New York University
Physics Department
Class GA.2061 "Non-Equilibrium Statistical Physics", Fall 2021

Home Work 07 *Solutions*

1. Consider paper [1]. What are the variables y they used to monitor the fluctuations in their system? How many of them were used? What was the manifestation of broken detailed balance? Was it visible equally well on every plane (y_i, y_j)? Based on this paper, if some system exhibits sign of broken detailed balance in some variables (y_1, y_2), does it always mean that this system is in equilibrium? Conversely, if you see the signature of broken detailed balance on some plane, what is the conclusion?

Solution

They used three coarse grained variables, the amplitudes of three Fourier modes for their fluctuating filament. They do observe loopy currents on planes "Mode 1 – Mode 2" and "Mode 2 – Mode 3". This means, detailed balance is broken. As you can see in the paper, current projected on the plane "Mode 1 – Mode 3" is practically non-loopy, simply because of projection. Thus, if you do see a loop of current on some 2D plane, it is a reliable indication of the lack of detailed balance and, therefore, lack of equilibrium. But if you see no loop on some plane, this does not prove that the system is in equilibrium.

2. Consider a physical system being simulated on a computer. Suppose possible states of the system are labeled i (a good example would be an Ising model, on which case i means $\{\sigma_x\}$, the values of all spins in the system). The simulation proceeds by running the algorithm, which we can view as an artificial dynamics described by the master equation with transition rates

$$k_{i\to j} = e^{E_i} \min\left\{\frac{1}{\mu_i}e^{-E_i}, \frac{1}{\mu_j}e^{-E_j}\right\} \ , \tag{1}$$

where E_i is the system energy in the state i, while μ_i is the number of other states to which state i can be converted in one step of the artificial dynamics. For simplicity, energies here are measured in the units of thermal energy T, while single step of the algorithm is taken to be the unit of time. If this dynamics arrives to a steady state, is this steady state equilibrium or not?

Note: The single word answer, like "yes" or "no" will be considered unsatisfactory, even though one of them is right. You have to explain and justify your answer.

Solution

This algorithm is called Metropolis Monte Carlo, its steady state is equilibrium, because it satisfies the detailed balance. Indeed, $P^{\mathrm{eq}}(i) = e^{-E_i}/Z$, therefore

$$P^{\mathrm{eq}}(i)k_{i\to j} = \min\left\{\frac{1}{\mu_i}e^{-E_i}, \frac{1}{\mu_j}e^{-E_j}\right\} = P^{\mathrm{eq}}(j)k_{j\to i} \ . \tag{2}$$

The way it works is usually as follows. If the system is in state i, we randomly choose one of the possible μ_i possible steps as a "suggestion", and then accept this suggestion with probability $\min\left\{1, \frac{\mu_i}{\mu_j}\exp\left(E_i - E_j\right)\right\}$; if suggestion is accepted, we move to j, otherwise we remain in i and play the game again, etc.

Note that in general detailed balance is satisfied as soon as rate constants are presented in the form e^{+E_i} times a symmetric function of i and j.

3. Consider a colloidal particle in a viscoelastic medium, captured in a laser trap. Laser trap acts as a harmonic potential well, $U(\mathbf{x}) = {}^1\!/\!{}_2 k\mathbf{x}^2$, while friction force in viscoelastic medium is given by the causal kernel $\zeta(\tau)$, $f_{\mathrm{friction}} = -\int_{-\infty}^{t}\zeta(t-t')\dot{x}(t')dt'$. Find time-time correlation function of the Langevin random force.

Solution

Langevin random force can be understood as the random force imbalance in the statement of the Newton's second law:

$$m\ddot{x} - f_{\mathrm{friction}} + \nabla U(x) = f_{\mathrm{random}}(t) \ . \tag{3}$$

Or more explicitly

$$m\ddot{x} + \int_{-\infty}^{t}\zeta(t-t')\dot{x}(t')dt' + kx = f_{\mathrm{random}}(t) \ . \tag{4}$$

Upon Fourier transforming, we have in frequency domain

$$\left[-m\omega^2 - \imath\omega\zeta_\omega + k\right] x_\omega = f_{\mathrm{random}\ \omega} \implies \chi_\omega = \frac{1}{\left[-m\omega^2 - \imath\omega\zeta_\omega + k\right]} \ , \tag{5}$$

where χ is the response function which describes the response of variable x to the conjugate force. The sign convention for Fourier transforms is as follows:

$$x_\omega = \int_{-\infty}^{\infty} x(t) e^{\imath\omega t} dt \ ; \quad x(t) = \int_{-\infty}^{\infty} x_\omega e^{-\imath\omega t} \frac{d\omega}{2\pi} \ . \tag{6}$$

