
I don't recall the source where I found this method. It is based on having the position and velocity values a half time step out of phase. I used the following:

1. Position half-step: $r \leftarrow r + \frac{1}{2} v \Delta t$. with $t \leftarrow t + \frac{1}{2} \Delta t$.
2. Velocity update: $v \leftarrow v + f \Delta t - \alpha v \Delta t + \sigma_a(\Delta t) w$.
3. Position half-step: $r \leftarrow r + v \frac{1}{2} \Delta t$. with $t \leftarrow t + \frac{1}{2} \Delta t$.
4. Repeat the cycle.

Because of the time update and half steps, this may look confusing. But the scheme has two position updates per step, but only one velocity update. That is actually so that there is at least one point per cycle where both are defined, even though the minimum requirement is that r and v are defined at the alternating half steps. It should be equivalent to the following:

1. Position half-step: $r(t + \frac{\Delta t}{2}) = r(t) + \frac{1}{2} v(t) \Delta t$, with $t \leftarrow t + \frac{1}{2} \Delta t$.
2. Velocity update: $v(t + \Delta t) = v(t) + f(t + \frac{\Delta t}{2}) \Delta t - \alpha v(t) \Delta t + \sigma_a(\Delta t) w$.
3. Position half-step: $r(t + \Delta t) = r(t + \frac{\Delta t}{2}) + \frac{1}{2} v(t + \Delta t) \Delta t$. with $t \leftarrow t + \frac{1}{2} \Delta t$.
4. Repeat the cycle.

Let's look at the corresponding theory for this, which best seen in a diagram of the time axis. For compactness, use the index notation, with $t_n = n\Delta t$ and even half steps like $t_{n+\frac{1}{2}} = (n+\frac{1}{2})\Delta t$, etc. The symbols on the diagram are the numbers that actually get calculated in the algorithm. There are velocities missing at the half steps, because those are not calculated.



The diagram shows the different sub-steps ①, ②, ③. Let's look at the parts ① and ③, including the error terms. For part ①, with a half time step, the Taylor expansion from time t_n is

$$r_{n+\frac{1}{2}} = r_n + \frac{\Delta t}{2} v_n + \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2 v_n' + \frac{1}{3!}\left(\frac{\Delta t}{2}\right)^3 v_n'' + ... \tag{3.97}$$

Also write this for a reversed half time step,

$$r_{n-\frac{1}{2}} = r_n - \frac{\Delta t}{2} v_n + \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2 v_n' - \frac{1}{3!}\left(\frac{\Delta t}{2}\right)^3 v_n'' + ... \tag{3.98}$$

Then for part ③ of the algorithm, going *into* the time t_n on the previous cycle, r_n is found by solving this last equation,

$$r_n = r_{n-\frac{1}{2}} + \frac{\Delta t}{2} v_n - \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2 v_n' + \frac{1}{3!}\left(\frac{\Delta t}{2}\right)^3 v_n'' + ... \tag{3.99}$$

Then the combination of the ③-step and the subsequent ①-step produces some cancellations [use r_n from (3.99) substituted into (3.97)] is equivalent to

$$r_{n+\frac{1}{2}} = r_{n-\frac{1}{2}} + \Delta t\, v_n + \frac{2}{3!}\left(\frac{\Delta t}{2}\right)^3 v_n'' + ... \tag{3.100}$$

That is the usual symmetric formula for the velocity v_n at the midpoint of these two half-steps. Considered as an update of the position, which it is, the error is proportional to $(\Delta t)^3$, so it is accurate to second order in the time step.

Look at the velocity update. In finding v_{n+1} from v_n, it is using the force calculated at the middle of that time interval, $f_{n+\frac{1}{2}}$. This likely improves the precision. To see why this is so, look at the integral needed to derive this stochastic update (note that there was no stochastic term in the position update, so finite differences were OK there). From the Langevin equation, $\dot v = f(t) + f_s(t)$, integrated once, one gets

$$v(t+\Delta t) = v(t) + \int_t^{t+\Delta t} dt'\, f(t') + \int_t^{t+\Delta t} dt'\, f_s(t') \tag{3.101}$$

The last term is the stochastic push which is replaced ("exactly") by $\sigma_a(\Delta t)w$. The other integral can be approximated different ways, according to the time at which the force is used. Look at the expansion of that force (conservative + damping) around the *middle* of the interval–this would seem to be the best alternative to try. The mid-point time is $\bar t = t + \frac{\Delta t}{2}$.

$$f(t') = f(\bar t) + (t'-\bar t)\cdot f'(\bar t) + \frac{1}{2!}(t'-\bar t)^2 \cdot f''(\bar t) + ... \tag{3.102}$$

With this expansion, the force integral can be evaluated:

$$\begin{aligned}\int_t^{t+\Delta t} dt'\, f(t') \;&=\; f(\bar t)\int_t^{t+\Delta t} dt' + f'(\bar t)\int_t^{t+\Delta t} dt'\,(t'-\bar t) \\ &\quad + \frac{1}{2!} f''(\bar t)\int_t^{t+\Delta t} dt'\,(t'-\bar t)^2 + ...\end{aligned} \tag{3.103}$$

But changing to the relative variable $z = t' - \bar{t}$, the integrals are of the general form

$$\int_{-\frac{\Delta t}{2}}^{+\frac{\Delta t}{2}} dz\ z^n = \left.\frac{z^{n+1}}{n+1}\right|_{-\frac{\Delta t}{2}}^{+\frac{\Delta t}{2}} = \begin{cases} \frac{2}{n+1}\left(\frac{\Delta t}{2}\right)^{n+1} & \text{for even } n \\ 0 & \text{for odd } n \end{cases} \tag{3.104}$$

So the force integral has only terms with odd powers of Δt:

$$\int_t^{t+\Delta t} dt'\, f(t') = \Delta t\, f(\bar{t}\,) + \frac{1}{24}(\Delta t)^3 f''(\bar{t}\,) + ... \tag{3.105}$$

So this gives a good velocity updating procedure,

$$v(t+\Delta t) = v(t) + \Delta t\, f(\bar{t}\,) + \sigma_a(\Delta t)w + \frac{1}{24}(\Delta t)^3 f''(\bar{t}\,) \tag{3.106}$$

where the last term is the error estimate. Written in the index notation, it is the same as what was described for the rotor.c program:

$$v_{n+1} = v_n + \Delta t\, f_{n+\frac{1}{2}} + \sigma_a(\Delta t)w_n + \frac{1}{24}(\Delta t)^3 f''_{n+\frac{1}{2}} \tag{3.107}$$

Surprisingly, the error is proportional to $(\Delta t)^3$, the same order as the position updating! This makes this method quite accurate.

There is only one technical detail that would limit the accuracy, which is the usual problem of dealing with the damping. The algorithm had to use the term $-\alpha v_n$, although the theory says to use $-\alpha v_{n+\frac{1}{2}}$. But the velocities are not being calculated at the half time steps. So, let's put in the estimate of v at the half step, based on the average of the end points for that interval. The expansions of v around the mid-point $\bar{t} = t + \frac{\Delta t}{2}$ are

$$v(t) = v(\bar{t}\,) - \frac{\Delta t}{2}v'(\bar{t}\,) + \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2 v''(\bar{t}\,) - \frac{1}{3!}\left(\frac{\Delta t}{2}\right)^3 v'''(\bar{t}\,) + ... \tag{3.108}$$

$$v(t+\Delta t) = v(\bar{t}\,) + \frac{\Delta t}{2}v'(\bar{t}\,) + \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2 v''(\bar{t}\,) + \frac{1}{3!}\left(\frac{\Delta t}{2}\right)^3 v'''(\bar{t}\,) + ... \tag{3.109}$$

Then these added together give a good estimate of the mid-point velocity,

$$v(\bar{t}\,) = \frac{1}{2}\left[v(t) + v(t+\Delta t)\right] - \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2 v''(\bar{t}\,) + ... \tag{3.110}$$

Using this to write the damping force $-\alpha v(\bar{t}\,)$, we have in the velocity update, with index notation,

$$\begin{aligned} v_{n+1} = {} & v_n - \frac{\alpha\Delta t}{2}[v_n + v_{n+1}] + \Delta t\, f_{n+\frac{1}{2}} + \sigma_a(\Delta t)w_n \\ & + \alpha\Delta t\, \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2 v''_{n+\frac{1}{2}} + \frac{1}{24}(\Delta t)^3 f''_{n+\frac{1}{2}} \end{aligned} \tag{3.111}$$

or just summarizing together with the error term,

$$\boxed{(1+\beta)v_{n+1} = (1-\beta)v_n + \Delta t\, f_{n+\frac{1}{2}} + \sigma_a(\Delta t)w_n + \mathcal{O}(\Delta t^3), \qquad \beta = \frac{\alpha\Delta t}{2}.} \tag{3.112}$$

In this way, the update is indeed accurate to second order in the time step, and the inclusion of the damping is totally stable and gives the correct non-forced solution.

So let's summarize this out-of-phase 2nd order algorithm, with stable damping and two position updates per step, but only one velocity update per step. Suppose I start from a v_n and an $r_{n-\frac{1}{2}}$, and do the ③ part first:

$$r_n = r_{n-\frac{1}{2}} + \frac{\Delta t}{2} v_n - \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2 v_n' + \frac{1}{3!}\left(\frac{\Delta t}{2}\right)^3 v_n'' + ... \tag{3.113}$$

$$r_{n+\frac{1}{2}} = r_n + \frac{\Delta t}{2} v_n + \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2 v_n' + \frac{1}{3!}\left(\frac{\Delta t}{2}\right)^3 v_n'' + ... \tag{3.114}$$

$$(1+\beta) v_{n+1} = (1-\beta) v_n + \Delta t\, f_{n+\frac{1}{2}} + \sigma_a(\Delta t) w_n + \mathcal{O}(\Delta t^3), \qquad \beta = \frac{\alpha \Delta t}{2}. \tag{3.115}$$

It may seem unnecessary to do the two half steps in sequence. Why not just do one whole step from $r_{n-\frac{1}{2}}$ to $r_{n+\frac{1}{2}}$ for the position update? In fact, you could. But then would have the positions only at the half-step times and the velocities only at the whole step times. For plotting, correlations or other analysis, you would still need to shift one of them half a step to look correctly at the output.

The first error terms in the position update cancel, so the algorithm with the errors summarized, and in my original ①, ②, ③ ordering, is

$$r_{n+\frac{1}{2}} = r_n + \frac{\Delta t}{2} v_n + \mathcal{O}(\Delta^3), \tag{3.116}$$

$$(1+\beta) v_{n+1} = (1-\beta) v_n + \Delta t\, f_{n+\frac{1}{2}} + \sigma_a(\Delta t) w_n + \mathcal{O}(\Delta t^3), \qquad \beta = \frac{\alpha \Delta t}{2}, \tag{3.117}$$

$$r_n = r_{n-\frac{1}{2}} + \frac{\Delta t}{2} v_n + \mathcal{O}(\Delta^3). \tag{3.118}$$

It is certainly simpler than the Langevin-velocity-Verlet I proposed earlier. For the rotor problem, it worked fine. The big advantage, is the evaluation of the forces in the middle of the interval for the velocity update. On the other hand, an advantage of the Langevin-velocity-Verlet is that it has stochastic terms in both the position and velocity updates, which could give it some better balance and symmetry.

I had a lot of discussion about numerics for a moving mass, however, all of it could be applied to the rotor problem by the translations previously mentioned: $m \leftrightarrow I$ and $v \leftrightarrow \omega$ and $f \leftrightarrow \tau$.

4 Langevin Dynamics for 3D Spins

The real problem I want to address is how to look at the dynamics for three-component spins in thermal equilibrium at some temperature. It should be a simple generalization of the dynamics for the rotor model, i.e., changed into the dynamics for spins, as in the Landau-Gilbert equation.

The damping for the Landau-Gilbert equation has already been discussed, so now, we need to know what type of random "forces" must be included, and how are they correlated to each other and to the temperature.

