Stochastic Mode Reduction: From Klein-Kramers to Smoluchowski Equation

Tuesday, March 24, 2009
11:58 AM

Talk relevant to class today at 4 PM in Amos Eaton 216:

Paul Atzberger will talk about stochastic and computational modeling of microbiological systems (membranes, polymers)

We now visit the question of: How is the Langevin model that takes into account momentum/velocity fluctuations

$$m\,d\vec{V} = \left(-\gamma \vec{V} + \vec{F}_{ext}(\vec{X})\right) dt + \sqrt{2\gamma k_B T}\, d\vec{W}(t)$$

$$d\vec{X} = \vec{V}\,dt \qquad \text{Langevin}$$

related to the simpler model that just takes into account the position variable

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

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

We can check for the exact solutions in the absence of the external force that

$$\lim_{\frac{\gamma}{m}\to\infty} \langle \vec{X}^{(L)}(t)\rangle = \langle \vec{X}^{(S)}(t)\rangle$$

$$\lim_{\frac{\gamma}{m}\to\infty} \frac{\mathrm{Cov}(\vec{X}^{(L)}(t), \vec{X}^{(L)}(t))}{2t} = \frac{\mathrm{Cov}(\vec{X}^{(S)}(t), \vec{X}^{(S)}(t))}{2t} = D\,\mathcal{I}$$

and both solutions are Gaussian if the initial data is Gaussian.

$\vec{X}^{(L)}(t)$: solution to Langevin

$\vec{X}^{(S)}(t)$: solution to Smoluchowski equation

So the observation is that the force-free Langevin equation appears to approach the behavior of the force-free Smoluchowski equation (which is just the Wiener process model) when friction becomes large or mass becomes small.

We want to see whether this kind of connection can be extended to the case with an external force where we don't have the exact solutions to look at.

Many books do this connection and call it "inverse friction expansion" or "small mass expansion" of the Langevin equation or the associated Fokker-Planck equation known as the Klein-Kramers equation. This is actually a little bit weird and limiting because what does it mean for friction to be large or mass to be small?

The problem is that γ, m, $\frac{\gamma}{m}$

are all dimensional quantities and so their "size" is ambiguous as it depends on measuring units.

This points out the importance of conducting and interpretation perturbation theories in terms of nondimensional quantities. Lin and Segel, Mathematics Applied to Deterministic Problems in the Natural Sciences
also Barenblatt, Scaling, Self-Similarity, and Intermediate Asymptotics

From this point of view, the better way to think of the connection between the force-free Langevin equation and the force-free Smoluchowski equation is that the former is well approximated by the latter when

$$\frac{\gamma t}{m} \to \infty$$

nondimensional

This can be checked directly from the tediously derived exact solution.

You'll asked to show this by using a PDE-based perturbation theory approach which mirrors what we will do in the case of an external force on HW3.

So we now proceed to consider how the two equations are related to each other when external force is present. Here we can't generally solve the equations exactly but we can use perturbation techniques combined with dimensional analysis to make the connection even though we can't solve the equations exactly. For the extension of this procedure to a more complicated setting with interacting particles with thermal forces, see my paper with Andy Majda called "Stochastic Mode reduction for particle-based methods."

The approach I will use is a little different than what you see in textbooks under the phrase "adiabatic elimination of fast variables" which often use ad hoc shortcuts, etc....I prefer to be systematic.

To prepare properly for a perturbation theory, we first nondimensionalize carefully.

Begin by accounting for all governing parameters and variables and their dimensions.

Typically perturbation methods (Holmes, Introduction to Perturbation Methods as well as Lin and Segel)
for stochastic problems are most easily done on the associated partial differential equations (like the Fokker-Planck equation) rather than the system of stochastic differential equations.

So we want to show then, how the Klein-Kramers equation (which is the Fokker-Planck equation for the Langevin model with external force)

$$\begin{aligned}\frac{\partial p_{\vec{X},\vec{V}}}{\partial t}(\vec{x},\vec{v};t) = &-\vec{\nabla}_x \cdot \left(\vec{v}\, p_{\vec{X},\vec{V}}\right) \\ &- \vec{\nabla}_v \cdot \left(\left(-\frac{\gamma \vec{v}}{m} + \frac{\vec{F}_{ext}(\vec{x})}{m}\right) p_{\vec{X},\vec{V}}\right) \\ &+ \frac{\gamma k_B T}{m^2} \Delta_v\, p_{\vec{X},\vec{V}}\end{aligned}$$