Now, let us use the Fluctuation-Dissipation Theorem:

$$\left(x^2\right)_\omega = \frac{2T}{\omega}\chi''_\omega \ . \tag{7}$$

Since we want correlation of forces, we can address that directly, noting that $f_\omega = x_\omega/\chi_\omega$ and, therefore, $\left(f^2\right)_\omega = \left(x^2\right)_\omega / \left|\chi_\omega\right|^2$. Therefore,

$$\left(f^2\right)_\omega = \frac{2T}{\omega}\frac{\chi''_\omega}{\left|\chi_\omega\right|^2} = -\frac{2T}{\omega}\left(\frac{1}{\chi_\omega}\right)'' \ . \tag{8}$$

This is nice, because $1/\chi_\omega$ is known to us, and we directly find its imaginary part: $\left(\frac{1}{\chi_\omega}\right)'' = -\omega\zeta'_\omega$. Thus,

$$\left(f^2\right)_\omega = 2T\zeta'_\omega \ . \tag{9}$$

Now, what is left is to invert the Fourier transform. According to Wiener-Khinchin theorem, time-time correlation function is the inverse Fourier transform of the power spectrum:

$$\langle f(t)f(0)\rangle = \int_{-\infty}^{\infty} \left(f^2\right)_\omega e^{-\imath\omega t}\frac{d\omega}{2\pi} = 2T\int_{-\infty}^{\infty} \zeta'_\omega e^{-\imath\omega t}\frac{d\omega}{2\pi} \ . \tag{10}$$

In the definition of ζ_ω, we identify the real part:

$$\zeta_\omega = \int_0^\infty \zeta(\tau) e^{\imath\omega\tau} d\tau \implies \zeta'_\omega = \int_0^\infty \zeta(\tau)\cos\omega\tau d\tau \ . \tag{11}$$

Plugging this back to the expression above and re-grouping the integrals leads to the integral which is easy to evaluate:

$$\int_{-\infty}^{+\infty} e^{-\imath\omega t}\cos\omega\tau\frac{d\omega}{2\pi} = \frac{1}{2}\int_{-\infty}^{+\infty}\left[e^{-\imath\omega(t-\tau)} + e^{-\imath\omega(t+\tau)}\right]\frac{d\omega}{2\pi} = \frac{1}{2}\left[\delta(\tau - t) + \delta(\tau + t)\right] \ . \tag{12}$$

This finally yields

$$\langle f(t)f(0)\rangle = T\left(\zeta\left(t\right) + \zeta\left(-t\right)\right) \ . \tag{13}$$

To understand this result, remember that $\zeta(t)$ is a causal kernel, which means $\zeta(t) = 0$ at $t < 0$. Pay attention to the fact that this condition is imposed at $t < 0$, with point $t = 0$ <u>excluded</u>. In particular, if there is no instantaneous action, which means if $\zeta(0) = 0$, then either $\zeta(-t) = 0$ (at $t < 0$) or $\zeta(t) = 0$ (at $t > 0$), or both $\zeta(-t) = \zeta(t) = 0$ (at $t = 0$); in this case, the result can be re-written as

$$\langle f(t)f(0)\rangle = T\zeta\left(|t|\right) \ . \tag{14}$$

In the opposite limit, if there is no memory, when friction force at time t is determined solely by the velocity at that same moment t, then $\zeta(t) = \zeta_0\delta(t)$, and both terms $\zeta(t)$ and $\zeta(-t)$ contribute, leading to the familiar result for the white noise case

$$\langle f(t)f(0)\rangle = 2T\zeta_0\delta\left(t\right) \ . \tag{15}$$

4. Imagine a rod-like particle that undergoes random turns – random walk in the "space of orientations". You can imagine that this particle is a vector and its end undergoes a random walk around a sphere. Suppose it starts at $t = 0$ in the North pole (you can always choose North pole properly). If a particle were to diffuse on a plane, its displacement would be distributed according to $\propto e^{-x^2/4Dt}$, with mean-squared-average $\left\langle x^2 \right\rangle = 4Dt$. But on a sphere you cannot diffuse like that, there is no room. Assuming the direction of your particle in $3D$ is a unit vector $\mathbf{u}(t)$, find time-dependent correlation function $\langle \mathbf{u}(t) \cdot \mathbf{u}(t') \rangle$.

   What are the units of angular diffusion coefficient? If the particle starts pointing to the North pole, with time its distribution will spread and eventually relax to a uniform distribution around the sphere. What is the relaxation time – the time over which the particle "forgets" its initial orientation?