The obvious physical idea, is that the spins should be subjected to random *torques* τ_s. But the torqus cannot be arbitrary, because they must conserve the spin lengths. Then it makes more sense and is more practical to imagine that there are *random magnetic fields* $\mathbf{F}_s$ that affect the spins. In this way, their spin length will be absolutely conserved. So if I assume that, the possible equation of motion for an individual spin with the first form of damping, Eq. (1.9), is

$$\dot{\mathbf{S}} = \mathbf{S} \times (\mathbf{F} + \mathbf{F}_s) + \alpha [\mathbf{S} \times (\mathbf{F} + \mathbf{F}_s)] \times \mathbf{S}, \tag{4.1}$$

I would hope that the conditions of thermal equilibrium (using classical mechanics with a Boltzmann distribution) will be enough to determine the correlations of the random fields. One should assume that they are uncorrelated in time, just as we had earlier for random forces,

$$\langle F_s^i(t) F_s^j(t') \rangle = A\, \delta_{ij}\, \delta(t - t') \tag{4.2}$$

where i and j label Cartesian components. The constant A needs to be determined.

The simplest situation to consider, that has some defined energy in the limit of zero temperature, is a spin in a fixed magnetic field, which can be taken pointing along the z-axis, with $F = F_z = \gamma B$. If we don't have at least this, there is no energy function for the system and no unique ground state. So by having this, the spin's minimum energy state is aligned to $\mathbf{B}$, and fluctuations will cause it to tilt away from this magnetic field, the more so with higher temperature.

The damping double cross product can be expanded in the usual way, and the equations of motion are

$$\dot{\mathbf{S}} = \mathbf{S} \times \mathbf{F} + \mathbf{S} \times \mathbf{F}_s + \alpha \left[S^2(\mathbf{F} + \mathbf{F}_s) - \mathbf{S} \cdot (\mathbf{F} + \mathbf{F}_s)\mathbf{S} \right]. \tag{4.3}$$

If the equations of motion are considered in Cartesian coordinates, they are

$$\begin{aligned}
\dot{S}_x &= S_y(F + F_s^z) - S_z F_s^y + \alpha S^2 F_s^x - \alpha[S_x F_s^x + S_y F_s^y + S_z(F + F_s^z)]S_x \\
\dot{S}_y &= S_z F_s^x - S_x(F + F_s^z) + \alpha S^2 F_s^y - \alpha[S_x F_s^x + S_y F_s^y + S_z(F + F_s^z)]S_y, \\
\dot{S}_z &= S_x F_s^y - S_y F_s^x + \alpha S^2(F + F_s^z) - \alpha[S_x F_s^x + S_y F_s^y + S_z(F + F_s^z)]S_z.
\end{aligned} \tag{4.4}$$

This looks tough to analyze, and it probably means we need some approximations. Or, alternatively it will be good to look also at the motion in spherical coordinates, or, at least in the two basic coordinates, (ϕ, S_z). So transform to

$$\begin{aligned}
S_x &= S \sin\theta \cos\phi = S\sqrt{1 - m^2}\, \cos\phi, \\
S_y &= S \sin\theta \sin\phi = S\sqrt{1 - m^2}\, \sin\phi, \\
S_z &= S \cos\theta = Sm.
\end{aligned} \tag{4.5}$$

Further, one expects in the absence of the random forces, that the spin will align with the applied field, and quickly (in atomic time scales) go to $S_z \approx S$ or $m \approx 1$. This means that S_x and S_y are small parameters. Indeed, then it is actually better to use $\theta \ll 1$ as a small parameter that scales the in-plane components. So instead, use the transformation to

$$\begin{aligned}
S_x &= S \sin\theta \cos\phi \approx S\theta\, \cos\phi, \\
S_y &= S \sin\theta \sin\phi \approx S\theta\, \sin\phi, \\
S_z &= S \cos\theta \approx S\left(1 - \frac{1}{2}\theta^2\right).
\end{aligned} \tag{4.6}$$

This will be fine because we only want to know about the fluctuations away from or near the stable state where the spin is aligned to the applied field. The alignment is only related to θ. The ϕ variable should be free to move around at will, there is no potential to restrict it, because the energy in the applied field is

$$H = -\vec{\mu} \cdot \mathbf{B} = -\gamma \mathbf{S} \cdot \mathbf{B} = -\gamma SB \cos\theta \approx -\gamma SB \left(1 - \frac{1}{2}\theta^2\right), \tag{4.7}$$

which is a parabolic potential only for θ. The ground state energy is $-\gamma SB$ and the term $\frac{1}{2}\gamma SB\theta^2$ is the excitation energy above that value. On the other hand, there will be ϕ fluctuations, which we might be able to relate to the temperature by looking at the autocorrelation of the velocity $\dot{\phi}$.

4.1 About spin and equipartition of thermal energy

As far as relating the dynamics to equipartition at some point, we know that an individual spin has two degrees of freedom (the two angles). Classically each degree of freedom on average has a kinetic energy of $\frac{1}{2}k_B T$, *if it appears quadratically in the Hamiltonian.* Only the deviation θ satisfies this. So assuming quadratic equipartition applies, we would have for the mean excitation energy

$$\langle E_\theta \rangle = \left\langle \frac{1}{2}\gamma SB\, \theta^2 \right\rangle = \frac{1}{2}k_B T, \qquad \text{or} \quad \langle \theta^2 \rangle = \frac{k_B T}{\gamma SB}. \tag{4.8}$$

Thinking about this, though, one can suspect something is wrong. Where is the other $\frac{1}{2}k_BT$ of thermal energy, if there are two degrees of freedom? Where is the other degree of freedom? The angle ϕ does not appear in the Hamiltonian, and there is no KE term. So something does not add up here.

To check whether the last result is correct (at least at low temperature where the fluctuations are small), one can compare the average that would be obtained with the correct statistical average using $z = \cos\theta$,

$$\langle \cos\theta \rangle = \langle z \rangle = \frac{\int_{-1}^{+1} dz\ z e^{-\beta H}}{\int_{-1}^{+1} dz\ e^{-\beta H}} = \frac{\int_{-1}^{+1} dz\ z e^{\beta\gamma S B z}}{\int_{-1}^{+1} dz\ e^{\beta\gamma S B z}} \tag{4.9}$$

With the parameter $\lambda = \beta\gamma SB$, the lower integral is the partition function, whose exact value is

$$Z = \int_{-1}^{+1} dz\ e^{\lambda z} = \frac{1}{\lambda}(e^{\lambda} - e^{-\lambda}) = \frac{2}{\lambda}\sinh\lambda \tag{4.10}$$

The upper integral is the derivative of this

$$C = \frac{\partial}{\partial\lambda}\int_{-1}^{+1} dz\ e^{\lambda z} = \frac{\partial Z}{\partial\lambda} = \frac{\partial}{\partial\lambda}\left(\frac{2}{\lambda}\sinh\lambda\right) = \frac{2}{\lambda}\left(\cosh\lambda - \frac{1}{\lambda}\sinh\lambda\right) \tag{4.11}$$

Then the statistical average is

$$\langle \cos\theta \rangle = \frac{C}{Z} = \frac{\frac{2}{\lambda}\left(\cosh\lambda - \frac{1}{\lambda}\sinh\lambda\right)}{\frac{2}{\lambda}\sinh\lambda} = \coth\lambda - \frac{1}{\lambda}. \tag{4.12}$$

Now look at what this gives for low temperature, where the spin deviates slightly from the field direction and θ is small. The LHS is approximately $1 - \frac{1}{2}\langle\theta^2\rangle$. The RHS must be approximated for large λ. Write it in exponential form, using

$$\langle \cos\theta \rangle \approx 1 - \frac{1}{2}\langle\theta^2\rangle \approx \frac{\frac{1}{2}(e^{\lambda} + e^{-\lambda})}{\frac{1}{2}(e^{\lambda} - e^{-\lambda})} - \frac{1}{\lambda} \approx 1 - \frac{1}{\lambda} \tag{4.13}$$

So this implies a similar relation for the squared variance, but *twice as large* as that from the quadratic approximation,

$$\langle\theta^2\rangle \approx \frac{2}{\lambda} = \frac{2k_BT}{\gamma SB}. \tag{4.14}$$

It means that only this one degree of freedom, θ, is taking *all* of the thermal energy:

$$\langle E_\theta \rangle = \left\langle \frac{1}{2}\gamma SB\,\theta^2 \right\rangle = 2\left(\frac{k_BT}{2}\right). \tag{4.15}$$

This makes sense because the other degree of freedom (ϕ) is completely free to move around 0 to 2π at no cost in energy. It is important to realize this if at some point a matching to thermal equilibrium properties is required.

To try to see why these two averages don't match, look at the details of the (wrong!) quadratic approximation. The energy above the ground state is $E = \frac{1}{2}SF\theta^2$. If one is just averaging θ^2 rather than $\cos\theta$, the usual integral to do for a quadratic variable is

$$\langle\theta^2\rangle_q = \frac{\int_0^{\pi} d\theta\ \theta^2 e^{-\beta\frac{1}{2}FS\theta^2}}{\int_0^{\pi} d\theta\ e^{-\beta\frac{1}{2}FS\theta^2}} = \frac{-2\frac{\partial}{\partial\lambda}Z_q(\lambda)}{Z_q(\lambda)}, \tag{4.16}$$

where the partition function is

$$Z_q(\lambda) = \int_0^{\pi} d\theta\ e^{-\frac{1}{2}\lambda\theta^2} \to \int_0^{\infty} d\theta\ e^{-\frac{1}{2}\lambda\theta^2} = \frac{1}{2}\sqrt{\frac{2\pi}{\lambda}}, \tag{4.17}$$

The derivative in the numerator is

$$\int_0^\pi d\theta\ \theta^2 e^{-\frac{1}{2}\lambda\theta^2} = -2\frac{\partial Z_q}{\partial\lambda} = \frac{1}{2}\sqrt{\frac{2\pi}{\lambda^3}} = \frac{1}{\lambda}Z_q(\lambda) \tag{4.18}$$

and thus the average is

$$\left\langle\theta^2\right\rangle_q = \frac{1}{\lambda} = \frac{1}{\beta FS} = \frac{k_BT}{FS} = \frac{k_BT}{\gamma BS}, \tag{4.19}$$

and as well, the averaged energy follows the equipartition rule,

$$\langle E_\theta\rangle_q = \frac{1}{2}\gamma BS\left\langle\theta^2\right\rangle_q = \frac{1}{2}k_BT. \tag{4.20}$$

But this does not actually apply to the spin problem!

Comparing the detail of the exact calculation, why do these differ? The answer is a actually obvious. It is because this is not a usual quadratic degree of freedom, because the phase space allows the spins to point anywhere on the *surface of a sphere* of radius S. When integrating correctly over the polar angle (I ignored the 2π range of the in-plane angle), the differential element is $\sin\theta\,d\theta$ and not just $d\theta$ as was assumed incorrectly for the quadratic integral. Let's fix this and see what is the average squared polar angle. Find the corrected partition function, applying further the small angle approximation, $\sin\theta\approx\theta$, good for low temperature,

$$Z(\lambda) = \int_0^\pi d\theta\ \sin\theta\ e^{-\beta\frac{1}{2}SF\theta^2} \approx \int_0^\pi d\theta\ \theta\ e^{-\frac{1}{2}\lambda\theta^2} = -\frac{e^{-\frac{1}{2}\lambda\theta^2}}{\lambda}\bigg|_0^\pi = \frac{1-e^{-\frac{1}{2}\lambda\pi^2}}{\lambda} \approx \frac{1}{\lambda} \tag{4.21}$$

The last approximation is that for low temperature. The desired average squared angle is twice the derivative w.r.t. λ, divided by Z,

$$\left\langle\theta^2\right\rangle = -\frac{2}{Z}\frac{\partial Z}{\partial\lambda} \approx 2\lambda\frac{1}{\lambda^2} = \frac{2}{\lambda} = \frac{2k_BT}{FS} \tag{4.22}$$

That *is* the same as the result from the averaging of $\cos\theta$. So we can really see, the polar angle takes all of the thermal energy, which is twice the value naively expected from the quadratic equipartition theorem (for a uniformly distributed variable)!

For reference also look at the averages of the terms that were dropped in the expansion of $\cos\theta = 1-\frac{1}{2}\theta^2+\frac{1}{4!}\theta^4+...$ I expect the higher terms just depend on higher powers of T. All of these higher terms could take some of the energy k_BT, which was *all* attributed to θ^2, possibly. Look at the quartic, and see what energy it gets, which can be done in the linearized model, using the partition function already found,

$$\langle\theta^4\rangle = \frac{2^2}{Z}\frac{\partial^2 Z}{\partial\lambda^2} = 4\lambda\frac{2}{\lambda^3} = \frac{8}{(\beta SF)2} = \frac{8(k_BT)^2}{(SF)^2}. \tag{4.23}$$

This is what I expected, however, at low temperature this is irrelavant compared to the quadratic term we kept.