can be approximated by (and under what circumstances) the Smoluchowski equation which is the Fokker-Planck equation associated to the stochastic model that just takes into account the position variable

$$\frac{\partial p_{\vec{X}}(\vec{x};t)}{\partial t} = -\vec{\nabla}_x \cdot \left(\frac{\vec{F}_{ext}(\vec{x})}{m}\, p_{\vec{X}}\right) + D\,\Delta_x\, p_{\vec{X}}$$

$$D = k_B T/\gamma$$

$$p_{\vec{X}}(\vec{x};t) = \int_{\mathbb{R}^3} p_{\vec{X},\vec{V}}(\vec{x},\vec{v};t)\, d\vec{v}$$

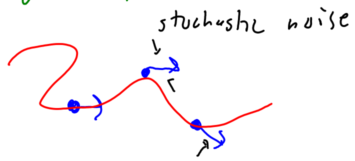
marginal PDF

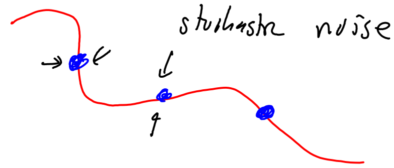
joint PDF

marginal PDF $\qquad\qquad$ joint PDF

This is a coarse-graining projection that retains information about the position of the particle but not its velocity.

Langevin / Klein-Kramers $\qquad\qquad\qquad\qquad$ Smoluchowski





Let's start with the Klein-Kramers equation and see if we can obtain the Smoluchowski equation as some sort of asymptotic description in some certain limit.

Begin by accounting for the variables, parameters, and dimensions in the Klein-Kramers equation. We'll ignore the initial data because that will get forgotten eventually and is irrelevant if we just start observing the system in thermal equilibrium.

Variables and parameter and dimension accounting:

$$[\vec{x}] = \mathcal{L} \qquad \text{length}$$
$$[t] = \mathcal{T} \qquad \text{time}$$
$$[\vec{v}] = \mathcal{L}/\mathcal{T}$$
$$[m] = \mathcal{M}$$
$$[\gamma] = \mathcal{M}/\mathcal{T}$$
$$[k_B T] = \mathcal{M}\frac{\mathcal{L}^2}{\mathcal{T}^2}$$
$$[\vec{F}] = \mathcal{M}\frac{\mathcal{L}}{\mathcal{T}^2}$$
$$[\ell_F] = \mathcal{L}$$

(dimensional consistency)

$$\left[\frac{\partial \rho_{\vec{x},\vec{v}}}{\partial t}\right] = \left[\vec{\nabla}_v \cdot \left(-\frac{\gamma \vec{v}}{m}\rho_{\vec{x},\vec{v}}\right)\right]$$

$$\frac{\cancel{[\rho_{\vec{x},\vec{v}}]}}{[t]} = [\vec{\nabla}_v]\left[\frac{\gamma \vec{v}}{m}\right]\cancel{[\rho_{\vec{x},\vec{v}}]}$$

$$\frac{1}{\mathcal{T}} = \frac{1}{\mathcal{L}/\mathcal{T}}\,\frac{[\gamma]\;\mathcal{L}/\mathcal{T}}{\mathcal{M}}$$

$$[\gamma] = \mathcal{M}/\mathcal{T}$$

The external force is a given function...how do we extract dimensional quantities from a function?

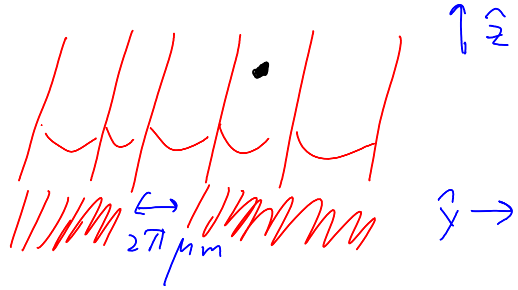
Typically to a given function, we can associate two scales -- one associated to its amplitude and one associated to its scale of variation. For the case of the external force, we could try to associate to it a force amplitude and a length scale on which the force varies.

$$\vec{F}(\vec{x}) = \bar{F}\,\vec{f}(\vec{x}/\ell_F)$$

force amplitude $\qquad$ length scale of the f force amplitude

force

Example: $\vec{F}(\vec{x}) = -30\ pN\ \hat{z}\left(\cos\left(\frac{\hat{y}\cdot\vec{x}}{1\ \mu m}\right)+1\right)$



$$\bar{F} = 30\ pN$$

$$l_F = 1\ \mu m$$

$$\vec{f}(\vec{x}') = -\hat{z}\left(\cos\left(\hat{y}\cdot\vec{x}'\right)+1\right)$$

Notice that $\vec{f}(\vec{x}')$ is nondimensional.

