TD4 : The Langevin equation, in and out of equilibrium

Statistical Mechanics – iCFP M2

The Langevin equation will be our tool of choice to describe stochastic systems in the rest of this course. Here we train in its use, and familiarize ourselves with the notion that it can describe equilibrium as well as nonequilibrium systems.

1 The Ornstein-Uhlenbeck process

We consider a particle diffusing in a harmonic potential, described by the Langevin equation:

$$\partial_t x(t) = -\mu \partial_x U[x(t)] + \mu f(t) + \xi(t), \tag{1}$$

where μ is known as the mobility of the particle, $U = kx^2/2$ is the confining potential, $f(t)$ is a deterministic, externally imposed force, and ξ is a Gaussian white noise with

$$\langle \xi(t) \rangle = 0 \tag{2a}$$

$$\langle \xi(t)\xi(t') \rangle = 2D\delta(t-t'). \tag{2b}$$

Here D denotes the diffusion constant.

1.1 What famous relation relates μ and D at equilibrium?

1.2 Formally solve Eq. (1), expressing $x(t)$ as a function of $x(t=0) = x_0$, $\xi(t)$ and $f(t)$.

1.3 Express $\langle x(t) \rangle$ for $f(t) \neq 0$.

1.4 Express $\langle x(t_1)x(t_2) \rangle$ for $f(t) = 0$.

1.5 Write the propagator $P(x, t|x_0, 0)$ in the case $f(t) = 0$.

1.6 The response function $\chi(\tau)$ is defined as

$$\langle x(t) \rangle = \int_{-\infty}^{+\infty} [\chi(\tau) f(t-\tau)] \, \mathrm{d}\tau. \tag{3}$$

In the next few lectures we will dedicate a substantial amount of attention to the fluctuation-dissipation theorem, which states a relationship between $\chi(\tau)$ and the equilibrium autocorrelation function $C(\tau) = \langle x(t_0+\tau)x(t_0) \rangle_c$, namely

$$\chi(\tau) = -\frac{H(\tau)}{k_B T} \frac{\mathrm{d}C}{\mathrm{d}\tau}, \tag{4}$$

where H is the Heaviside step function. Refrain from computing $\chi(\tau)$ explicitely for now; just combine Eqs. (3) and (4) to describe the response of our system to a constant force $f(t) = f$. Using your considerable knowledge of Hookean springs, which familiar equilibrium relation do you recover from the fluctuation-dissipation theorem in this simple case?

1.7 Consider a system at steady-state, meaning a system has had sufficient time to go to thermal equilibrium since it was initiated at $t = 0$. Compute $\chi(\tau)$ explicitly for in this case, and check that Eq. (4) is indeed correct.

1.8 Now consider a system that hasn't yet relaxed to its steady state. Is the fluctuation-dissipation relation satisfied?

2 Nonequilibrium Langevin dynamics: the Hopf bifurcation

Consider the following two-dimensional relaxation equation:

$$\partial_t x_1 = -r x_1 + \omega_1 x_2 + \xi_1(t) + f_1(t) \quad (5a)$$

$$\partial_t x_2 = -\omega_2 x_1 - r x_2 + \xi_2(t), \quad (5b)$$

with $r > 0$, and where $\langle \xi_i(t) \rangle = 0$, $\langle \xi_i(t)\xi_j(t') \rangle = 2k_B T \delta_{ij} \delta(t - t')$ (note that we set the mobility to one in this exercise). A similar equation is commonly used to describe the relaxational dynamics of the hair bundle, the rod-shaped sensory organ of our inner ear anchored at its base [1]. In this context, x_1 represents the displacement of the tip of the bundle relative to the base (which can be directly observed experimentally), while x_2 is an internal active force (which cannot).

2.1 Setting the noise and force to zero for now, trace a typical relaxation trajectory for the system for $\omega_1 = \omega_2 = 1$ and $r \ll 1$.

2.2 Fourier transforming with respect to time, we define the response function in the frequency domain $\tilde{\chi}(\omega) = \int_{-\infty}^{+\infty} \chi(t) e^{i\omega t} \, \mathrm{d}t = \langle \tilde{x}_1(\omega) \rangle / \tilde{f}(\omega)$. What physical interpretation do you give to its real and imaginary part, respectively?

2.3 The measured values of its real part $\tilde{\chi}'(\omega)$ and its imaginary part $\tilde{\chi}''(\omega)$ are plotted in the left-hand side of Fig. 1. Why is this data surprising? Is it sufficient to conclude that the system is out of equilibrium?

2.4 Derive the expression of $\tilde{\chi}(\omega)$ in our system, and write $\tilde{\chi}''(\omega)$ separately.

2.5 Translate the fluctuation-dissipation theorem Eq. (4) into the frequency domain by writing $\tilde{\chi}''(\omega)$ as a function of $\tilde{C}(\omega)$. Do not to worry about $\tilde{\chi}'(\omega)$; there is a good reason why you shouldn't (see Appendix A).

2.6 Compute $\tilde{C}(\omega)$, the Fourier transform of the autocorrelation of x_1.

2.7 we now define the fluctuation-dissipation ratio

$$\frac{T_{\text{eff}}(\omega)}{T} = \frac{\omega \tilde{C}(\omega)}{2k_B T \tilde{\chi}''(\omega)}. \quad (6)$$

What is its expected value for an equilibrium system? What do you predict it to be for our system?

2.8 Could you have predicted that Eqs. (5) wouldn't give rise to an equilibrium dynamics from the onset?

2.9 Show that for some special choices of ω_1, ω_2 the system admits a thermal equilibrium. Now consider one such case, but assume that the noises ξ_1 and ξ_2 are associated with different temperatures. Is this sufficient to break the fluctuation-dissipation relation again?