4.1.1 Average of polar angle θ

Another average that may be helpful for the calculations and testing of programming is the average of the polar angle away from the magnetic field, θ. This will be a nonzero value that should be proportional to T. Using the approximate differential element $\sin\theta d\theta\approx\theta d\theta$, good for low temperature, and the low-T Hamiltonian,

$$\langle\theta\rangle \approx \frac{\int_0^\pi d\theta\ \theta\ \theta e^{-\beta\frac{1}{2}FS\theta^2}}{\int_0^\pi d\theta\ \theta\ e^{-\beta\frac{1}{2}FS\theta^2}} = \frac{-2\frac{\partial Z_q}{\partial\lambda}}{Z(\lambda)} = \frac{\frac{1}{2}\sqrt{\frac{2\pi}{\lambda^3}}}{\frac{1}{\lambda}} = \sqrt{\frac{\pi}{2\lambda}} = \sqrt{\frac{\pi k_BT}{2SF}} \tag{4.24}$$

Thus, it is not linearly proportional to T, which is interesting, as is the curious factor of $\pi/2$. But it shows how much the spin acquires xy components, proportional to $\sin\theta$, as it precesses around the magnetic field in a cone-like state. For example, at a moderately low temperature $k_BT/SF = 0.1$, the formula gives $\langle\theta\rangle \approx 0.4$, which is already quite large. That produces surprisingly large in-plane components. The conclusion is that even at low T, the in-plane spin fluctuations are already quite strong.

4.2 Dynamics in angular coordinates

We will consider, eventually, the equivalent linearization of the equations of motion. Cartesian coordinates may not be the best choice. We know that S_x and S_y relate to the ϕ degree of freedom, so it can possibly be ignored, initially. Only the S_z component is doing anything interesting. In any case, look at both in the linearized sense, for small θ. One has from $\dot{S}_z = -S\sin\theta\,\dot{\theta}$,

$$\begin{aligned} -S\sin\theta\,\dot{\theta} &= S\sin\theta(\cos\phi\,F_s^y - \sin\phi\,F_s^x) + \alpha S^2(F + F_s^z) \\ &\quad -\alpha S^2\left[\sin\theta(\cos\phi\,F_s^x + \sin\phi\,F_s^y) + \cos\theta(F + F_s^z)\right]\cos\theta \end{aligned} \tag{4.25}$$

The damping terms involving the z-components are varying as $1 - \cos^2\theta = \sin^2\theta$. The other terms are proportional to $\sin\theta$, that itself divides out. So now there is still the exact relation,

$$\boxed{-\dot{\theta} = (\cos\phi\,F_s^y - \sin\phi\,F_s^x) - \alpha S\left[\cos\theta(\cos\phi\,F_s^x + \sin\phi\,F_s^y) - \sin\theta(F + F_s^z)\right]} \tag{4.26}$$

Or it could be written

$$-\dot{\theta} = (F_s^y - \alpha S F_s^x\cos\theta)\cos\phi - (F_s^x + \alpha S F_s^y\cos\theta)\sin\phi + \alpha S(F + F_s^z)\sin\theta \tag{4.27}$$

At low temperature one could then use the approximations $\cos\theta \approx 1$ and $\sin\theta \approx \theta$ to simplify some of the terms.

Also look at the in-plane stochastic motion equation, First, the exact equation is

$$\begin{aligned} \dot{\phi} &= \frac{S_x\dot{S}_y - S_y\dot{S}_x}{S_x^2 + S_y^2} = \frac{S_x\dot{S}_y - S_y\dot{S}_x}{S^2 - S_z^2} \\ &= -(F + F_s^z) + \frac{(S_xF_s^x + S_yF_s^y)S_z}{S^2 - S_z^2} + \alpha S^2\frac{S_xF_s^y - S_yF_s^x}{S^2 - S_z^2} \end{aligned} \tag{4.28}$$

Then also consider the small angle approximation for S_z, where $S^2 - S_z^2 = S^2\sin^2\theta$ is a small quantity (small xy spin components).

$$\dot{\phi} = -(F + F_s^z) + \frac{(\cos\phi\,F_s^x + \sin\phi\,F_s^y)\cos\theta}{\sin\theta} + \alpha S\frac{\cos\phi\,F_s^y - \sin\phi\,F_s^x}{\sin\theta} \tag{4.29}$$

The first term on the RHS is the usual precessional motion, but modified by the z-component of the noise. The other parts are somewhat singular due to the presence of $\sin\theta$ in the denominators. Partly, though, this shows how there can be wild variations in ϕ, although those variations may not have any true physical significance, rather, being an artifact of the singularity of polar spherical coordinates near the pole. Even so, it can be written instead as

$$\boxed{\dot{\phi}\,\sin\theta = -(F + F_s^z)\sin\theta + (\cos\phi\,F_s^x + \sin\phi\,F_s^y)\cos\theta + \alpha S\,(\cos\phi\,F_s^y - \sin\phi\,F_s^x)} \tag{4.30}$$

That is still exact. Again, at low temperature, the approximation is that $\cos\theta \approx 1$ and $\sin\theta \approx \theta$. Next, one has to look at this together with the dynamic equation for $\dot{\theta}$, and see if a solution can be found, that can be related to equilibrium properties.

4.3 The dynamics with only a longitudinal random field, $F_s^z(t)$

The general dynamics for $\dot{\theta}$ and $\dot{\phi}$ in an arbitrary case could be challenging to solve. Physically, I am not sure that is necessary. In the limit of small polar displacements θ, the ϕ coordinate becomes irrelevant to the real physical mechanics, because there a change in ϕ gives the corresponding change in spin components only after multiplication by $\sin\theta$, which is becoming small. In addition to this, the ϕ coordinate is not connected to the energy, hence, it is hard to find a relation connecting it to a thermal equilibrium statistical average.

Although I cannot completely justify it, I now consider a situation where the in-plane stochastic fields are turned off, and the only nonzero noise comes from F_s^z. It could be considered that the only fluctuations present are the fluctuations in the actual applied field strength that is there, but not in its direction.[3] This itself might not be considered very physical. In the end, however, the $\mathbf{F_s}$ is not a real magnetic field. It is meant only to represent the effect of temperature, so at least as a mathematical device, this assumption is acceptable. Then the equations are greatly simplified,

$$\dot{\theta} = -\alpha S(F + F_s^z)\sin\theta, \qquad \dot{\phi} = -(F + F_s^z). \tag{4.31}$$

The $\dot{\phi}$ equation indicates some random jumping of that angle, but, I don't know how to connect averages like $\langle\phi(t)\phi(t)\rangle$ or even $\langle\dot{\phi}(t)\dot{\phi}(t)\rangle$ from this equation to equilibrium averages, so for now let's ignore that equation.

The $\dot{\theta}$ equation looks more challenging, however, it was already solved in an earlier section, in the absence of the stochastic forces (it was written in terms of S_z there). In the way it is written here, one might say it has "multiplicative noise" instead of a noise term that is added. However, I am not sure this is so important, because equations can always be transformed to different appearences. The equation can be expressed

$$\frac{\dot{\theta}}{\sin\theta} = \frac{\dot{\theta}\sin\theta}{1-\cos^2\theta} = \frac{-\frac{d}{dt}\cos\theta}{1-\cos^2\theta} = -\alpha S(F + F_s^z) \tag{4.32}$$

At this point, the equation is still exact. Since I only desire to connect to low temperature properties, we could assume $\theta \ll 1$ and simplify some algebra, but I can see that is not necessary, because the LHS can be integrated exactly. That integral is the inverse hyperbolic tangent, or, it can be expressed with a logarithm. Integrating both sides, starting from an arbitrary initial angle $\theta_0 = \theta(0)$,

$$\begin{aligned}
\int_0^t dt' \; \frac{\frac{d}{dt'}\cos\theta}{1-\cos^2\theta} &= \alpha S \int_0^t dt' \; [F + F_s^z(t')] \\
\tanh^{-1}\cos\theta(t) - \tanh^{-1}\cos\theta_0 &= \alpha S F t + \alpha S \int_0^t dt' \; F_s^z(t') \\
\frac{1}{2}\left\{\ln\left[\frac{1+\cos\theta(t)}{1-\cos\theta(t)}\right] - \ln\left[\frac{1+\cos\theta_0}{1-\cos\theta_0}\right]\right\} &= \alpha S F t + \alpha S \int_0^t dt' \; F_s^z(t')
\end{aligned} \tag{4.33}$$

Finally the last can be rearranged in a familar form,

$$\frac{1}{2}\ln\left[\frac{1+\cos\theta(t)}{1-\cos\theta(t)}\cdot\frac{1-\cos\theta_0}{1+\cos\theta_0}\right] = \alpha S F t + \alpha S \int_0^t dt' \; F_s^z(t') \tag{4.34}$$

Now although that was exact, perhaps the reason for doing it has been lost. Let me also show the linearized approximate version. The differential equation becomes simple in a new variable $u = \theta^2$, because then $\frac{du}{dt} = 2\theta\,\dot{\theta}$, and

$$\frac{du}{dt} = -2\alpha S[F + F_s^z(t)]\theta\sin\theta \approx -2\alpha S[F + F_s^z(t)]u, \qquad \text{then} \quad \frac{1}{u}\frac{du}{dt} = -2\alpha S(F + F_s^z(t)). \tag{4.35}$$

[3] It turns out that this does not give any equilibrium condition to determine the correlation constant A. But it is good to try it. A better approach is given in a following section.

This is easily integrated in the same way, starting from initial angle θ_0,

$$\ln\left[\frac{\theta^2(t)}{\theta_0^2}\right] \approx -2\alpha SFt - 2\alpha S\int_0^t dt'\ F_s^z(t'). \tag{4.36}$$

It means this process is going to give the autocorrelation function for the polar angle, which is the quantity for which we know the equilibirum value. For one particular realization of the stochastic field, we have found the solution,

$$\theta^2(t) \approx \theta_0^2 e^{-2\alpha SFt}\ \exp\left\{-2\alpha S\int_0^t dt'\ F_s^z(t')\right\} \tag{4.37}$$

The exact solution above will surely give the same result, when it is expanded for small angles. In fact, to check that, let

$$\Xi(t) = \alpha SFt + \alpha S\int_0^t dt'\ F_s^z(t') = \alpha SFt + \xi(t). \tag{4.38}$$

We already found the exact solution of (4.34), see for example equation (1.26) or (1.45),

$$\cos\theta(t) = \frac{(1+\cos\theta_0)e^{\Xi(t)} - (1-\cos\theta_0)e^{-\Xi(t)}}{(1+\cos\theta_0)e^{\Xi(t)} + (1-\cos\theta_0)e^{-\Xi(t)}} \tag{4.39}$$

Now taking this and supposing the polar angle is small, as is its initial angle,

$$1-\frac{1}{2}\theta^2(t) \approx \frac{(2-\frac{\theta_0^2}{2})e^{\Xi(t)} - \frac{\theta_0^2}{2}e^{-\Xi(t)}}{(2-\frac{\theta_0^2}{2})e^{\Xi(t)} + \frac{\theta_0^2}{2}e^{-\Xi(t)}} = \frac{2e^{\Xi(t)} - \theta_0^2\cosh\Xi(t)}{2e^{\Xi(t)} - \theta_0^2\sinh\Xi(t)} \tag{4.40}$$

carry out a few more steps,

$$1-\frac{1}{2}\theta^2(t) \approx \frac{1-\frac{1}{2}\theta_0^2 e^{-\Xi(t)}\cosh\Xi(t)}{1-\frac{1}{2}\theta_0^2 e^{-\Xi(t)}\sinh\Xi(t)} \approx \left[1-\frac{1}{2}\theta_0^2 e^{-\Xi}\cosh\Xi\right]\left[1+\frac{1}{2}\theta_0^2 e^{-\Xi}\sinh\Xi\right] \tag{4.41}$$

Keeping only the quadratic term, this is

$$\frac{1}{2}\theta^2(t) \approx \frac{1}{2}\theta_0^2\, e^{-\Xi}(\cosh\Xi - \sinh\Xi) = \frac{1}{2}\theta_0^2\, e^{-2\Xi(t)}. \tag{4.42}$$

That gives the same as we found from the linearized dynamic equation, namely,

$$\theta^2(t) \approx \theta_0^2\, e^{-2\Xi(t)} = \theta_0^2\, e^{-2\alpha SFt}e^{-2\xi(t)}. \tag{4.43}$$