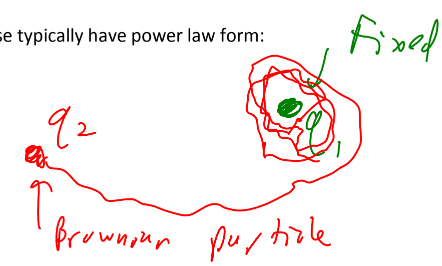
$$\vec{x}' = \frac{\vec{x}}{l_F}$$

This works well when the force function has a single relevant length scale. It could have multiple length scales...straightforward but more complicated generalization.

But some important physical forces have no length scales!

Like (unscreened) electromagnetic interaction, van der Waals force, etc. These typically have power law form:

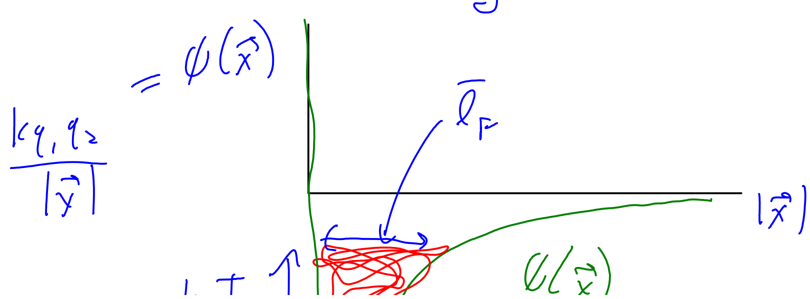
$$\vec{F}(\vec{x}) = \frac{k q_1 q_2 \vec{x}}{|\vec{x}|^3}$$



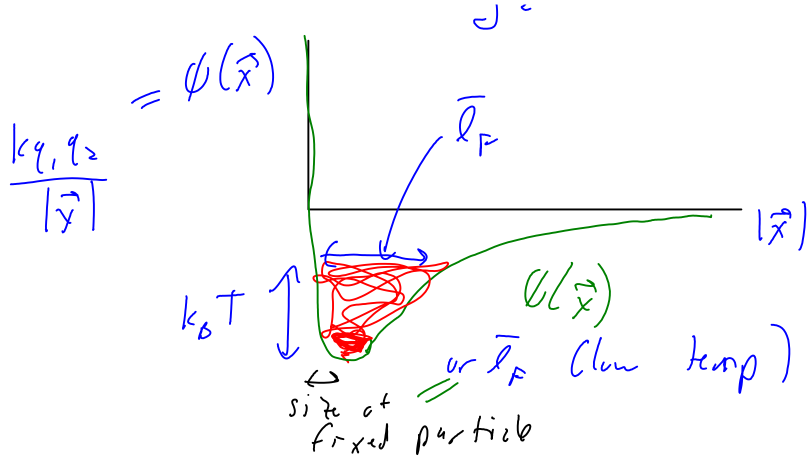
There's no length scale, and in fact no real force scale either

$$[k q_1 q_2] = \frac{M L^3}{T^2} \qquad q_1 q_2 < 0$$

In this case,



In this case,



At low temperatures, one could take the force length scale to be the length scale of the repulsive core of the fixed charge.

At temperatures high enough so that the Brownian particle can make large excursions relative to the size of the repulsive core, a better choice of length scale would be the one corresponding to how far away it typically gets.

Once you choose a length scale, then you can associate a force scale

$$\bar{F} = \frac{|k q_1 q_2|}{l_{\bar{F}}^2}$$

Alternatively, one can nondimensionalize directly without reference to a force amplitude and length scale, but we won't do this separate calculation -- it leads to the same result essentially.

Now that we have listed all the parameters and variables in the problem, along with their dimensions, the next step is to reformulate the system in terms of nondimensional variables. This is guaranteed to work and not only that, the nondimensionalized system will have fewer parameters/variables than the original system. The number of degrees of freedom that are reduced by nondimensionalization is equal to the number of independent dimensions in the problem (in our case 3: mass, length, time). This will allow us to go from dealing with 3 variables and 5 parameters to 3 nondimensional variables and 2 nondimensional parameters. This is fully equivalent to the original system.