

Langevin equation for Brownian motion

Friday, February 13, 2009
12:02 PM

Homework 1 extended to Friday, February 20 at 12 PM.

We now proceed to the next level of complexity in describing Brownian motion. We'll try to build a model that is based on Newton's law rather than a random walk intuition.

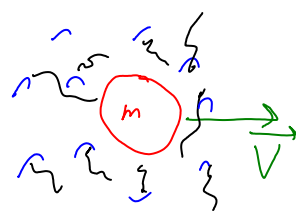
Reference: [Gardiner Sec. 1.2](#)

Recall that one peculiarity of our random walk model was that the velocity of the Brownian particle was not defined in the continuous-time limit of the random walk. On the one hand, this was useful because it explained why experimental measurements for velocity of Brownian particles were giving inconsistent results. Still, this is not theoretically satisfying because the laws of statistical mechanics and physics should still hold and the Brownian particle really should have a finite velocity.

Start with Newton's second law:

$$\frac{d\vec{V}}{dt} = \vec{V}$$

↑ velocity



$$m \frac{d\vec{V}}{dt} = -\gamma \vec{V} + \vec{F}_{th}(t)$$

↑ mass ↑ acceleration

↑ friction force (low Reynolds number)
↑ friction coefficient

↑ thermal force

The thermal force represents interactions with the water molecules with which the particle "collides."

How do we model the thermal force? If we try to represent it in full physical detail, then we would have to write down equations for where all the water molecules are and this would be very expensive. Sometimes this is done in molecular dynamics simulations for small pieces of proteins, etc. But this limits the size of the systems you can simulate and the times over which they can be simulated. This is because resolving the motion of the water molecules requires taking time steps on the order of 10^{-15} seconds.

If you want to simulate somewhat larger systems over reasonable time scales (microseconds), a very reasonable approach is to model the thermal force statistically. Rather than model the interactions with the surrounding water molecules in complete detail, simply represent the effects of the water molecules on the particle of interest in a statistical sense. That means we should develop a random model for the thermal force.

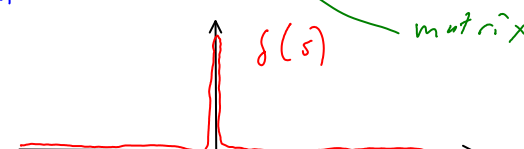
What should its properties be?

$$\langle \vec{F}_{th}(t) \rangle = 0$$

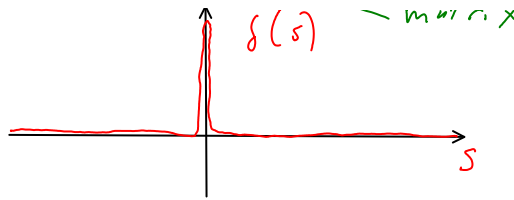
↑ because the mean component was already accounted for in the deterministic friction force.
The thermal force is just supposed to model the fluctuations about the deterministic component.

$$\langle \vec{F}_{th}(t) \otimes \vec{F}_{th}(t') \rangle = \text{Cov}(\vec{F}_{th}(t), \vec{F}_{th}(t'))$$

We use here the observation that the time scale over which a colliding water molecule interacts with the Brownian particle is something like 10^{-21} seconds. This is much faster than any practical observation or even molecular dynamics simulation. Together with the intuition that the thermal motion of different water molecules is not well correlated (more precisely, the thermal motion of particles influence the thermal motion of other particles that are within a few particle diameters). This means that on the scale of the particle of interest (typically tens, hundreds, thousand times bigger than the water molecules), the particle is feeling many brief collisions that have no correlation with each other. This suggests that the thermal force felt at different times should be essentially independent, and thus uncorrelated. This is represented physically as follows:

$$\langle \vec{F}_{th}(t) \otimes \vec{F}_{th}(t') \rangle = \int \delta(t-t')$$


↑ matrix



This is a little worrisome because it gives the thermal force an infinite variance! This is actually just an idealized approximation; of course the real thermal force has finite variance but the point of the statistical model is that the actual physical collision forces, because they are so short-lived and independent of each other, will have their effects well represented by this idealized model. This idealization is almost never refined in any practical classical mechanics model for microscopic motion in physics or biology. But it is refined when the statistical interaction is with larger objects like gels, turbulent structures, polymers.

This idealization will be fine provided that the time scales we are resolving are $\gtrsim 10^{-15}$ s (long compared to mean collision time)

Recall that our previous model for Brownian motion based on random walk approximations required that we did not resolve the motion below a time scale of

10^{-12} s molecules
 10^{-6} s collisions, microparticles

To complete our description of the thermal force model, we have to prescribe its probability distribution.

A Gaussian model for the random thermal force is an excellent approximation because the fact that the force results from many independent collisions over any resolvable time step means that the force is essentially the sum of a large number of independent mini-forces, and by the central limit theorem, this result should have a Gaussian (normal) distribution.

To summarize, the model for the thermal force is that

$$\vec{F}_{th}(t)$$

is a Gaussian random vector-valued function (just think of a large collection of jointly Gaussian random variables describing the components of the force at various moments of time).

with mean: $\langle \vec{F}_{th}(t) \rangle = \vec{0}$

covariance (aka correlation function): $\langle \vec{F}_{th}(t) \otimes \vec{F}_{th}(t') \rangle = \mathcal{L} \delta(t-t')$

and for an isotropic Brownian motion: $\mathcal{L} = g \mathcal{I}$
↑ identity matrix

This provides a complete description of the thermal force (this kind of model is known as **white noise**)

How do we work with such white noise forces in differential equations:

Many physicists just proceed by working formally with these thermal forces with correlation function represented by Dirac delta function.