   Hint: Write down the diffusion equation for the time-dependent probability distribution $\pi_t(\mathbf{u}(t))$. Look for a solution in the form of expansion over spherical harmonics; since the system is isotropic around North-South axis, it follows that $m = 0$ (in standard quantum mechanics notations) and angular harmonics are reduced simply to Legendre polynomials $P_\ell(\cos\theta)$. Knowing the initial condition, find time-dependent coefficients of the expansion. Make sure to establish that at short times, when you diffuse over a small almost flat patch around North pole you obtain the standard result of $2D$ diffusion.

   Solution

   Diffusion equation looks the usual way

$$\partial_t \pi_t(\mathbf{u}) = D_{\mathrm{ang}} \Delta_{\mathrm{ang}} \pi_t(\mathbf{u}) \ , \tag{16}$$

   except Laplace operator is only the angular part of the laplace operator in spherical coordinates, because we only move around the sphere. Angular diffusion coefficient D_{ang} has units of inverted time.

   Thus, we look for the solution in the form $\pi_t(\mathbf{u}) = \sum_{\ell=0}^{\infty} C_\ell(t) P_\ell(\cos\theta)$. You hopefully remember from quantum mechanics that $\Delta_{\mathrm{ang}} P_\ell(\cos\theta) = -\ell(\ell+1) P_\ell(\cos\theta)$ and thus you can obtain

$$\sum_{\ell=0}^{\infty} \dot{C}_\ell(t) P_\ell(\cos\theta) = -D_{\mathrm{ang}} \sum_{\ell} \ell(\ell+1) C_\ell(t) P_\ell(\cos\theta) \quad \Longrightarrow \quad \dot{C}_\ell(t) = -\ell(\ell+1) D_{\mathrm{ang}} C_\ell(t) \ . \tag{17}$$

   This must be valid at $t > 0$. But at $t = 0$ our particle points to the North pole, meaning $\pi_0 = \frac{1}{4\pi}\delta(0)$. North pole corresponds to $\theta = 0$ or $\cos\theta = 1$. Since all Legendre polynomials are normalized such that $P_\ell(1) = 1$, we obtain $C_\ell(0) = (2\ell+1)/4\pi$. This means, $C_\ell(t) = \frac{1}{4\pi}(2\ell+1)e^{-D_{\mathrm{ang}}\ell(\ell+1)t}$, and the solution is now

$$\pi_t(\mathbf{u}) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} e^{-D_{\mathrm{ang}}\ell(\ell+1)t} P_\ell(\cos\theta) \ . \tag{18}$$

   With growing time, exponentials rapidly die out, and only the $\ell = 0$ term survives, which is the constant $1/4\pi$: as expected, the rod direction gets uniformly spread around the sphere. The slowest dying correction to it is at $\ell = 1$, and it has relaxation time $1/2D$.

   Now we need the correlation function $\langle \mathbf{u}(0) \cdot \mathbf{u}(t) \rangle$. Since $\mathbf{u}(0)$ points to the North pole, this correlation function is nothing else but $\langle \cos\theta \rangle$, or $\langle P_1(\cos\theta) \rangle$. The later average is the integral around the sphere $\int P_1(\cos\theta) \pi_t(\mathbf{u}) d^2\mathbf{u}$. Because of orthogonality of Legendre polynomials, only the $\ell = 1$ term survives and gives

$$\langle \mathbf{u}(0) \cdot \mathbf{u}(t) \rangle = \langle \cos\theta \rangle = e^{-2D_{\mathrm{ang}}t} \ . \tag{19}$$

   Very simple answer! At $t \ll 1/D_{\mathrm{ang}}$, the particle only slightly deviates from its original direction. More specifically, angle θ is small, $\cos\theta \simeq 1 - \theta^2/2$ while $e^{-2D_{\mathrm{ang}}t} \simeq 1 - 2D_{\mathrm{ang}}t$, which means $\left\langle \theta^2 \right\rangle = 4D_{\mathrm{ang}}t$ – exactly the answer you expect for diffusion on the plane. Over the relaxation time $1/2D_{\mathrm{ang}}$ the intial direction gets forgotten, with $\langle \cos\theta \rangle \approx 0$, meaning all values of angle are equally probable.

5. Consider Smoluchowski equation (i.e., diffusion equation in an external potential field $U(x)$ (in any dimension you like). We usually say that the current there includes diffusion and drift. Show that it can be equivalently presented as containing drift only, except it is "drift" not in the regular potential $U(x)$, but in chemical potential $\mu(x)$. Show that "diffusion" in this interpretation means simply the drift driven by the "entropic force".

