

## PDE perspective on Langevin equation

Friday, March 06, 2009  
12:05 PM

From last time, we integrated then averaged the solution to the Langevin model for Brownian motion:

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

$$m d\vec{V} = -\gamma \vec{V} dt + \sqrt{2\gamma k_B T} d\vec{W}(t)$$

to obtain mean and correlation function of the velocity as well as the mean and covariance of the position of the Brownian particle, which we wrote down explicitly at long time:

$$\langle \vec{X}(t) \rangle = \langle \vec{X}(0) \rangle + \langle \vec{V}(0) \rangle \frac{m}{\gamma} (1 - e^{-\gamma/m t})$$

$$\text{Cov}(\vec{X}(t), \vec{X}(t)) = \frac{2k_B T t}{\gamma} \text{ (bounded)} + O(1)$$

So we see that at long times, the particle position behaves just like our simpler continuous model for Brownian motion

$$d\vec{X} = \sqrt{2D} d\vec{W}(t)$$

because the mean of the position is shifted by only a finite amount (which looks negligible compared to the growth in the random component of the position with time) and the particle position in the Langevin equation has a diffusive behavior in time, meaning the covariance of the particle position grows linearly with time. In fact the global (long-time) diffusivity of the particle in the Langevin model is just:

$$D = \lim_{t \rightarrow \infty} \frac{\text{Cov}(\vec{X}(t), \vec{X}(t))}{2t}$$

$$D = \frac{k_B T}{\gamma} \text{ (Einstein relation)}$$

with isotropic diffusivity constant

$$D = \frac{k_B T}{\gamma} \quad \text{Einstein relation}$$

This is not however the way that Einstein derived this relation --- this is a rederivation using the techniques of Langevin, Ornstein, Uhlenbeck.

A very important point that has applicability to much modern research on more complex stochastic systems is how the Langevin model is and can be related to the simpler Brownian motion model just involving the Wiener process.

We'll do this more systematically next lecture but for now, let's look at the basic way in which the solution to the Langevin model differs from solution to the simpler Wiener process model -- they have similar behavior at long time. But what about at short time?

Wiener process model has short-time behavior:

$$\langle \vec{x}(t) \rangle = \langle \vec{x}(0) \rangle$$

$$\text{Cov}(\vec{x}(t), \vec{x}(t)) = 2Dt \mathbb{1} + \text{Cov}(\vec{x}(0), \vec{x}(0))$$

Langevin equation model?

$$\langle \vec{x}(t) \rangle = \langle \vec{x}(0) \rangle + \langle \vec{v}(0) \rangle \frac{m}{\gamma} (1 - (1 - \frac{\gamma}{m}t + O(t^2)))$$

$$= \langle \vec{x}(0) \rangle + \langle \vec{v}(0) \rangle t + O(t^2)$$

$$\text{Cov}(\vec{x}(t), \vec{x}(t)) = ?$$

For short times  $\vec{v}(t) \approx \vec{v}(0)$

$$t \ll m/\gamma$$

↑  
time scale on which velocity decorrelates

$$\vec{x}(t) \approx \vec{x}(0) + \vec{v}(0)t + O(t^2)$$

$$\text{Cov}(\vec{x}(t), \vec{x}(t)) = \text{Cov}(\vec{x}(0) + \vec{v}(0)t, \vec{x}(0) + \vec{v}(0)t) + O(t^2)$$

$$= \text{Cov}(\vec{x}(0), \vec{x}(0))$$

$$+ \text{Cov}(\vec{x}(0), \vec{v}(0))t$$

$$+ \text{Cov}(\vec{v}(0), \vec{x}(0))t$$

$$+ \text{Cov}(\vec{v}(0), \vec{v}(0))t^2$$

$$+ O(t^2) \rightarrow O(t^3) \text{ in thermal equi!}$$

(equipartition)

$$k_B T / m$$

To make sense of this suppose that we are observing a particle which is in thermal equilibrium already at time 0, then we can use the probability distribution for the state variables of the system in thermal equilibrium for the initial values of position and velocity:

$$P(\vec{x}, \vec{v})$$

$$P_{\vec{x}, \vec{v}}(\vec{x}, \vec{v}) = \frac{\exp\left(-\frac{1}{2} \frac{m |\vec{v}|^2}{k_B T}\right)}{Z}$$

