

Applications of the Fokker-Planck (Forward Kolmogorov) Equation

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12:08 PM

From last time, the probability density function for the position and velocity of a Brownian particle under the Langevin model is:

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

Laplacian

This is the **Fokker-Planck equation** for the Langevin model, describes how the probability density of the state variables evolves in time.

This equation can actually be solved exactly using, for example, Fourier transform with respect to both variables, which gives a first order PDE in Fourier space, then solve this by method of characteristics. This is a long computation -- see the article by **Chandrasekhar Sec. 4, iii** (who does it in an even more confusing way).

The result is (assuming the initial data is either deterministic or Gaussian):

$$p(\vec{x}, \vec{v}; t) = \frac{1}{(2\pi)^d \sqrt{\det C_v \det C_x}} \exp \left(-\frac{1}{2} \begin{pmatrix} \vec{v} - \vec{\mu}_v(t) \\ \vec{x} - \vec{\mu}_x(t) \end{pmatrix} \cdot \begin{pmatrix} C_{vv}(t) & C_{v\vec{x}}(t) \\ C_{\vec{x}v}(t) & C_{\vec{x}\vec{x}}(t) \end{pmatrix}^{-1} \cdot \begin{pmatrix} \vec{v} - \vec{\mu}_v(t) \\ \vec{x} - \vec{\mu}_x(t) \end{pmatrix} \right)$$

where

$$\vec{\mu}_{\vec{x}}(t) = \langle \vec{X}(t) \rangle$$

$$\vec{\mu}_v(t) = \langle \vec{V}(t) \rangle$$

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

$$C_{\vec{x}v}(t) = \text{Cov}(\vec{X}(t), \vec{V}(t))$$

etc.

where the right hand sides are just the exact formulas that we derived directly from the stochastic differential equation, however, you do not actually solve the SDE's to get these expressions.

This just says that solving the Fokker-Planck equation gives consistent results with solving the stochastic differential equation exactly, in that, under the assumptions about the initial data, the solution for the PDF has a Gaussian form with mean and covariance structure agreeing with what we obtained from the solution of the SDE. Obtaining this exact solution is less work using the SDE approach than the PDE approach for most people.

The Fokker-Planck approach, however, can become very useful when we look at more complex problems.

Let's add some sort of external force on the Brownian particle.

- electrostatic
- gravity
- attraction or binding energy to a surface
- laser trap
- cargo with spring

The external force changes the Langevin equation model in a straightforward way since it's based on Newton's laws:

$$m d\vec{V} = (-\gamma \vec{V} + \vec{F}(\vec{X}, t)) dt + \sqrt{g} d\vec{W}$$

↑ external force

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

Note that we have reverted to putting an unknown constant in front of the white noise term because it's not clear a priori that the thermal force will be the same when the system is also feeling another force.

Let's try to fix the amplitude of the thermal noise by the same fluctuation-dissipation argument as before, which is that in thermal equilibrium, we should have:

$$p(\vec{x}, \vec{v}; t) = \frac{1}{Z} \exp\left(-\frac{E(\vec{x}, \vec{v})}{k_B T}\right) \equiv p_s(\vec{x}, \vec{v})$$

where $E(\vec{x}, \vec{v})$ is energy of system.

This approach can only work when the external force has a conservative, time-independent form

$$\vec{F} = \vec{F}(\vec{x}) = -\vec{\nabla} \phi(\vec{x})$$

↑ potential energy

Then $E(\vec{x}, \vec{v}) = \frac{1}{2} m |\vec{v}|^2 + \phi(\vec{x})$

What value of g will ensure that the probability distribution for the state variables will be consistent with this thermal equilibrium? Not clear how to do this from the SDE perspective because with a nonharmonic potential, we can't solve the SDE's exactly!

But we can do a simple calculation using the Fokker-Planck formulation.

$$\begin{aligned} \frac{\partial p(\vec{x}, \vec{v}; t)}{\partial t} = & -\vec{\nabla}_v \cdot \left[\left(\frac{-\gamma \vec{v}}{m} - \frac{\vec{\nabla} \phi(\vec{x})}{m} \right) p(\vec{x}, \vec{v}; t) \right] \\ & - \vec{\nabla}_x \cdot \left(\vec{v} p(\vec{x}, \vec{v}; t) \right) \\ & + \frac{1}{2} \vec{\nabla}_v \vec{\nabla}_v : \left(\left(\frac{\sqrt{g}}{m} d \right) \left(\frac{\sqrt{g}}{m} d \right)^T p(\vec{x}, \vec{v}; t) \right) \end{aligned}$$

↑ coefficient of noise term only in v eqn.