4.3.1 Finding an equilibrium condition??

Now do an averaging over the random field. This may be tricky but interesting. The averaged autocorrelation of the angle is

$$\left\langle\theta^2(t)\right\rangle \approx \theta_0^2\, e^{-2\alpha SFt}\ \left\langle\exp\left\{-2\alpha S\int_0^t dt'\ F_s^z(t')\right\}\right\rangle. \tag{4.44}$$

This should be found by expanding the exponential,

$$\left\langle e^{-2\xi(t)}\right\rangle \approx \left\langle 1-2\xi(t)+\frac{1}{2!}(2\xi(t))^2 - \frac{1}{3!}(2\xi(t))^3 + ...\right\rangle \tag{4.45}$$

But upon averaging over different histories of the stochastic fields, which should be assumed to be unbiased, there obviously results

$$\langle\xi(t)\rangle = \alpha S\int_0^t dt'\,\langle F_s^z(t')\rangle = 0. \tag{4.46}$$

Next, for the squared term, we need to use two copies of the integral,

$$\left\langle \xi^2(t) \right\rangle = (\alpha S)^2 \int_0^t dt' \int_0^t dt'' \, \langle F_s^z(t') F_s^z(t'') \rangle \tag{4.47}$$

Now here is where we can make the assumption of uncorrelated random fields, with some undetermined coefficient,

$$\langle F_s^z(t') F_s^z(t'') \rangle = A \, \delta(t' - t''). \tag{4.48}$$

That makes this integral easy to do:

$$\left\langle \xi^2(t) \right\rangle = (\alpha S)^2 \int_0^t dt' \int_0^t dt'' \; A \, \delta(t' - t'') = (\alpha S)^2 \int_0^t dt' \; A = (\alpha S)^2 A t. \tag{4.49}$$

Next, the cubic term,

$$\left\langle \xi^3(t) \right\rangle = (\alpha S)^3 \int_0^t dt' \int_0^t dt'' \int_0^t dt''' \, \langle F_s^z(t') F_s^z(t'') F_s^z(t''') \rangle \tag{4.50}$$

Here, some new approximation or postulate must be applied. The usual thing that is done is to suppose the F factors can be averaged in pairs, since that is the basic correlator we have already (random phase approximation?). But if these are paired up, then there is always one left alone, and that averaged would be zero. So I think the reasonable approximation, is that this is zero, as would be all the odd powers of $\xi(t)$.

Finally, it will be good to do this rule to the fourth (and higher) power.

$$\left\langle \xi^4(t) \right\rangle = (\alpha S)^4 \int_0^t dt_1 \int_0^t dt_2 \int_0^t dt_3 \int_0^t dt_4 \, \langle F_s^z(t_1) F_s^z(t_2) F_s^z(t_3) F_s^z(t_4) \rangle \tag{4.51}$$

The integration variables are all equivalent, and un-ordered. They need to be paired, and there are $\frac{4\times 3}{2\times 1} = 6$ possible ways to do that. But all these ways to do the pairs give the same result, so

$$\left\langle \xi^4(t) \right\rangle = 6(\alpha S)^4 \int_0^t dt_1 \int_0^t dt_2 \int_0^t dt_3 \int_0^t dt_4 \; A^2 \, \delta(t_1 - t_2) \, \delta(t_3 - t_4) = 6(\alpha S)^4 A^2 t^2 \tag{4.52}$$

If the same rules are applied to all the even powers of $\xi(t)$, then the typical integral will be

$$\left\langle \xi^{2n}(t) \right\rangle = \frac{2n(2n-1)}{2!} (\alpha S)^{2n} (At)^n = \frac{2n(2n-1)}{2!} (\alpha^2 S^2 A t)^n. \tag{4.53}$$

Now putting the results together and praying for some magic, the sum of these terms is

$$\begin{aligned} \left\langle e^{-2\xi(t)} \right\rangle &\approx 1 + \frac{1}{2!} \left\langle (2\xi(t))^2 \right\rangle + \frac{1}{4!} \left\langle (2\xi(t))^4 \right\rangle + ... \\ &= 1 + \frac{1}{2!} (2\alpha S)^2 (At) + \frac{6}{4!} (2\alpha S)^4 (At)^2 + ... \end{aligned} \tag{4.54}$$

Unfortunately, the magic does not happen here. If I want the result for the autocorrelation to be independent of time for large time, and go to the equilibrium value, this is not going to work. This calculation gives

$$\left\langle \theta^2(t) \right\rangle \sim \theta_0^2 \tag{4.55}$$

if the result will be time-independent–that does not make sense. At long time the result should be independent of the particular starting value. It appears that at some point an approximation was too extreme, probably the idea that only F_s^z field was needed. My guess is that all the components are needed to be logically consistent.

4.4 Dynamics dominated by in-plane random fields, $F_s^x(t)$ and $F_s^y(t)$

As seen in the previous section, the dynamics with the longitudinal stochastic field only does not lead to anything resembling a Langevin equation, and hence it was not possible to get a condition for the field correlations in equilbrium or give the constant A. One can possibly see why that is. If all three components (F_s^x, F_s^y, F_s^z) are present, the total field is still nearly aligned on the z-axis, due to the static field $F = F_z = \gamma B$. The primary deviations from that state have to do with fluctuations not in its *magnitude*, but in its *direction*. These directional fluctuations come from $F_s^x(t)$ and $F_s^y(t)$. So, in this section, I concentrate on their effects.

In fact, it is good to give orders of smallness for different items. We are considering low temperature, so T is the basic scale of smallness. Arbitrarily, one might assume the damping is also a similar order. The angle θ actually should scale like $\langle\theta^2\rangle \propto T$, i.e. as the square root of T, at most. The fluctuating fields are expected to scale like $\langle F_s F_s\rangle \propto \alpha T$, i.e., F_s is the same order as the temperature or the damping.

With that, look again at the dynamics equations. On the RHS of the equation for $\dot\theta$, there is a stochastic term with the in-plane fields, and another one with the in-plane fields multiplied by α. The second is one order smaller, so let's ignore it. In addition, the field F_s^z is added to the static field F, the latter of which is much larger, so in this section we are ignoring F_s^z! Also, this makes sense as saw it did not play any role in evolution towards equilibrium.

With these approximations, there results the following equation for the low-T in-plane dynamics,

$$\dot\phi \sin\theta \approx (F_s^x \cos\phi + F_s^y \sin\phi) - F\sin\theta \tag{4.56}$$

The average dynamics of the in-plane angle is precession at frequency $\omega = -F$, however, it gets kicks from the random fields, but, there is no damping to leading orders. The kicks could be considered quite strong, because of the factors of $\sin\theta$ diminishing the other terms. For now, I don't care what ϕ is doing in details, except that it is somewhat random, due to the dominance of the stochastic forces there.

With the same type of approximations for the in-plane dynamics, there does result an equation that resembles the Langevin equation. One gets

$$\dot\theta \approx (F_s^x \sin\phi - F_s^y \cos\phi) - \alpha SF\sin\theta \tag{4.57}$$

It resembles the Langevin equation for a rotor,

$$\dot\omega = \tau_s(t) - \alpha\omega \tag{4.58}$$

where $\tau_s(t)$ is the stochasic torque per unit rotational inertia. Note also the energetic similarities: The rotor has $KE = \frac{1}{2}I\omega^2$ while the spin has potential energy above the ground state $E = \frac{1}{2}SF\theta^2$.

One can think it is impossible to solve this without knowing what $\phi(t)$ is doing. However, I think that $\phi(t)$ is a fairly chaotic function, because although it could be roughly precessing at an average rate $\omega = F$, the kicks it receives are large. In addition, a regular function multiplied by a stochastic function is mostly hard to predict, i.e., it will also likely be stochastic. So this combination that appears here is a stochastic function. Let me call the combination $\tau_s(t)$, (it is similar to a stochastic torque or a stochastic magnetic field),

$$\tau_s(t) = (F_s^x \sin\phi - F_s^y \cos\phi) \tag{4.59}$$

We may as well do the linearization also and change $\sin\theta \to \theta$. Then the polar dynamics is just like the rotor,

$$\dot\theta = \tau_s(t) - \alpha SF\theta \tag{4.60}$$

Now at this point its solution would be just like the solution we have already found, if the torque has the properties expected for a stochastic function, even though it has some dependence on the in-plane angle. But we can look at the correlations in τ_s:

$$\langle\tau_s(t)\tau_s(t')\rangle = \langle(F_s^x(t)\sin\phi(t) - F_s^y(t)\cos\phi(t))(F_s^x(t')\sin\phi(t') - F_s^y(t')\cos\phi(t'))\rangle \tag{4.61}$$

It is usual to assume the different Cartesian coordinates of $\mathbf{F}_s$ are not correlated. So this assumption is

$$\langle F_s^x(t) F_s^y(t') \rangle = \langle F_s^x(t) \rangle \langle F_s^y(t') \rangle = 0 \tag{4.62}$$

Then this means the cross terms in $\langle \tau_s(t) \tau_s(t') \rangle$ are zero. What about the direct terms? We want to relate them to the fundamental assumed correlations,

$$\langle F_s^x(t) F_s^x(t') \rangle = \langle F_s^y(t) F_s^y(t') \rangle = A\, \delta(t - t'). \tag{4.63}$$

Now the correlations here have the additional factors of sine and cosine. Consider them to be zero unless the times match (which is very reasonable, because $F_s^x(t)$ is wildly changing and uncorrelated at different times, regardless of the behavior of $\phi(t)$). And, when the times do match, assume that the regular function just factors out,

$$\langle F_s^x(t) \sin\phi(t)\ F_s^x(t') \sin\phi(t') \rangle \;=\; A\, \delta(t - t') \sin^2\phi(t) \tag{4.64}$$

$$\langle F_s^y(t) \cos\phi(t)\ F_s^y(t') \cos\phi(t') \rangle \;=\; A\, \delta(t - t') \cos^2\phi(t) \tag{4.65}$$

The constant A on the right is the same for both components, because the system is assumed rotationally invariant (i.e., no force bias in thermal equilibrium, like always). Then when these are summed, the net result is simple!

$$\langle \tau_s(t) \tau_s(t') \rangle = A\, \delta(t - t'). \tag{4.66}$$

With that now as an assumption for the torques in the effective Langevin equation, although we already solved it, just review that, and here with slightly different parameters:

$$\left(\frac{d}{dt} + \alpha S F \right) \theta(t) = \tau_s(t). \tag{4.67}$$

The solution is elucidated by taking out the long-time homogeneous behavior and letting

$$\theta(t) = h(t)\, e^{-\alpha S F t}, \qquad \text{gives } \Rightarrow \left(\frac{d}{dt} + \alpha S F \right) \theta(t) = \frac{dh}{dt}\, e^{-\alpha S F t}. \tag{4.68}$$

This is like an integrating factor, and gives

$$\int_0^t \frac{dh}{dt'}\, dt' = \int_0^t dt'\, \tau_s(t')\, e^{\alpha S F t'} \tag{4.69}$$

Then following the solution already developed earlier in these notes, the result will be that obtained earlier, but with the changes $I \to 1$ and $\alpha \to \alpha S F$. The polar angle comes out as

$$\theta(t) = \theta_0\, e^{-\alpha S F t} + \int_0^t dt'\ e^{-\alpha S F (t - t')}\, \tau_s(t') \tag{4.70}$$

Obviously this is a good solution because it goes to zero at long times in the absence of the stochastic force, and the time scale is correctly $(\alpha S F)^{-1}$. Then the procedure to get the autocorrelation function works correctly here, and following the previous calculations, gives,

$$\langle \theta(t) \theta(t) \rangle = \theta_0^2\, e^{-2\alpha S F t} + \frac{A}{2\alpha S F} \left(1 - e^{-2\alpha S F t} \right) \tag{4.71}$$

Finally, finally, in the limit of long times, this needs to reach the thermal equilibrium value (with applied field $F = \gamma B$):

$$\langle \theta(t) \theta(t) \rangle_{t \to \infty} = \frac{A}{2\alpha S F} = \frac{2 k_B T}{S F} = \left\langle \theta^2 \right\rangle_{\text{eq.}} \tag{4.72}$$

(Here I am using the correct value for the RHS where all of the energy is in the θ degree of freedom.) Now luckily the applied field cancels out, which is both surprising and very good. This gives the needed constant

$$A = 4\alpha k_B T, \qquad \left(\text{based on } \ \langle E_\theta \rangle = \frac{1}{2} S F \left\langle \theta^2 \right\rangle_{\text{eq.}} = k_B T. \right) \tag{4.73}$$

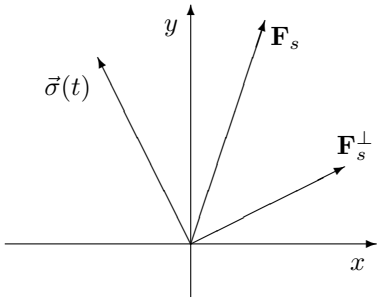
The numerical factor seems too large, but this averaged energy was found two different ways and is correct. In fact, that value of A is correct for the correlations in τ_s, but *not* for the correlations in the stochastic Cartesian components. The correct result for those is actually,

$$A = 2\alpha k_B T \quad \Longrightarrow \quad \langle F_s^x(t) F_s^x(t') \rangle = 2\alpha k_B T \, \delta(t - t'). \tag{4.74}$$

Based on the algebra I did above, it is hard to see what went wrong. It is subtle. Apparently, there is a correlaton between the in-plane fluctuating fields and the in-plane spin flucuations $\phi(t)$, that was not correctly accounted for.