$Z$  ← normalizing factor

In thermal equilibrium, the particle position is uniformly distributed over the domain, the velocity has a Gaussian distribution, and the initial position and velocity are independent of each other. Our expression then simplifies to:

$$\text{Cov}(\vec{X}(t), \vec{X}(t)) = \text{Cov}(\vec{X}(0), \vec{X}(0)) + \frac{k_B T}{m} t^2 + O(t^3)$$

$t^2$  ballistic scaling

One can show through careful consideration of all the error terms, that in thermal equilibrium, this short-time approximation is valid for

$$t \ll m/\gamma$$

whereas the long-time asymptotics (with diffusive behavior that we saw before) is accurate when

$$t \gg m/\gamma$$

Putting our observations together, we make the following conclusions:

- The behavior of the particle position in the Langevin model behaves very similarly to the particle position in the simpler Wiener process model at long times

$$(t \gg m/\gamma)$$

The Langevin equation model differs however from the Wiener process model on time scales

$$t \lesssim m/\gamma$$

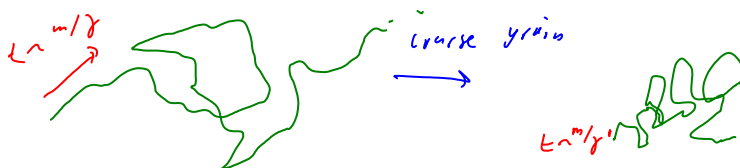
The source of this difference is that by tracking the momentum dynamics of the particle, and thereby taking inertia into account, and therefore keeps the velocity of the Brownian particle correlated for a period of time  $\sim m/\gamma$

The Langevin equation model also has built into it that the friction force (and thermal fluctuations) will together cause the velocity to decorrelate on longer time scales and therefore, on these longer time scales to behave as if the particle position were undergoing independent increments.

Recall from last time that for a micron-size particle (typical microfluidic, colloidal systems, cellular level)

$$m/\gamma \sim 10^{-7} \text{ s}$$

$$\text{small molecules: } m/\gamma \sim 10^{-10} \text{ s}$$



So this basically says that the Langevin equation model is an improvement of the simpler Wiener process model in that:

- it's more physically based (Newton's law)
- for practical purposes, it is more accurate when describing dynamics on time scales  $\lesssim m/\gamma$

Therefore, for practical purposes, one should use the simpler Wiener process model if one is interested in dynamics only on time scales large compared to this momentum decorrelation time scale, and use the more detailed Langevin equation model if these short time scales are relevant and accessible to the system of interest.

Later developments spurred by numerical simulations around 1960 show that the Langevin equation model does not quite properly describe the autocorrelation function of the velocity -- first homework problem touches on how to correct that for hydrodynamic interactions. For practical purposes, this does not have serious consequences for the dynamics of the **position** of the Brownian particle, and so the basic Langevin equation is still generally used even in some molecular dynamics simulations. One reason is that to take into account the hydrodynamic corrections requires a much more complicated equation with memory.

### PDE (Eulerian) perspective on Langevin dynamics

In general, a system of stochastic differential equations can always be associated rigorously (with some technical conditions) to a deterministic partial differential equation describing the dynamics of the probability density for the state variables.