Simplify:

$$\frac{\partial p(\vec{x}, \vec{v}; t)}{\partial t} = -\vec{\nabla}_v \cdot \left[\frac{(-\gamma \vec{v} - \vec{\nabla} U(\vec{x}))}{m} p(\vec{x}, \vec{v}; t) \right] - \vec{\nabla}_x \cdot (\vec{v} p(\vec{x}, \vec{v}; t)) + \frac{g}{2m^2} \underbrace{(\partial_v)}_{= \vec{\nabla}_v \cdot \vec{v}} p(\vec{x}, \vec{v}; t)$$

This is the Fokker-Planck equation for the position and velocity of a Brownian particle subjected to a conservative force; it is also known as the **Klein-Kramers** equation.

Just like you can't solve the SDE exactly, you can't solve this PDE exactly when the potential is not harmonic. But you can still use it to figure out what g must be through a self-consistency check.

When you plug in the Gibbs-Boltzmann thermal equilibrium distribution into the Fokker-Planck equation, it should be a self-consistent steady solution.

$$\begin{aligned} 0 &= \vec{\nabla}_v \cdot \left[\left(\frac{-\gamma \vec{v} - \vec{\nabla} U(\vec{x})}{m} + \frac{g}{2m^2} \vec{\nabla}_v \right) p_s(\vec{x}, \vec{v}) \right] - \vec{\nabla}_x \cdot (\vec{v} p_s(\vec{x}, \vec{v})) \\ &= \vec{\nabla}_v \cdot \left[\left(\frac{\gamma \vec{v}}{m} + \frac{\vec{\nabla} U(\vec{x})}{m} + \frac{g}{2m^2} \underbrace{(-\vec{\nabla}_v \frac{E(\vec{x}, \vec{v}))}{k_B T}}_{= m \vec{v}} \right) p_s(\vec{x}, \vec{v}) \right] + \vec{v} \cdot \left(- \underbrace{(-\vec{\nabla}_x \frac{E(\vec{x}, \vec{v}))}{k_B T})}_{= \vec{\nabla} U} p_s(\vec{x}, \vec{v}) \right) \\ &= \vec{\nabla}_v \cdot \left[\left(\frac{\gamma \vec{v}}{m} + \underbrace{\frac{\vec{\nabla} U(\vec{x})}{m}}_{\text{expand this}} - \frac{g \vec{v}}{2m k_B T} \right) p_s(\vec{x}, \vec{v}) \right] + \frac{\vec{v}}{k_B T} \cdot \vec{\nabla} U(\vec{x}) p_s(\vec{x}, \vec{v}) \\ &= \vec{\nabla}_v \cdot \left[\left(\frac{\gamma \vec{v}}{m} - \frac{g \vec{v}}{2m k_B T} \right) p_s(\vec{x}, \vec{v}) \right] + \frac{\vec{\nabla} U(\vec{x})}{m} \cdot \underbrace{\vec{\nabla}_v p_s(\vec{x}, \vec{v})}_{= -\frac{m \vec{v}}{k_B T} p_s(\vec{x}, \vec{v})} + \frac{\vec{v}}{k_B T} \cdot \vec{\nabla} U(\vec{x}) p_s(\vec{x}, \vec{v}) \\ \text{Cancel } (& \left[\frac{\vec{\nabla} U(\vec{x})}{m} \cdot \left(-\frac{m \vec{v}}{k_B T} p_s(\vec{x}, \vec{v}) \right) + \frac{\vec{v}}{k_B T} \cdot \vec{\nabla} U(\vec{x}) p_s(\vec{x}, \vec{v}) \right] \\ 0 &= \vec{\nabla}_v \cdot \left[\left(\frac{\gamma \vec{v}}{m} - \frac{g \vec{v}}{2m k_B T} \right) p_s(\vec{x}, \vec{v}) \right] \end{aligned}$$

This will be satisfied provided that

$$\frac{\gamma}{m} = \frac{g}{2m k_B T}$$

$$g = 2\gamma k_B T$$

This is the same relationship we had before; and we have shown through a direct calculation that the presence of the external force does not modify it.

This **fluctuation-dissipation** relationship between the amplitude of the thermal noise term and the friction coefficient is here rigorously derived for a conservative, steady external force. This relationship is generally assumed to hold also when the external force varies in time, provided the time variation is gradual enough.

Can we develop a coarse-grained version of the Langevin equation with external force, just like the Wiener process model was a coarse-grained version of the Langevin equation without external force?

First we'll proceed intuitively then back this up later through a mathematical calculation.

