Physics (6)562:
Problem Set 11: Correlations and dynamics

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1 Damped oscillator

Do Sethna Ex. 10.3.

I’m sure many of you have been teaching the damped harmonic oscillator in introductory mechanics. This exercise shows you can get nontrivial results just a step or two beyond that.

Also keep in mind that we may always approximate the free energy functional of a translationally invariant system by a sum over independent Fourier modes. If you allow each of these modes to have its own resonant frequency and damping, the treatment in this problem carries over to give the full space/time dependent dynamic behavior, both correlation and response functions.

2 Einstein relation

This short exercise is somewhat marooned, as it was covered in Sethna 6.7 but seems more at home in the present unit on dynamics. It is closely related to the ideas of Langevin dynamics found in Sethna Ex. 10.7.

Review diffusion (from Unit 2): the diffusion current was

$$J_{\text{diff}} = -D \nabla \rho(\mathbf{r})$$

(2.1)

where $D$ is the diffusion constant, which also quantifies the random walks e.g. $\langle |\Delta \mathbf{r}|^2 \rangle = (2d)Dt$ in spatial dimension $d$, and $\rho(\mathbf{r})$ is the density. (I’ve been deliberately vague as to whether this is the probability density for an ensemble describing the motion of one particle, or the macroscopic density of a large number of independent copies of the particle. As we showed back in Unit 2, both densities obey the same equations.)

Say also that, besides the random component of the particle’s motion, there is a “drift” part

$$\mathbf{v}_{\text{drift}}(\mathbf{r}) = +\gamma \mathbf{f}_{\text{ext}}(\mathbf{r})$$

(2.2)
where \( f_{\text{ext}}(r) \) is any external force.

On the other hand, in the presence of an external potential \( V(r) \) — e.g. due to gravity — the equilibrium density is given by the Boltzmann distribution:

\[
\rho(r) \propto e^{-\beta V(r)}.
\] (2.3)

Finally, in a steady state

\[
\frac{\partial \rho(r)}{\partial t} = \nabla \cdot \left( \rho v_{\text{drift}}(r) \right) = 0.
\] (2.4)

Put all this together to infer \( D = \gamma T \), the Einstein relation.

The Einstein is the original fluctuation-dissipation relation. The “\( D \)” expresses the “fluctuation” i.e. the random walk excursions, related to correlation functions; the \( \gamma \) is an example of a linear response coefficient.

## 3 Fluctuation-dissipation relation: numerical

Do Sethna Ex. 10.6, which uses the same “ising” program you downloaded previously.

There is a subtlety in “measuring \( m(t) \)”. In principle, all we are guaranteed by the response function is an ensemble average, which would require repeating the simulation with different random numbers and averaging. Fortunately, the Ising model is “self averaging”, meaning that spatially disjoint chunks of the sample behave as almost independent random variables, so (thanks to the central limit theorem) the system total magnetization does a good approximation of the ensemble average. You just need to make the system big enough to beat down the statistical noise.