2.10 Now consider the data on the right-hand side of Fig. 1. Is the hair bundle at equilibrium?

The fluctuation-dissipation theorem is the tool of choice to unambiguously characterize the non-equilibrium character of the dynamics of biological [2, 3] and glassy systems, among others. Some like to refer to T_{eff} as the system's "effective temperature". Be aware that this use of terminology is controversial, partly because it hardly makes any sense outside of the linear response regime.

3 Drawing lessons

Recapitulate the three distinct sources of nonequilibrium-ness that we have encountered in this exercise sheet.

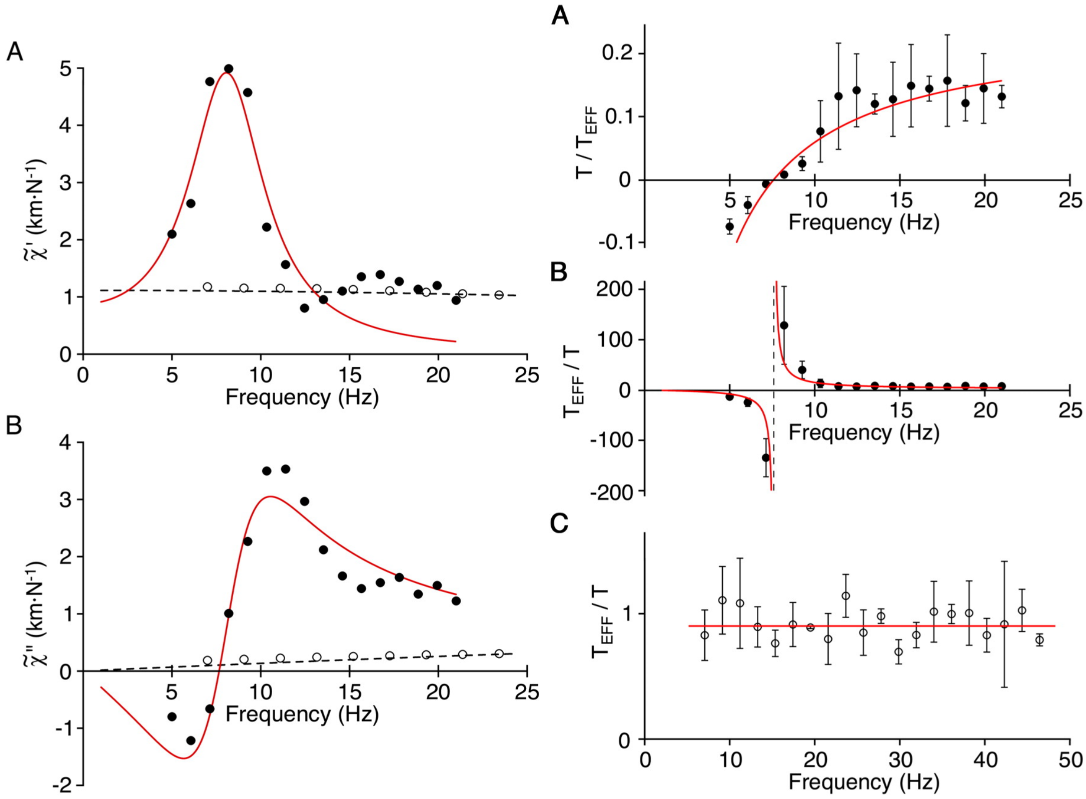

Figure 1: (*left*) Linear response functions as a function of stimulus frequency for an oscillatory hair bundle. (*right*) The "effective temperature" of spontaneous hair bundle motion. All open symbols represent data for a hair bundle whose displacement does not display large spontaneous fluctuations (*i.e.*, presumably a beat-up hair bundle).

References

[1] P Martin, A J Hudspeth, and F Jülicher. Comparison of a hair bundle's spontaneous oscillations with its response to mechanical stimulation reveals the underlying active process. *Proc. Natl. Acad. Sci. U.S.A.*, 98(25):14380–14385, December 2001.

[2] Daisuke Mizuno, Catherine Tardin, C F Schmidt, and F C Mackintosh. Nonequilibrium mechanics of active cytoskeletal networks. *Science*, 315(5810):370–373, January 2007.

[3] H. Turlier, D. A. Fedosov, B. Audoly, T. Auth, N. S. Gov, C. Sykes, J.-F. Joanny, G. Gompper, and T. Betz. Equilibrium physics breakdown reveals the active nature of red blood cell flickering. *Nat. Phys.*, 12:513–519, 2016.

A Kramers-Kronig relations

Physical causality implies that $\chi(\tau) = 0$ for $\tau < 0$. From this statement, it can be shown that the real and imaginary parts of $\tilde{\chi}(\omega)$ are not independent of one another, and that one can always be computed from the other as

$$\mathcal{P}\int_{-\infty}^{+\infty} \frac{\tilde{\chi}'(z)}{z-\omega}\,\mathrm{d}z = \pi\tilde{\chi}''(\omega), \qquad \mathcal{P}\int_{-\infty}^{+\infty} \frac{\tilde{\chi}''(z)}{z-\omega}\,\mathrm{d}z = -\pi\tilde{\chi}'(\omega), \tag{7}$$

where $\mathcal{P}\int$ denotes the principal value of the integral. These relations are known as the Kramers-Kronig relations. They imply that the fluctuation dissipation theorem is valid for $\tilde{\chi}(\omega)$ as a whole iff the right-hand side of Eq. (6) is equal to one.