Reference: Gardiner Secs. 3.4-3.6

Given a system of Ito stochastic differential equations in vector form:

$$d\vec{Y} = \underbrace{\vec{a}(\vec{Y}, t)}_{\text{vector (drift)}} dt + \underbrace{\mathcal{L}(\vec{Y}, t)}_{\text{matrix function}} \cdot \underbrace{d\vec{W}(t)}_{\text{Wiener process}}$$

The dynamics of the probability density of  $\vec{Y}$  is given by the **forward Kolmogorov (Fokker-Planck) equation**:

$$\frac{\partial p(\vec{y}; t)}{\partial t} = -\vec{\nabla} \cdot (\vec{a}(\vec{y}, t) p(\vec{y}, t)) + \frac{1}{2} \vec{\nabla} \cdot \vec{\nabla} : (\mathcal{B}(\vec{y}, t) p(\vec{y}, t))$$

↘ correction after lecture

$p(\vec{y}; t)$  is PDF for  $\vec{Y}(t)$

$$p(\vec{y}; t) = P_{\vec{Y}(t)}(\vec{y})$$

$\mathcal{B}(\vec{y}; t)$  is local diffusivity matrix

$$\mathcal{B} = \begin{pmatrix} 1 \\ 2 \end{pmatrix} \mathcal{L} \mathcal{L}^T \leftarrow \text{transpose}$$

$\vec{\nabla} \otimes \vec{\nabla}$  — ↘ correction after lecture

$$\vec{\nabla} \cdot \vec{\nabla} : (\mathcal{B}(\vec{y}, t) p(\vec{y}, t))$$

$$= \sum_{i,j} \frac{\partial}{\partial y_i} \frac{\partial}{\partial y_j} (\mathcal{B}_{ij}(\vec{y}, t) p(\vec{y}, t))$$

$$a : \mathcal{B} \equiv a_{ij} \mathcal{B}_{ij}$$

So let's apply this to Langevin equation:

$$\vec{Y} = \begin{pmatrix} \vec{x} \\ \vec{v} \end{pmatrix}$$

$$d \begin{pmatrix} \vec{x} \\ \vec{v} \end{pmatrix} = \begin{pmatrix} \vec{v} \\ -\frac{\gamma}{m} \vec{v} \end{pmatrix} dt + \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{\frac{2k_B T \gamma}{m}} d\vec{W}(t) \end{pmatrix}$$

$\vec{a}(\vec{x}, \vec{v})$        $\mathcal{B}(\vec{x}, \vec{v})$

6 components!

3x3 block matrices

$$\frac{\partial p(\vec{x}, \vec{v}; t)}{\partial t} = - \left( \vec{\nabla}_x \cdot (\vec{v} p(\vec{x}, \vec{v}; t)) + \vec{\nabla}_v \cdot \left( -\frac{\gamma \vec{v}}{m} p(\vec{x}, \vec{v}; t) \right) \right) + \vec{\nabla}_v \vec{\nabla}_v : \left( \frac{k_B T \gamma}{m^2} p(\vec{x}, \vec{v}; t) \right)$$

$$\mathcal{B}(\vec{x}, \vec{v}, t) = \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & \frac{\sqrt{2k_B T \gamma}}{m} d \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & \frac{\sqrt{2k_B T \gamma}}{m} d \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & \frac{2k_B T \gamma}{m^2} d \end{pmatrix}$$

$\mathcal{B}^{xx}$        $\mathcal{B}^{xv}$   
 $\mathcal{B}^{vx}$        $\mathcal{B}^{vv}$

Note that this local diffusivity matrix only has nonzero entries corresponding to the vv block.

$$\vec{\nabla} \vec{\nabla} : (\mathcal{B} p) = \vec{\nabla}_x \vec{\nabla}_x : (\mathcal{B}^{xx} p) + \vec{\nabla}_x \vec{\nabla}_v : (\mathcal{B}^{xv} p) + \vec{\nabla}_v \vec{\nabla}_x : (\mathcal{B}^{vx} p) + \vec{\nabla}_v \vec{\nabla}_v : (\mathcal{B}^{vv} p)$$

$\frac{2k_B T \gamma}{m^2}$