4.4.1 The corrected calculation of the equilibrium condition

To do this in a different way, consider what the fluctuating "torque" $\tau_s(t)$ really means. A diagram might help. The spin factors present are $\sigma_x = \cos\phi$ and $\sigma_y = \sin\phi$, which form a unit vector $\vec{\sigma}$ from the projection of the spin onto the xy plane. Then the combination in the equation of motion for $\dot{\theta}$ is the in-plane component of the fluctuating field $\mathbf{F}_s$ that is perpendicular to $\vec{\sigma}$. This fluctuating field can be written as



$$\begin{aligned} \tau_s(t) &= F_s^x \sin\phi - F_s^y \cos\phi \\ &= (F_s^x \sigma_y - F_s^y \sigma_x) \\ &= (\mathbf{F}_s \times \vec{\sigma})_z = F_s^{\perp}. \end{aligned} \tag{4.75}$$

The symbol $F_s^{\perp}$ indicates the instantaneous component of the stochastic field that is perpendicular to the instantaneous projection of the spin in the xy-plane. There is another component of the stochastic field that is parallel to the spin, namely,

$$F_s^{\parallel} = F_s^x \cos\phi + F_s^y \sin\phi = \mathbf{F}_s \cdot \vec{\sigma} \tag{4.76}$$

This term was multiplied by damping α in the equation of motion and thus plays only a weak role in the dynamics. The combination of $F_s^{\perp}$ and $F_s^{\parallel}$ could be a new basis for the stochastic field. Of course, that axis $\vec{\sigma}$ is changing wildly with the fluctuations. Indeed, the angle ϕ responds very quickly to the stochastic torques in a way we can't predict, and that gave difficulties in the earlier analysis.

In our algebra above, at one point, we assumed the correlations of τ_s proportional to the constant A, and that constant was found to be $A = 4\alpha k_B T$, which is the correct constant for that variable:

$$\langle \tau_s(t) \tau_s(t') \rangle = 4\alpha k_B T \, \delta(t - t'). \tag{4.77}$$

Then, the correlations for $F_s^{\perp} = \tau_s$ correspond to a degree of freedom taking $k_B T$ of thermal energy (twice the usual $\frac{1}{2} k_B T$), and they do really have the "4" on the RHS,

$$\left\langle F_s^{\perp}(t) F_s^{\perp}(t') \right\rangle = 4\alpha k_B T \, \delta(t - t'). \tag{4.78}$$

But the parallel component, on the other hand, does not contain any thermal energy, in the sense of its correlations, to leading order,

$$\left\langle F_s^{\parallel}(t) F_s^{\parallel}(t') \right\rangle = 0. \tag{4.79}$$

In fact, this is because this parallel stochastic field component does not have any torque which would change θ, *hence it is not connected to the system energy.* Its effect on the spin is a torque acting around the z-axis, tending to push the spin in the azimuthal direction at constant θ. (Stated otherwise, the vector $F_s^{\parallel} \hat{\sigma} \times \mathbf{S}$ has no z-component.)

Now at this point, we *ignore* the underlying fluctuating axis $\vec{\sigma}$, and instead refer to the Cartesian components for $\mathbf{F}_s$, which is described either by the combination of perpendicular and parallel components, or by Cartesian components to *a fixed coordinate frame*,

$$F_s^2 = (F_s^\perp)^2 + (F_s^\parallel)^2 = (F_s^x)^2 + (F_s^y)^2 \tag{4.80}$$

Then the same transformation should be done for the autocorrelations, to their representation in the fixed coordinate frame of the laboratory. Due to rotational symmetry, the x and y components, take the same amount of energy, on average, which is half of what $F_s^\perp$ contains. So we can expect that the Cartesian correlations are related to the perpendicular correlations by an obvious relation,

$$\left\langle F_s^\perp(t) F_s^\perp(t') \right\rangle = \langle F_s^x(t) F_s^x(t') \rangle + \langle F_s^y(t) F_s^y(t') \rangle = 4\alpha k_B T\, \delta(t-t'). \tag{4.81}$$

Then since the Cartesian factors are equivalent, we have the correct equipartition result,

$$\langle F_s^x(t) F_s^x(t') \rangle = \langle F_s^y(t) F_s^y(t') \rangle = 2\alpha k_B T\, \delta(t-t'). \tag{4.82}$$

This shows the even sharing between different Cartesian components. Obviously the same can be said for the z-component too, although we already saw that $F_s^z(t)$ does not evolve the system towards equilibrium when the magnetic field is along the z-axis.

Then, for the total stochastic field, each Cartesian component will involve an amount of energy corresponding actually to $\frac{1}{2}k_B T$, however, in an instantaneous sense, only two of these will be active at any time. Thus, a spin in equilibrium will only get $k_B T$ of thermal energy, corresponding to two effective degrees of freedom. The net fluctuation-dissipation theorem for the vector stochastic field is thus,

$$\boxed{\langle \mathbf{F}_s(t) \cdot \mathbf{F}_s(t') \rangle = 6\alpha k_B T\, \delta(t-t').} \tag{4.83}$$

This includes the factor of $2\alpha k_B T$ for each Cartesian component. Then this has shown that the correlations of the effective torques are varying as

$$\boxed{\langle \tau_s(t) \tau_s(t') \rangle = 4\alpha k_B T\, \delta(t-t'). \qquad (\text{using } \langle E_\theta \rangle = k_B T)} \tag{4.84}$$

And the correlations of the stochastic field, when refered to fixed Cartesian axes, has the factor divided by 2, for example,

$$\boxed{\langle F_s^x(t) F_s^x(t') \rangle = 2\alpha k_B T\, \delta(t-t'). \qquad (\text{using } \langle E_\theta \rangle = k_B T)} \tag{4.85}$$

This is the fluctuation-dissipation theorem for the (scaled) random magnetic fields.

Curiously, there is no mass or rotational inertia present, which is good because there really isn't such a quantity for a spin. Check this by checking dimensions. The F_s are the same dimensions as $F = \gamma B$, which is frequency or inverse time. So the LHS is squared frequency. On the RHS α in my formulation is unfortunately not dimensionless, rather, it has dimensions of inverse of spin (see the dynamic equation of motion), where spin is angular momentum (units = J$\cdot$ s). The delta function is inverse of its argument, which makes it also inverse time. So in SI, the equation has dimensions

$$\text{LHS} = \frac{1}{s^2}, \quad \text{RHS} = \frac{\text{J}}{(\text{Js}) \cdot \text{s}} = \frac{1}{\text{s}^2}, \qquad \text{All OK.} \tag{4.86}$$

Some may prefer to write the relation not with these scaled fields but with ones measured in tesla. Also usually a dimensionless damping is defined, for example, by writing the damped dynamics like

$$\dot{\mathbf{S}} = \mathbf{S} \times \mathbf{F} + \frac{\alpha_o}{S} (\mathbf{S} \times \mathbf{F}) \times \mathbf{S}, \qquad \text{where } \alpha_o = \alpha S. \tag{4.87}$$

This new parameter α_o is dimensionless. All the terms on the RHS have dimensions as FS. Also, define the stochastic magnetic fields in tesla via $\mathbf{F}_s = \gamma \mathbf{B_s}$. Then in these terms the correlation relation or fluctuation-dissipation theorem is

$$\boxed{\gamma^2 S\, \langle B_s^x(t) B_s^x(t') \rangle = 2\alpha_o k_B T\, \delta(t-t').} \tag{4.88}$$

One can ask, what about the F_s^z fields, this calculation doesn't say anything about them? They have the same correlations as F_s^x and F_s^y, due to rotational symmetry in thermal equilibrium, its just that they have a limited effect on this polar angle. They instead would produce motions for a spin aligned to the x of y axes.

One may also try to consider a more general situation, say, that of a spin surrounded by others and interacting via exchange. That could be general enough, still, it would require some good approximations to be able to do the kind of analysis presented here.

4.5 Equilibrium condition based on $\langle\theta\rangle$?

Now try to find a condition on the stochastic fields based on the average of θ, which is nonzero, rather than the average of θ^2. This may result in some other interesting relations between equilibrium quantities, and also, give relations for testing numerics. I will try to use the equations of motion with some reasonable assumptions in equilibrium. After a long time, the polar angle stays near some average value that is its equilibrium value, and

$$\langle\theta\rangle \approx \sqrt{\frac{\pi k_B T}{2SF}}, \qquad \langle\dot{\theta}\rangle \approx 0. \tag{4.89}$$

For the in-plane motion, the good approximation is not as clear. For very low T and weak perturbations, the motion should be a uniform precession at frequency $\omega = -F$. So it is reasonable to assume over long times,

$$\langle\dot{\phi}\sin\theta\rangle \approx \langle\dot{\phi}\rangle\langle\theta\rangle \approx -F\langle\theta\rangle. \tag{4.90}$$

Looking at the dynamics equations,

$$\begin{aligned}
\langle\dot{\theta}\rangle &= -\alpha S\langle(F+F_s^z)\sin\theta\rangle \\
&\quad +\langle(F_s^x\sin\phi - F_s^y\cos\phi)\rangle + \alpha S\langle(F_s^x\cos\phi + F_s^y\sin\phi)\cos\theta\rangle = 0, \qquad (4.91)\\
\langle\dot{\phi}\,\sin\theta\rangle &= -\langle(F+F_s^z)\sin\theta\rangle \\
&+ \langle(F_s^x\cos\phi + F_s^y\sin\phi)\cos\theta\rangle + \alpha S\langle(F_s^y\cos\phi - F_s^x\sin\phi)\rangle = -F\langle\sin\theta\rangle. \qquad (4.92)
\end{aligned}$$

and knowing the thermal equilibrium value of $\langle\theta\rangle$, this gives some surprising relations. They become

$$\begin{aligned}
\langle F_s^x\sin\phi - F_s^y\cos\phi\rangle + \alpha S\langle F_s^x\cos\phi + F_s^y\sin\phi\rangle &= \alpha SF\langle\sin\theta\rangle, \qquad (4.93)\\
-\alpha S\langle F_s^x\sin\phi - F_s^y\cos\phi\rangle + \langle F_s^x\cos\phi + F_s^y\sin\phi\rangle &= 0. \qquad (4.94)
\end{aligned}$$

Here I also assumed $\langle F_s^z\sin\theta\rangle = 0$, because that term is much smaller than $\langle F\sin\theta\rangle \neq 0$. This is a 2×2 system for the two combined correlations. They can be easily solved, and the results are the averaged perpendicular and parallel stochastic field components,

$$\begin{aligned}
\left\langle F_s^{\parallel}\right\rangle &= \langle F_s^x\cos\phi + F_s^y\sin\phi\rangle = \frac{\alpha^2S^2}{1+\alpha^2S^2}F\langle\sin\theta\rangle, \qquad (4.95)\\
\left\langle F_s^{\perp}\right\rangle &= \langle F_s^x\sin\phi - F_s^y\cos\phi\rangle = \frac{\alpha S}{1+\alpha^2S^2}F\langle\sin\theta\rangle. \qquad (4.96)
\end{aligned}$$

The sum is smaller than the difference, by a factor of the damping. If I assume a certain symmetry between x and y components, then the first implies approximatley,

$$\langle F_s^x\cos\phi\rangle = \langle F_s^y\sin\phi\rangle \approx \frac{1}{2}(\alpha S)^2F\langle\sin\theta\rangle \approx 0. \tag{4.97}$$

For low enough T, with small damping, the RHS is quite small, and approximates zero. Those correlations involve a field component with the *same component* of the spin. It would make sense that those are zero; we saw that F_z does not really cause S_z to relax towards equilibrium, and these are similar. For the other equation, let me assume there is some symmetry relation of the off-diagonal correlations like

$$\langle F_s^y\cos\phi\rangle = -\langle F_s^x\sin\phi\rangle. \tag{4.98}$$

Applying $\langle \sin\theta \rangle \approx \langle \theta \rangle$, this would imply

$$\langle F_s^x \sin\phi \rangle = -\langle F_s^y \cos\phi \rangle = \frac{1}{2}\alpha SF \langle \sin\theta \rangle \approx \frac{1}{2}\alpha SF \sqrt{\frac{\pi k_B T}{2SF}} = \alpha \sqrt{\frac{\pi}{8} SF k_B T}. \tag{4.99}$$

In some sense, this must mean that ϕ has to jump around suddenly in response to the random fields, to make this correlation consistently nonzero. But this calculation did not give a constraint on the field-field correlations like $\langle F_s^x(t) F_s^x(t') \rangle$.

