# PHYS CS 5: Non-Equilibrium Statistical Mechanics - Problem Set 2

Sidharth Kannan

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1. ($\star\star$) **Position of a Brownian Walker** *(15 pts)*

   In the lecture notes, I threatened to ask you to compute the mean squared displacement of the Brownian walker. Do it! You should get that at equilibrium,

$$\langle(\Delta x)^2\rangle_{eq} = \frac{2kT}{\gamma}\left[t - \frac{m}{\gamma} + \frac{m}{\gamma}e^{-\frac{\gamma t}{m}}\right]$$

   A warning: This calculation is a bit tedious, but not very difficult problem. If you are feeling uncomfortable with the mechanics of working with expectations and correlation functions, then it is highly recommended you work through this one!

2. ($\star\star$) **Optical Tweezers** *(15 pts)*

   An optical tweezer is a device which uses highly concentrated laser light to trap and manipulate particles of matter. Biophysicists use such optical tweezers to "trap" single bacteria or DNA molecules. The laser acts like a Hookean spring, exerting a force $F = -kx$. In such micro and nanoscale interactions, Brownian motion is non-negligible. For such experiments, the overdamped Langevin equation (no inertial term) provides a good approximation:

$$0 = -\gamma\dot{x} - kx + \delta F(t)$$

   Compute the expected variance of the position of this particle, $\langle(\Delta x)^2\rangle$. This is an example of a system where there are competing forces: the trap tries to keep the particle near the bottom of the potential well, while the Brownian motion tries to kick it out.

3. ($\star\star$) **Self-Adjointness of the Fokker-Planck Operator** (*15 pts*)

   Define the Fokker-Planck operator as

$$\mathcal{L} = \frac{1}{\gamma}\frac{\partial}{\partial x}\left(\cdot\,,\frac{\partial V}{\partial x}\right) + D\frac{\partial^2}{\partial x^2}$$

   The $\cdot$ in the parenthesis indicates that the function the operator is acting on goes there. Show that $\mathcal{L}$ is *not* Hermitian with respect to the $L_2$ norm. That is, show that for some arbitrary (normalizable) functions $f, g$

$$\langle f, \mathcal{L}g\rangle \neq \langle \mathcal{L}f, g\rangle$$

where as usual,

$$\langle f, g \rangle \equiv \int_{-\infty}^{\infty} dx f(x) g(x)$$

Unlike in your prior courses in linear algebra, recall that here, the FP operator acts on *real* valued function spaces, so there's no need to worry about complex conjugation.

4. ($\star\star\star$) **Fokker-Planck in a Harmonic Potential** *(30 pts)*

   In this problem, we will solve the Fokker-Planck equation for a harmonic potential by using the harmonic oscillator solutions for Schrödinger's equation.

   (a) *(2 pts)* The harmonic oscillator potential is given by $V(x) = \frac{1}{2}kx^2$. Plug this into the Fokker-Planck equation. This is the equation we are going to solve.

   (b) *(5 pts)* Recall that the first step in using the analogy to Schrödinger's equation is to find the equilibrium distribution. To do this, we should set $\frac{dP}{dt} = 0$ and solve the resulting differential equation for $P_{\text{eq}}(x)$.

   This is not a trivial differential equation to solve. The principled way to do it, if you don't already have some idea what the solution should be, would be to assume a series solution, and then derive a recurrence for the coefficients of the series solution.

   Instead, I will ask you to just show by plugging it in, that

   $$P(x) = c_1 \exp\left(\frac{-kx^2}{2D\gamma}\right)$$

   solves the equation. Also compute the normalization constant, $c_1$. There is another linearly independent solution (written in terms of the error function), but it is not normalizable so we will disregard it.

   (c) *(5 pts)* Using the result from lecture, determine the effective potential $U_{\text{eff}}(x)$ that the corresponding Schrodinger equation satisfies. Write down the equation of motion for $\tilde{P}$.

   $$-\frac{\partial \tilde{P}}{\partial t} = \left[-D\frac{\partial^2}{\partial x^2} + \frac{k^2x^2}{4\gamma^2 D} - \frac{k}{2\gamma}\right]\tilde{P}$$

   The last term is a constant, so we can see that the resulting equation is the same as the quantum harmonic oscillator Hamiltonian, with a constant energy shift.

   (d) *(3 pts)* The standard quantum harmonic oscillator Hamiltonian is written as

   $$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$$

   Drop the constant term in our transformed FP operator and identify the expressions for $\hbar$ and $\omega$, in terms of the constants in our transformed Fokker-Planck equation.

   $$\omega = \frac{k}{\gamma\hbar}, \quad \hbar = \sqrt{2mD}$$

(e) *(10 pts)* We know the energies of the quantum harmonic oscillator are given by

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

Plug in the expressions for $\hbar$ and $\omega$ from the last part. Show that if you plug the constant energy shift back in, you get $E_0 = 0$. Finally, now that you know the energies, write out the solution for Schrodinger's equation, transform it back, and write the final solution for $P(x, t)$.

(f) *(5 pts)* The higher energy eigenmodes of Schrodinger's equation correspond to the non-equilibrium modes of our solution to the Fokker-Planck equation. Comment briefly on how the various constants in the Schrodinger equation affect the energy spacing, and what this implies about the way the various constants in the Fokker-Planck equation affect the spectral gap and thus the relaxation time of our solution.

*Remark: This method can be used to compute various other solutions for the Fokker-Planck equation. For example, the case of a linear potential is related via similarity transform to the delta well problem in quantum mechanics. For more on this, I refer you to 'The Fokker-Planck Equation: Methods of Solution and Applications' by Risken.*