   Solution

   Moved to the next HW

6. Consider the following simple three state model: a system has three states, 1, 2, and 3, with rate constants as indicated: $k_{1\to 2}$, $k_{2\to 1}$, and $k_{2\to 3}$. We want to know MFPT from 1 to 3. Since we want first passage to the state 3, we impose absorbing boundary condition at 3, which means nothing comes out of state 3, state 3 is a perfect trap, which is why we do not need to specify $k_{3\to 2}$. We know that each rate constant is the inverse of the MFPT for the same step, i.e. $\langle \tau_{i\to j}\rangle = 1/k_{i\to j}$. Knowing the time needed to go from 1 to 2 and then from 2 to 3, one should expect overall time from 1 to 3 to be $\langle \tau_{1\to 2}\rangle + \langle \tau_{2\to 3}\rangle = \frac{1}{k_{1\to 2}} + \frac{1}{k_{2\to 3}}$: if a train takes 2 hours from NYC to Philly, and then 3 hours from Philly to DC – then you expect the time from NYC to DC to be 5 hours, isn't that right[1]? Now let us approach this problem differently, using the auxiliary steady process: let us feed a constant current J into the state 1, collect the outgoing current J from state 3, and adjust J such that there is just one particle in the system. Solve the problem this way. Do you obtain the same or a different answer? If different, then why? Which one is right? What specifically is wrong with the wrong one?

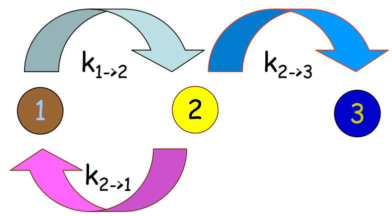

FIG. 1. Three state model.

Solution

Suppose in the steady state the probability to be on state 1 is c_1 and on state 2 it is c_2, and we want to have one particle in the system, then $c_1 + c_2 = 1$. Equation $\mathrm{div}\mathbf{J} = 0$ in this discrete case means that currents flowing into any node must be balanced by the currents flowing out. For node 1 this means $J_{\mathrm{in}} + c_2 k_{2\to 1} = c_1 k_{1\to 2}$, and for node 2 this reads $c_1 k_{1\to 2} = c_2 k_{2\to 1} + c_2 k_{2\to 3}$, and for the node 3 it is $c_2 k_{2\to 3} = J_{\mathrm{out}}$.

A few lines of algebra then shows that $J_{\mathrm{in}} = J_{\mathrm{out}}$, as expected, and then MFPT

$$\langle \tau \rangle = \frac{1}{J} = \underbrace{\frac{1}{k_{1\to 2}} + \frac{1}{k_{2\to 3}}}_{\langle \tau_{1\to 2}\rangle + \langle \tau_{2\to 3}\rangle} + \frac{k_{2\to 1}}{k_{1\to 2}k_{2\to 3}} \ . \tag{20}$$

Thus, we obtain mean first passage time which is longer than just $\langle \tau_{1\to 2}\rangle + \langle \tau_{2\to 3}\rangle$. Continuing the analogy with trains, this is because our "train", upon arrival to Philadelphia, has some probability to continue towards DC, but it has also some probability to go back to NYC. Thus, last term in our result for overall time is due to the possibility of un-productive going back and forth between nodes 1 and 2.

The problems below are not required and will not be graded, but recommended to those students who want to improve their knowledge and performance.

7. Professor Alexandra Zidovska of our Department in the paper [2] examined velocity correlations of moving chromatin (chromatin is a functional form of DNA in cell nucleus). In the results, what is common and what is different from the primitive model which you examined in the home works, where you studied fluctuations of velocity in an incompressible fluid?

Solution

The most obvious difference is the presence of coherently moving domains in chromatin. Nothing of this sort is observed in a simple incompressible fluid.

8. Consider again Rouse model of a polymer chain. Find mean-square average displacement of a monomer after time t, both for times short compared at Rouse relaxation time, and for longer times. Explain your results.

Solution

See, e.g., in my book [3, Sec. 31] or the book [4].

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[1] Just in case you don't know, Philadelphia is located between New York City and Washington DC, and there is no other way for a train to go from NYC to DC but via Philadelphia.

[1] C. Battle, C. P. Broedersz, N. Fakhri, V. F. Geyer, J. Howard, C. F. Schmidt, and F. C. MacKintosh, Broken detailed balance at mesoscopic scales in active biological systems, Science **352**, 604 (2016).
[2] A. Zidovska, D. A.Weitz, and T. J.Mitchison, Micron-scale coherence in chromatin interphase dynamics, Proc. Natl. Acad. Sci. USA **110**, 15555 (2013).
[3] A. Y. Grosberg and A. R. Khokhlov, *Statistical Physics of Macromolecules* (AIP, 1994) p. 350.
[4] M. Rubinstein and R. Colby, *Polymer Physics* (Oxford University Press, 2005) p. 442.