5 Numerics for 3D Langevin spin dynamics

Now one needs some numerical scheme to integrate the dynamics with the random fields and damping included. We suppose all Cartesian components of $\mathbf{F}_s$ are present, and have the correlations in Eq. (4.85). The dynamics are controlled by

$$\dot{\mathbf{S}} = \mathbf{S} \times (\mathbf{F} + \mathbf{F}_s) + \alpha [\mathbf{S} \times (\mathbf{F} + \mathbf{F}_s)] \times \mathbf{S}, \tag{5.1}$$

where $\alpha S = \alpha_o$ is the dimensionless damping. If one looks at just the form of the stochastic field terms, they are mulitplicative, which means these fields are multiplying functions of the unknown spin solution. There is only one damping term that is an additive noise, for instance, look at one Cartesian component of a spin precessing around the constant applied field in the z-direction,

$$\dot{S}_x = S_y(F + F_s^z) - S_z F_s^y + \alpha S^2 F_s^x - \alpha [S_x F_s^x + S_y F_s^y + S_z(F + F_s^z)] S_x \tag{5.2}$$

The general form of this is rather nonlinear, but might be expressed

$$\dot{r}(t) = f[t, r(t)] + f_s(t) \cdot g[t, r(t)] \tag{5.3}$$

The first term is the parts that don't depend on stochastic fields, but do depend on the current spin position $r(t)$, a symbol used to generally represent all the spin components (i.e., a 3D vector). The second term represents the stochastic terms. To see that form in the spin dynamics equations, again, consider a scalar product of 3D vector functions, for example, in the $\dot{S}_x$ equation, the terms

$$f_s(t) \cdot g[t, r(t)] = F_s^x(\alpha S^2 - \alpha S_x^2) + F_s^y(-S_z - \alpha S_x S_y) + F_s^z(S_y - \alpha S_x S_z), \tag{5.4}$$

are represented with the vector functions,

$$\vec{f}_s = \begin{pmatrix} F_s^x \\ F_s^y \\ F_s^z \end{pmatrix}, \qquad \vec{\mathbf{g}} = \begin{pmatrix} \alpha(S^2 - S_x^2) \\ -S_z - \alpha S_x S_y \\ S_y - \alpha S_x S_z \end{pmatrix} \tag{5.5}$$

and the deterministic force function for $\dot{S}_x$ is

$$f_x = [\mathbf{S} \times \mathbf{F} + \alpha(\mathbf{S} \times \mathbf{F}) \times \mathbf{S}]_x = S_y F - \alpha F S_x S_z. \tag{5.6}$$

More simply and generally, the time dreivative of $\mathbf{S}$ is always easy to split into a deterministic term (but with damping) and a stochastic term (also with damping). Obviously the equation is linear in the fields $\mathbf{F}$ and $\mathbf{F}_s$ and one can write

$$\dot{\mathbf{S}} = \mathbf{S} \times [\mathbf{F} - \alpha(\mathbf{S} \times \mathbf{F})] + \mathbf{S} \times [\mathbf{F}_s - \alpha(\mathbf{S} \times \mathbf{F}_s)] \tag{5.7}$$

Then one can clearly read off the deterministic function $\mathbf{f}$ and the stochastic function that corresponds to $\vec{f}_s \cdot \vec{g}$ for each spin component's time derivative.

5.1 Euler method for 3D Langevin spin dynamics

Now how to solve a system like (5.3)? As always, it is best to start with the equivalent of an Euler method, using the lowest order approximations to effect a a time step Δt. Then later one can look at how to improve its precision.

The stochastic forces must be accounted for by *integrating* the differential equation, not by finite differences alone. This will give

$$\int_t^{t+\Delta t} dt'\ \dot{r}(t') = r(t+\Delta t) - r(t) = \int_t^{t+\Delta t} dt'\ f(t') + \int_t^{t+\Delta t} dt'\ f_s(t') \cdot g(t') \tag{5.8}$$

For an Euler method, the deterministic parts on the RHS can be taken as constants– use their values at the start of the time interval. This will only leave the integration of the stochastic part:

$$r(t+\Delta t) = r(t) + \Delta t\, f(t) + g(t) \cdot \int_t^{t+\Delta t} dt'\ f_s(t') \tag{5.9}$$

The stochastic "push" integral was already encountered for the Langevin equation for a mass. Give it the same name a here, for one of its Cartesian components,

$$a_i(\Delta t) = \int_t^{t+\Delta t} dt'\ f_s^i(t') \tag{5.10}$$

Its average over different histories of the noise is zero:

$$\langle a_i(\Delta t)\rangle = \int_t^{t+\Delta t} dt'\ \left\langle f_s^i(t')\right\rangle = 0. \tag{5.11}$$

This applies to any Cartesian component. On the other hand, there is a distribution of this integral, so get the squared variance based on the fluctuation-dissipation result for the fields $\mathbf{F}_s$ which are identified as the f_s here, so assume

$$\left\langle f_s^i(t) f_s^j(t')\right\rangle = 2\alpha k_B T\, \delta_{ij}\, \delta(t-t'). \tag{5.12}$$

Then the squared variance of any Cartesian component of a is the same as that of a_x,

$$\sigma_a^2 = \left\langle a_x^2(\Delta t)\right\rangle = \int_t^{t+\Delta t} dt'\ \int_t^{t+\Delta t} dt''\ \langle f_s^x(t') f_s^x(t'')\rangle = 2\alpha k_B T\, \Delta t. \tag{5.13}$$

Then, the corresponding term $a_i(\Delta t)$ in the integration step is replaced by a zero mean, unit variance random number w multiplied by σ_a. So the Euler integration step is really simple, as expected,

$$r(t+\Delta t) = r(t) + \Delta t\, f(t) + g(t) \cdot (\sigma_a w) \tag{5.14}$$

The stochastic term really is a sum over Cartesian components, so here w is actually three random numbers and this term is expanded out as

$$r(t+\Delta t) = r(t) + \Delta t\, f(t) + g^i(t) \cdot (\sigma_a w^i) \tag{5.15}$$

I will avoid writing those sums over Cartesian indeces, however, to keep the formulas cleaner. That is because I also want to use the index notation for the steps, with $t_n = n\Delta t$ and $r(t_n) = r_n$, etc. So the one Euler step in index notation (with implied sum over Cartesian components in the stochastic dot product) is

$$\boxed{r_{n+1} = r_n + \Delta t\, f_n + g_n \cdot (\sigma_a w_n), \qquad \sigma_a(\Delta t) = \sqrt{2\alpha k_B T\, \Delta t}\,.} \tag{5.16}$$

Here, n on w_n refers to the n^{th} step's triple random number, $w_n = (w_n^x, w_n^y, w_n^z)$, and in similar fashion, $g_n = (g_n^x, g_n^y, g_n^z)$.

If one ignored the stochastic part, this is a Taylor series with the next order (error) term being $\frac{1}{2}\Delta t^2 f_n'$. Then this step is accurate to first order in the time step.

5.2 A second order integration method?

Let's approach this with the goal of better precision. There are always different ways to proceed. Let me first try to get a second order approach that uses r_n *and* r_{n-1} to calculate the estimate for r_{n+1}. But remember that the only logical way to go about this is to *integrate* the differential equation, otherwise, one doesn't know how to deal with the stochastics.

On the RHS, both $f(t)$ and $g(t)$ can be expanded in Taylor series, like

$$f(t') = f(t) + (t'-t)f'(t) + \frac{1}{2}(t'-t)^2 f''(t) + ... \tag{5.17}$$

While $f(t)$ comes from the differential equation, $f'(t)$ must come from a finite difference estimate, using two values at neighboring time steps. Suppose I use the times $t - \Delta t$ and the current time t. Applying this same expansion with $t' = t - \Delta t$, we have

$$f(t-\Delta t) = f(t) - \Delta t\, f'(t) + \frac{1}{2}(-\Delta t)^2 f''(t) + ... \tag{5.18}$$

so this tells us that we can put

$$f'(t) \approx \frac{f(t) - f(t-\Delta t)}{\Delta t} + \frac{1}{2}\Delta t\, f''(t) \tag{5.19}$$

Then I have an expansion of the force at time t' around the current time t,

$$f(t') \approx f(t) + (t'-t)\left[\frac{f(t) - f(t-\Delta t)}{\Delta t} + \frac{1}{2}\Delta t\, f''(t)\right] + \frac{1}{2}(t'-t)^2 f''(t) + ... \tag{5.20}$$

In the Euler method, the integration of the ODE produced $\Delta t\, f(t)$ on the RHS. Here, instead of just multiplication by Δt, we need to integrate this over the time step from t to $t+\Delta t$. With integration over $\tau' = t' - t$, this gives

$$\begin{aligned}
\int_t^{t+\Delta t} dt'\ f(t') &\approx \Delta t\, f(t) + \frac{(\Delta t)^2}{2} f'(t) + \frac{1}{3!}(\Delta t)^3 f''(t) + ... \\
&= \Delta t\, f(t) + \frac{(\Delta t)^2}{2}\left[\frac{f(t) - f(t-\Delta t)}{\Delta t} + \frac{1}{2}\Delta t\, f''(t)\right] + \frac{1}{3!}(\Delta t)^3 f''(t) + ... \\
&= \Delta t\left(\frac{3}{2}f(t) - \frac{1}{2}f(t-\Delta t)\right) + \frac{5}{12}(\Delta t)^3 f''(t) + ...
\end{aligned} \tag{5.21}$$

OK, this is a well-known 2-point finite difference formula for the integral. It just used the linear fit to the function, then integrated. If this was the only thing in the ODE RHS, the algorithm would become

$$r_{n+1} = r_n + \Delta t\,\left(\frac{3}{2}f_n - \frac{1}{2}f_{n-1}\right) + \frac{5}{12}(\Delta t)^3 f_n'' \tag{5.22}$$

This is accurate to second order in the time step.