Intuition: Start with the deterministic version without thermal noise. One can show that, provided the external force is either steady or varies slowly in time, that the behavior of the deterministic system:

$$\begin{aligned} m \frac{d\vec{V}}{dt} &= -\gamma \vec{V} + \vec{F}(\vec{X}, t) \\ \frac{d\vec{X}}{dt} &= \vec{V} \end{aligned}$$

approaches at long times the solution of the reduced (**overdamped**) system:

$$\frac{d\vec{X}}{dt} = \frac{\vec{F}(\vec{X}, t)}{\gamma}$$

Intuition: the inertia term $m \frac{d\vec{V}}{dt} \approx 0$

The amount of time you have to wait for this overdamped approximation to be accurate depends on the friction, and the greater the friction, the shorter amount of time you have to wait. For microscale applications, friction tends to be very strong in some suitably normalized sense.

Two interesting talks: **John Bush** Monday, March 30 at 4 PM: cool things with fluids and maybe critters.

Paul Atzberger Tuesday, March 24 at 4 PM in Amos Eaton 216, discussing stochastic modeling of microfluid systems (membranes and polymers in biological setting)

Let's just try (it turns out to be correct, as we'll show later) to just add together the coarse-grained deterministic model with the Wiener process model:

$$d\vec{X} = \frac{\vec{F}(\vec{X}, t)}{\gamma} dt + \sqrt{2D} d\vec{W}(t)$$

diffusivity

We'll show later how to derive this as a coarse-grained approximation to the Langevin model with external force, but for now let's take it as given.

Is it still true that the diffusivity is related to the friction as it was in the absence of external force?

$$D = \frac{k_B T}{\gamma} ?$$

We'll check this in the same way as we obtained the fluctuation-dissipation relation for the Langevin equation with force.

Write down the Fokker-Planck equation corresponding to our reduced model.

$$\frac{\partial p(\vec{x}, t)}{\partial t} = -\vec{\nabla}_x \cdot \left(\frac{\vec{F}(\vec{x}, t)}{\gamma} p(\vec{x}, t) \right) + \frac{1}{2} \vec{\nabla}_x \cdot \vec{\nabla}_x : (\overline{\Delta \Delta}) (\overline{\Delta \Delta})^T p(\vec{x}, t)$$

$$\frac{\partial p(\vec{x}, t)}{\partial t} = -\vec{\nabla}_x \cdot \left(\frac{\vec{F}(\vec{x}, t)}{\gamma} p(\vec{x}, t) \right) + D \Delta_x p(\vec{x}, t)$$

Smoluchowski equation 1906

Now we will try to derive a relationship between the diffusivity and other parameters by again insisting that the stationary probability distribution agrees with the laws of equilibrium statistical mechanics.

$$p_s(\vec{x}) = \frac{\exp\left(-\frac{E(\vec{x})}{k_B T}\right)}{Z}$$

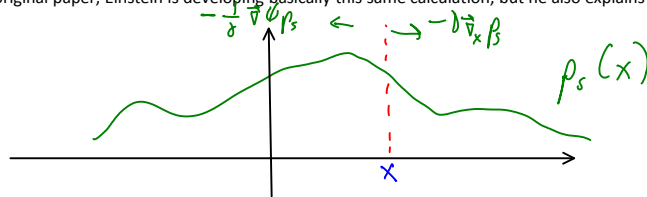
$$E(\vec{x}) = \mathcal{U}(\vec{x})$$

(for the case $\vec{F} = -\vec{\nabla} \mathcal{U}(\vec{x})$)

$$0 = -\vec{\nabla}_x \cdot \left(-\frac{\vec{\nabla} \mathcal{U}}{\gamma} p_s \right) + D \Delta_x p_s$$

$$0 = \vec{\nabla}_x \cdot \left(\underbrace{\frac{1}{\gamma} \vec{\nabla} \mathcal{U} p_s}_{\text{force-induced flux}} + \underbrace{D \vec{\nabla}_x p_s}_{\text{diffusive flux}} \right)$$

In his original paper, Einstein is developing basically this same calculation, but he also explains it through some intuition.



$$0 = \vec{\nabla}_x \cdot \left(\frac{1}{\gamma} \vec{\nabla} \mathcal{U} p_s + D \left(-\frac{\vec{\nabla} \mathcal{U}}{k_B T} \right) p_s \right)$$

$$D = \frac{k_B T}{\gamma}$$

Einstein relation 1905

Boltzmann's constant $k = R = \text{ideal gas constant}$

Boltzmann's constant $k_B = \frac{R}{N_A}$ = ideal gas constant
Avogadro number

$$D = \frac{RT}{N_A \delta}$$

$$N_A = \frac{RT}{D \delta}$$