- see **Risken, Fokker-Planck Equation**
- this is fine except when subtleties arise and you have to be careful to avoid making a mistake.

Mathematicians (and some applied practitioners as well) prefer to use the language of stochastic differential equations which is really no more difficult to work with but helps clarify what to do in situations with subtleties.

How do we transfer our set of equations into the framework of stochastic differential equations:

Note that the thermal force as prescribed above could be represented in terms of the Wiener process as follows:

$$\vec{F}_{th}(t) = \sqrt{g} \frac{d\vec{W}(t)}{dt}$$

Now, nothing here really makes sense; the left hand side has infinite variance, the right hand side involves the derivative of a nowhere differentiable function.

One has a similar situation with Feynman path integrals in theoretical physics:

$$\frac{1}{Z} \int f(\vec{w}(t)) e^{-\beta \int_0^t \left(\frac{d\vec{w}}{dt'}\right)^2 dt'} d\{\vec{w}(t)\}$$

Three things here are not even defined yet it's a computational tool.

Back to our thermal force, again the idealized delta-correlated forces are strictly unphysical yet yield useful results...we can see this more clearly by observing how these delta-correlated forces can be seen as the limit of a more physical model with finite variance for the force.

To see this, let's approximate:

$$\vec{F}_{th}^{ot}(t) = \sqrt{g} \frac{\vec{w}(t+\delta t) - \vec{w}(t)}{\delta t}$$

This is a smoothed version of the idealized thermal force.

This is still a Gaussian random function because it's a deterministic linear combination of Gaussian random variables.

$\{\mathcal{I}_j\}$ jointly Gaussian $\Rightarrow c_0 + \sum c_j \mathcal{I}_j$ also Gaussian for deterministic c_j

$$\begin{aligned} \langle \vec{F}_{th}^{ot}(t) \rangle &= \langle \sqrt{g} \frac{\vec{w}(t+\delta t) - \vec{w}(t)}{\delta t} \rangle \\ &= \frac{\sqrt{g}}{\delta t} (\langle \vec{w}(t+\delta t) \rangle - \langle \vec{w}(t) \rangle) \end{aligned}$$

$$\left(\mathbb{E} \left(c_0 + \sum_j c_j \mathcal{I}_j \right) = c_0 + \sum_j c_j \mathbb{E} \mathcal{I}_j \right)$$

for deterministic $\{c_j\}$

$$= \frac{\sqrt{g}}{\delta t} (\vec{0}) = \vec{0}$$

$$\langle \vec{F}_{th}^{ot}(t) \otimes \vec{F}_{th}^{ot}(t') \rangle =$$

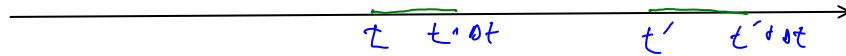
$$\left(\vec{0} \otimes \vec{0} \right) = \vec{0}$$

$$-\Gamma_{th}(t) \otimes \Gamma_{th}(t)'$$

$$= \left\langle \left(\sqrt{g} \frac{\vec{W}(t+\Delta t) - \vec{W}(t)}{\Delta t} \otimes \sqrt{g} \frac{\vec{W}(t'+\Delta t) - \vec{W}(t')}{\Delta t} \right) \right\rangle$$

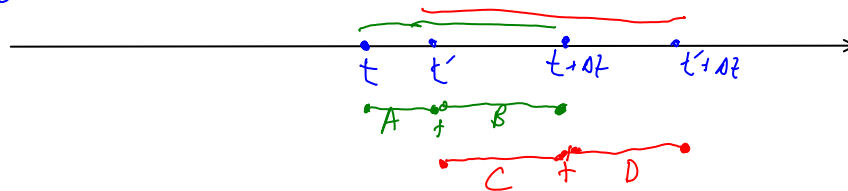
$$= \frac{g}{(\Delta t)^2} \langle (\vec{W}(t+\Delta t) - \vec{W}(t)) \otimes (\vec{W}(t'+\Delta t) - \vec{W}(t')) \rangle$$

$$|t-t'| > \Delta t$$



covariance = 0 since increments nonoverlapping so independent

$$t < t' < t+\Delta t$$



$$\langle \vec{F}_{th}(t) \otimes \vec{F}_{th}(t') \rangle = \frac{g}{(\Delta t)^2} \langle (A+B) \otimes (C+D) \rangle$$

$$= \frac{g}{(\Delta t)^2} \langle A \otimes C \rangle + \langle A \otimes D \rangle + \langle B \otimes C \rangle + \langle B \otimes D \rangle$$

non overlapping increments independent

$$= \langle (\vec{W}(t+\Delta t) - \vec{W}(t')) \otimes (\vec{W}(t+\Delta t) - \vec{W}(t')) \rangle$$

$$= \frac{g |t+\Delta t - t'|}{(\Delta t)^2} \Delta t$$

Variance of the increment of a component of the Wiener process is equal to the length of the interval, and the Wiener process in different directions is independent.