Now for the stochastic term in second order, more work is needed. A similar expansion is made for $g(t)$,

$$g(t') = g(t) + (t'-t)g'(t) + \frac{1}{2}(t'-t)^2 g''(t) + ... \tag{5.23}$$

But this is multiplied by the stochastic field, and then integrated. So the integral looks tricky,

$$q = \int_t^{t+\Delta t} dt' g(t')\cdot f_s(t') = \int_t^{t+\Delta t} dt'\ \left[g(t) + (t'-t)g'(t) + \frac{1}{2}(t'-t)^2 g''(t) + ...\right] f_s(t') \tag{5.24}$$

The integral itself cannot be evaluated, but its mean and variance can be found. The mean is zero, due to $\langle f_s(t')\rangle = 0$. Try to get the variance, using the fluctuation-dissipation theorem,

$$\begin{aligned}
\langle q^2\rangle &= \int_t^{t+\Delta t} dt'\ g(t') \int_t^{t+\Delta t} dt''\ g(t'')\,\langle f_s(t') f_s(t'')\rangle = 2\alpha k_B T \int_t^{t+\Delta t} dt'\ g^2(t') \\
&= 2\alpha k_B T \int_t^{t+\Delta t} dt'\ \left[g(t) + (t'-t)g'(t) + \frac{1}{2}(t'-t)^2 g''(t) + ...\right]^2
\end{aligned} \tag{5.25}$$

There are several trivial integrals, and the result is

$$\langle q^2\rangle = 2\alpha k_B T\left\{\Delta t\, g^2(t) + (\Delta t)^2 g(t)g'(t) + \frac{(\Delta t)^3}{3}\left[(g'(t))^2 + g(t)g''(t)\right] + ...\right\} \tag{5.26}$$

Now to use it, the finite difference value of $g'(t)$ must be substituted,

$$g'(t) \approx \frac{g(t) - g(t-\Delta t)}{\Delta t} + \frac{1}{2}\Delta t\, g''(t) \tag{5.27}$$

This could even be used in the term cubic in the time step. Some ugly algebra...

$$\begin{aligned}\langle q^2\rangle &= 2\alpha k_B T\left\{\Delta t\, g^2(t) + (\Delta t)^2 g(t)\left[\frac{g(t) - g(t-\Delta t)}{\Delta t} + \frac{1}{2}\Delta t\, g''(t)\right]\right.\\ &\left. + \frac{(\Delta t)^3}{3}\left[\frac{g(t) - g(t-\Delta t)}{\Delta t} + \frac{1}{2}\Delta t\, g''(t)\right]^2 + \frac{(\Delta t)^3}{3}g(t)g''(t) + ...\right\}\end{aligned} \tag{5.28}$$

Rearrange,

$$\begin{aligned}\frac{\langle q^2\rangle}{2\alpha k_B T\Delta t} &= g^2(t) + g(t)[g(t) - g(t-\Delta t)] + \frac{1}{3}[g(t) - g(t-\Delta t)]^2\\ &\quad + \frac{(\Delta t)^2}{3}\left(\frac{7}{2}g(t) - g(t-\Delta t)\right)g''(t) + ...\end{aligned} \tag{5.29}$$

$$\begin{aligned}\frac{\langle q^2\rangle}{2\alpha k_B T\Delta t} &= \frac{7}{3}g^2(t) - \frac{5}{3}g(t)g(t-\Delta t) + \frac{1}{3}g^2(t-\Delta t)\\ &\quad + \frac{(\Delta t)^2}{3}\left(\frac{7}{2}g(t) - g(t-\Delta t)\right)g''(t) + ...\end{aligned} \tag{5.30}$$

Then the variance of this stochastic "push" is actually dependent on the current and previous state of the system, correct to second order in the time step,

$$\sigma_q = \sqrt{\langle q^2\rangle} = \sqrt{2\alpha k_B T\Delta t}\left[\frac{7}{3}g^2(t) - \frac{5}{3}g(t)g(t-\Delta t) + \frac{1}{3}g^2(t-\Delta t)\right]^{1/2} + \mathcal{O}(\Delta t^3) \tag{5.31}$$

This is the same order of error as in the deterministic part. Putting them together, with index notation, and summing over the Cartesian components of the push, a single step is

$$r_{n+1} = r_n + \Delta t\left(\frac{3}{2}f_n - \frac{1}{2}f_{n-1}\right) + \sigma_{q,n}\cdot w_n + \mathcal{O}(\Delta t^3) \tag{5.32}$$

where the stochastic impulse (due to each Cartesian component) is determined by

$$\sigma_{q,n} = \sqrt{2\alpha k_B T\Delta t}\left[\frac{7}{3}g_n^2 - \frac{5}{3}g_n g_{n-1} + \frac{1}{3}g_{n-1}^2\right]^{1/2} \tag{5.33}$$

This should be a single step for the original differential equation,

$$\dot{r}(t) = f(t) + f_s(t)\cdot g(t) \tag{5.34}$$

where both f and g can depend on the desired solution function $r(t)$.

I cannot be sure about the stability, it is difficult to judge without knowing the force function explicitly.

There is a slight modification/simplification that could be applied. Above, I eliminated one term cubic in the time step, but there still remained a cubic error term. More consistent would be to

consider both cubic terms as the error. Then a simpler version of the algorithm will use the squared variance as follows:

$$\begin{aligned}\langle q^2\rangle &= 2\alpha k_B T\left\{\Delta t g^2(t)+(\Delta t)^2 g(t)\left[\frac{g(t)-g(t-\Delta t)}{\Delta t}+\frac{1}{2}\Delta t\, g''(t)\right]\right.\\ &\left.+\frac{(\Delta t)^3}{3}\left[(g'(t))^2+g(t)g''(t)\right]+...\right\}\end{aligned} \tag{5.35}$$

Do some arranging,

$$\frac{\langle q^2\rangle}{2\alpha k_B T\Delta t} = 2g^2(t)-g(t)g(t-\Delta t)+\frac{(\Delta t)^2}{3}\left[(g'(t))^2+\frac{5}{2}g(t)g''(t)\right]+... \tag{5.36}$$

So now, the variance of the stochastic impulse is much simpler,

$$\sigma_{q,n}=\sqrt{2\alpha k_B T\Delta t}\left[2g_n^2-g_n g_{n-1}\right]^{1/2}+\mathcal{O}(\Delta t^3) \tag{5.37}$$

The actual step is still the same as before, and the method is accurate to second order.

5.3 Second order Runge-Kutta method for Langevin spin dynamics

Sometimes these simple finite difference-like methods are numerically unstable. It is good to try to develop another method that might resemble Runde-Kutta, which tends to be very stable. It means to try to split a time step into two parts, using some evaluation at the center of the time step.

Consider a determinisitc ODE

$$\dot r(t)=f(t,r) \tag{5.38}$$

For second order Runge-Kutta, the first stage is to initially make a preliminary Euler half-step to the center of the desired integral, $\bar t = t+\frac{\Delta t}{2}$. Then that initial prediction is used to get a better estimate of the slope in the center of the interval, with which a whole "correction" step can be made, starting from the original starting point $r(t)$. I need to write this process as integrations, so it can be generalized to the stochastic problem.

We know the expansion of the force around the center of the interval is

$$f(t')=f(\bar t\,)+(t'-\bar t\,)\cdot f'(\bar t\,)+\frac{1}{2!}(t'-\bar t\,)^2\cdot f''(\bar t\,)+... \tag{5.39}$$

The individual step using this has also already been discussed. For RK2, only the first term is used and the correction step is

$$r(t+\Delta t)=r(t)+\int_t^{t+\Delta t}dt'\, f(t')=r(t)+\Delta t\, f(\bar t\,)+\frac{2}{3!}\left(\frac{\Delta t}{2}\right)^3 f''(\bar t\,)+... \tag{5.40}$$

where the last is the error estimate. But this cannot be applied directly, because the position $r(\bar t\,)$ is needed to generate the the mid-point force value. But that is where the preliminary Euler half-step is applied, which is just the integral of the Taylor series over the half step using the starting force value,

$$r(\bar t\,)=r(t)+\frac{\Delta t}{2}f(t)+\frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2 f'(t)+... \tag{5.41}$$

The force is really a function of time and the position, and this means really that $f(\bar t\,)=f(\bar t, r(\bar t\,))$, using an estimate from this last expression. So to summarize the one RK2 step, with $\bar t = t_{n+\frac{1}{2}}$,

$$\bar r = r_n+\frac{\Delta t}{2}f(t_n,r_n), \tag{5.42}$$

$$r_{n+1} = r_n+\Delta t\, f(t_{n+\frac{1}{2}},\bar r)+\mathcal{O}(\Delta t^3). \tag{5.43}$$

I have some doubt about how to get the accurate error estimate, but let it stand for the time being.

For the stochastic modifications, the preliminary Euler step should be like what has been already discussed, using though, a half-time-step, which introduces a factor of $\frac{1}{\sqrt{2}}$,

$$\bar{r} = r_n + \frac{\Delta t}{2} f_n + g_n \cdot \left(\frac{1}{\sqrt{2}}\, \sigma_a w_{1,n} \right), \qquad \frac{1}{\sqrt{2}}\, \sigma_a = \sqrt{2\alpha k_B T\, \frac{\Delta t}{2}}. \tag{5.44}$$

To be careful, note what the stochastic term/random number is replacing. It represents the integral over the half time step from t to $t + \frac{\Delta t}{2}$, of the stochastic force,

$$\frac{1}{\sqrt{2}}\, \sigma_a w_{1,n} \doteq \int_t^{t+\frac{\Delta t}{2}} dt'\, f_s(t') \tag{5.45}$$

Note that we may use this same partial history of $f_s(t')$ in the correction part of the RK2 step. That is why I called the random number $w_{1,n}$. There will be another random number, $w_{2,n}$ needed for the correction stage.

Now for the "correction whole step", the g-function can be expanded around the center point, instead of around the initial point as in the previous section,

$$g(t') = g(\bar{t}\,) + (t' - \bar{t}\,) \cdot g'(\bar{t}\,) + \frac{1}{2!}(t' - \bar{t}\,)^2 \cdot g''(\bar{t}\,) + ... \tag{5.46}$$

Multiplied by the stochastic field and integrated over the whole time step gives the stochastic "push",

$$q = \int_t^{t+\Delta t} dt'\, g(t') \cdot f_s(t') = \int_t^{t+\Delta t} dt' \left[g(\bar{t}\,) + (t' - \bar{t}\,) g'(\bar{t}\,) + \frac{1}{2!}(t' - \bar{t}\,)^2 g''(\bar{t}\,) + ... \right] f_s(t') \tag{5.47}$$

Of course, the mean of this integral is zero, but the variance is not, and

$$\begin{aligned} \langle q^2 \rangle &= \int_t^{t+\Delta t} dt'\, g(t') \int_t^{t+\Delta t} dt'' g(t'') \langle f_s(t') f_s(t'') \rangle = 2\alpha k_B T \int_t^{t+\Delta t} dt'\, g^2(t') \\ &= 2\alpha k_B T \int_t^{t+\Delta t} dt' \left[g(\bar{t}\,) + (t' - \bar{t}\,) g'(\bar{t}\,) + \frac{1}{2!}(t' - \bar{t}\,)^2 g''(\bar{t}\,) + ... \right]^2 \end{aligned} \tag{5.48}$$

Integration of the odd powers of $(t' - \bar{t}\,)$ gives zero because $\bar{t}$ is in the center of the interval. Besides the error term, only the zeroth and quadratic terms give a nonzero result. Their integration gives

$$\langle q^2 \rangle = 2\alpha k_B T \left\{ \Delta t\, g^2(\bar{t}\,) + \frac{2}{3} \left(\frac{\Delta t}{2} \right)^3 \left[(g'(\bar{t}\,))^2 + g(\bar{t}\,) g''(\bar{t}\,) \right] \right\} \tag{5.49}$$

By using the center of the interval, there is no term quadratic in the time step. The terms cubic in the time step can be considered the error terms. [One of them, $g'(\bar{t}\,)$, could be reduced but it really doesn't help because there will still be another cubic error term.] Then to leading order we can use just $q = g(\bar{t}\,) a(\Delta t)$, and the variance is

$$\sigma_q = \sqrt{\langle q^2 \rangle} = \sqrt{2\alpha k_B T \Delta t}\, g(\bar{t}\,) = \sigma_a\, g(\bar{t}\,) \tag{5.50}$$

It is the same as used in the discussion of Langevin Euler steps in a previous section.

The total correction step includes the simultaneous changes due to both the deterministic and stochastic terms. But for the stochastic part, we have to re-use *the same history* $f_s(t')$ during $t \le t' < t + \frac{\Delta t}{2}$, that was used in the preliminary Euler step, Eq. (5.44). So the actual stochastic push being used here, effectively determined only by $g(\bar{t}\,)$ and not depending on $g'(\bar{t}\,)$, etc, must partly use the random number $w_{1,n}$ in the preliminary step, and a new random number, $w_{2,n}$, due to

$$q = g(\bar{t}\,) \left\{ \int_t^{t+\frac{\Delta t}{2}} dt'\, f_s(t') + \int_{t+\frac{\Delta t}{2}}^{t+\Delta t} dt'\, f_s(t') \right\} = g(\bar{t}\,) \frac{\sigma_a}{\sqrt{2}} \left(w_{1,n} + w_{2,n} \right). \tag{5.51}$$

The net random number being used here is $w_n = w_{1,n} + w_{2,n}$. This is the sum of two unit-variance randoms, i.e, $\langle w_{1,n}\rangle = 0$ and $\langle w_{1,n}^2\rangle = 1$, and the same for the other one. Then the squared variance of the sum is $\langle (w_{1,n} + w_{2,n})^2\rangle = \langle w_{1,n}^2\rangle + \langle w_{2,n}^2\rangle = 2$. The variance of the sum is then $\sqrt{2}$, which combines with the factor of $\frac{1}{\sqrt{2}}$ so that the variance of $\frac{1}{\sqrt{2}}(w_{1,n} + w_{2,n})$ is 1, as required.

Then the correction step, including the deterministic and stochastic effects, is

$$r_{n+1} = r_n + \Delta t\, f(\bar{t}\,) + g(\bar{t}\,) \cdot \left(\frac{1}{\sqrt{2}} \sigma_a [w_{1,n} + w_{2,n}] \right) \tag{5.52}$$

The number $w_{1,n}$ *is required* to be the same number that was used in the preliminary Euler stage.

So let's summarize **a single second order Runge-Kutta step**. First there is the "trial" or preliminary Euler step to the center of the time interval,

$$\boxed{\bar{t} = t_{n+\frac{1}{2}} = t + \frac{\Delta t}{2},} \tag{5.53}$$

where the preliminary update is

$$\boxed{\bar{r} = r_n + \frac{\Delta t}{2} f(t_n, r_n) + g(t_n, r_n) \cdot \left(\frac{1}{\sqrt{2}} \sigma_a w_{1,n} \right).} \tag{5.54}$$

Then there is the correction stage all the way across the time interval,

$$\boxed{r_{n+1} = r_n + \Delta t\, f(\bar{t}, \bar{r}) + g(\bar{t}, \bar{r}) \cdot \left(\frac{1}{\sqrt{2}} \sigma_a [w_{1,n} + w_{2,n}] \right).} \tag{5.55}$$

Both of these are written in such a way that the variance to be included is the same,

$$\boxed{\sigma_a(\Delta t) = \sqrt{2\alpha k_B T \Delta t}\,.} \tag{5.56}$$

The errors should vary as $(\Delta t)^3$, so that it is accurate to second order in the time step. When actually applying the formulas, need to keep in mind that the dot products of g with the random numbers are 3D scalar products like

$$g_n \cdot w_n = \sum_{i=x,y,z} g_n^i w_n^i \tag{5.57}$$

That is, each of $w_{1,n}$ and $w_{2,n}$ are actually triplets of unit variance random numbers for the 3D spin dynamics problem.

5.4 Second order Heun method for Langevin dynamics

This is a scheme that is about as simpler and accurate as RK2. I can't say which is better. The advantage of the Heun method, is that it is a type of predictor-corrector scheme, which tend to be fairly stable. On the other hand, Runge-Kutta is also highly stable.

The predictor step is an Euler full step to some estimate of the solution at time t_{n+1}, call it $\tilde{r}_{n+1}$. Then that is corrected by using an average of the slope $f(r_n)$ and at the predicted point, $f(\tilde{r}_{n+1})$. That averaged slope is used to shoot from $r(t_n)$ to the new solution point, $r(t_{n+1})$.

To keep track of errors, start from expanding f and g around the initial point, as usual,

$$f(t') = f(t) + (t'-t)f'(t) + \frac{1}{2}(t'-t)^2 f''(t) + ... \tag{5.58}$$

$$g(t') = g(t) + (t'-t)g'(t) + \frac{1}{2}(t'-t)^2 g''(t) + ... \tag{5.59}$$

$$\tag{5.60}$$

For the ODE, $\dot{r} = f + g \cdot f_s$, integrated over one time step, the Euler uses only the first terms in these expansions. The deterministic part is

$$\begin{aligned} \tilde{r}(t+\Delta t) &= r(t) + \Delta t\, f(t) + \int_t^{t+\Delta t} dt' \left[(t'-t) f'(t) + \frac{1}{2}(t'-t)^2 f''(t) + ... \right] \\ &= r(t) + \Delta t\, f(t) + \frac{(\Delta t)^2}{2!} f'(t) + \frac{(\Delta t)^3}{3!} f''(t) + ... \end{aligned} \tag{5.61}$$

No surprise there! For the stochastic addition to this, there is

$$\begin{aligned} \tilde{q} &= \int_t^{t+\Delta t} dt'\, g(t') f_s(t') = \int_t^{t+\Delta t} dt'\, [g(t) + (t'-t) g'(t) + ...] f_s(t') \\ &= g(t) a(\Delta t) + g'(t) \int_t^{t+\Delta t} dt'\, (t'-t) f_s(t') + ... \end{aligned} \tag{5.62}$$

where the "acceleration" is

$$a(\Delta t) = \int_t^{t+\Delta t} dt'\, f_s(t'). \tag{5.63}$$

and the error scales with the integral

$$b(\Delta t) = \int_t^{t+\Delta t} dt'\, (t'-t) f_s(t'). \tag{5.64}$$

As usual, the mean of $\tilde{q}$ is zero, no matter how many terms you keep, and we can get the variance, but tracking the error seems tricky. However, we evaluated the squared variance to third order in the time step, it was

$$\langle q^2 \rangle = 2\alpha k_B T \left\{ \Delta t\, g^2(t) + (\Delta t)^2 g(t) g'(t) + \frac{(\Delta t)^3}{3} \left[(g'(t))^2 + g(t) g''(t) \right] + ... \right\} \tag{5.65}$$

The Euler approach uses only the first term here, so the error in the squared variance can be read off. To estimate the corresponding error in a particular evolution for $\tilde{q}(\Delta t)$, I think I need a new kind of mathematics. Let that be for now.

Then $\tilde{q}$ is replaced by a random number with the lowest approximation for the variance, σ_a, and the predictor step is

$$\tilde{r}_{n+1} = r_n + \Delta t\, f(t_n, r_n) + g(t_n, r_n) \cdot (\sigma_a w_n) + \mathcal{O}(\Delta t^2) \tag{5.66}$$

It will turn out we will re-use this same random number for the corrector.

For the correction part of the algorithm, that is used to produce a better estimate of the average slope. The exact solution could be obtained if we knew the exact average slope, for the deterministic part,

$$r(t+\Delta t) = r(t) + \Delta t\, \overline{f(t)} \tag{5.67}$$

That change in position uses the trapezoid rule for integration:

$$\begin{aligned} \int_t^{t+\Delta t} dt' f(t') &= \int_t^{t+\Delta t} dt' \left[f(t) + (t'-t) f'(t) + \frac{1}{2}(t'-t)^2 f''(t) + ... \right] \\ &= \Delta t\, f(t) + \frac{(\Delta t)^2}{2} f'(t) + \frac{(\Delta t)^3}{6} f''(t) + ... \\ &= \Delta t \left(\frac{f(t) + f(t) + \Delta t\, f'(t)}{2} \right) + \frac{(\Delta t)^3}{6} f''(t) + ... \end{aligned} \tag{5.68}$$

But one knows that the function value at the new time is

$$f(t+\Delta t) = f(t) + \Delta t\, f'(t) + \frac{1}{2}(\Delta t)^2 f''(t) + ... \tag{5.69}$$

Then the trapezoid rule with error estimate is

$$\int_t^{t+\Delta t} dt' f(t') \quad = \quad \Delta t \left(\frac{f(t) + f(t+\Delta t)}{2} \right) - \frac{(\Delta t)^3}{12} f''(t) \tag{5.70}$$

But since we don't know exactly $f(t+\Delta t)$ because we are still trying to find $r(t+\Delta t)$ the best we can do is use the predicted $\tilde{r}$ to get $f(t+\Delta t, \tilde{r})$. The error is hard to estimate, but still should be of order Δt^3.

Try to apply the same process to the correction for the stochastic part. With the trapezoid rule, applied to the product funcion $[g(t')f_s(t')]$ (ignoring problems about its differentiability!):

$$q = \int_t^{t+\Delta t} dt' \left[g(t') f_s(t') \right] \quad = \quad \Delta t \left(\frac{g(t)f_s(t) + g(t+\Delta t) f_s(t+\Delta t)}{2} \right) + \mathcal{O}(\Delta t^3) \tag{5.71}$$

Clearly this makes no sense, and at no point was the statistics of f_s used. The evolution could not possibly depend on the stochastic function only at the end points.

Instead, need to do the integration-equivalent of the trapezoid derivation, but only $g(t')$ can come from an expansion:

$$\int_t^{t+\Delta t} dt' \, g(t') f_s(t') \quad = \quad \int_t^{t+\Delta t} dt' \left[g(t) + (t'-t) g'(t) + \frac{1}{2}(t'-t)^2 g''(t) + ... \right] f_s(t') \tag{5.72}$$

This isn't looking very promising for giving a simple trapezoid rule, because how to get a term like $g(t+\Delta t)$ times a random number out of this? However, try instead to do the expansion around the center point of the interval:

$$g(t') = g(\bar{t}\,) + (t' - \bar{t}\,) g'(\bar{t}\,) + \frac{1}{2}(t' - \bar{t}\,)^2 g''(\bar{t}\,) + ... \tag{5.73}$$

If there weren't any stochastic force multiplying this, its integral over the interval would drop out the first derivative term. That would leave

$$\int_t^{t+\Delta t} dt' \, g(t') = \Delta t \, g(\bar{t}\,) + \frac{1}{3!} \left(\frac{\Delta t}{2} \right)^3 g''(\bar{t}\,) + ... \tag{5.74}$$

It doesn't look like trapezoid, but it will become that, with the following expansions around the center point,

$$g(t+\Delta t) \quad = \quad g(\bar{t}\,) + \frac{\Delta t}{2} g'(\bar{t}\,) + \frac{1}{2} \left(\frac{\Delta t}{2} \right)^2 g''(\bar{t}\,) + ... \tag{5.75}$$

$$g(t) \quad = \quad g(\bar{t}\,) - \frac{\Delta t}{2} g'(\bar{t}\,) + \frac{1}{2} \left(\frac{\Delta t}{2} \right)^2 g''(\bar{t}\,) + ... \tag{5.76}$$

From which one has the result that will give the trapezoid rule:

$$g(\bar{t}\,) = \frac{1}{2}(g_n + g_{n+1}) - \frac{1}{2} \left(\frac{\Delta t}{2} \right)^2 g''(\bar{t}\,) + ... \tag{5.77}$$

Now include the stochastic function with the same central expansion, and integrate to get the push,

$$q \quad = \quad \int_t^{t+\Delta t} dt' \left\{ g(\bar{t}\,) + (t' - \bar{t}\,) g'(\bar{t}\,) + \frac{1}{2}(t' - \bar{t}\,)^2 g''(\bar{t}\,) + ... \right\} f_s(t') \tag{5.78}$$

Really, the first term here is the only one we want. The second term, though, is not necessarily zero when a stochastic force is present, however. But the same can be said for all the terms beyond that.

We already found the squared variance for this in the discussion of RK2 (this analysis here is really now very similar!). It is

$$\left\langle q^2 \right\rangle = 2\alpha k_B T \left\{ \Delta t \, g^2(\bar{t}\,) + \frac{2}{3}\left(\frac{\Delta t}{2}\right)^3 \left[(g'(\bar{t}\,))^2 + g(\bar{t}\,) g''(\bar{t}\,) \right] \right\} \tag{5.79}$$

Then the cubic terms are the error. To make this fit the trapezoid idea, though, $g(\bar{t}\,)$ comes from the trapezoid rule. So really one needs to use

$$\left\langle q^2 \right\rangle = 2\alpha k_B T \Delta t \, \left(\frac{g_n + g_{n+1}}{2} \right)^2 + \mathcal{O}(\Delta t^3) \tag{5.80}$$

To do the actual update with this, the push comes from the *same random number* w_n that was used in the predictor Euler step. It's the same time sequence, same time interval, for $f_s(t')$. The push must be replaced by

$$q \doteq \frac{1}{2}(g_n + g_{n+1}) \cdot (\sigma_a w_n). \tag{5.81}$$

So finally we can summarize the **second order Langevin Heun method**, which has first an Euler predictor step, over the whole interval,

$$\tilde{r}_{n+1} = r_n + f(t_n, r_n)\Delta t + g(t_n, r_n) \cdot (\sigma_a w_n) + \mathcal{O}(\Delta t^2) \tag{5.82}$$

Then the same random number gets used again in the corrector step, because it is the motion re-calculated (better) over the same time interval, via the trapezoid rule,

$$\begin{aligned} r_{n+1} &= r_n + \frac{1}{2}[f(t_n, r_n) + f(t_{n+1}, \tilde{r}_{n+1})]\Delta t \\ &+ \frac{1}{2}[g(t_n, r_n) + g(t_{n+1}, \tilde{r}_{n+1})] \cdot (\sigma_a w_n) + \mathcal{O}(\Delta t^3) \end{aligned} \tag{5.83}$$

One can see a good advantage of the Heun method over the RK2. It only needs one random number (triplet) per step, since it uses that same number twice. That makes it very efficient.