Example Sheet #2

1. *Brownian motion with inertia.* Here we generalize the Langevin equation discussed in lecture to a particle with inertia.

(a) Consider the Langevin equation for a single particle of mass m, drag coefficient γ and random forcing $\mathbf{A}'(t)$,

$$m\frac{d\mathbf{u}}{dt} = -\gamma\mathbf{u} + \mathbf{A}'(t) \ . \tag{1}$$

Assume the random force has zero mean and a variance $< \mathbf{A}'(t) \cdot \mathbf{A}'(t') >$ that is a function $\phi(|t-t'|)$ decaying very rapidly with $t - t'$, satisfying $\int_{-\infty}^{\infty} dy\phi(y) = m^2\tau$. If $\mathbf{u}(0) = \mathbf{u}_0$ and $\mathbf{r}(0) = \mathbf{r}_0$ are the initial velocity and position, solve (1) to obtain $\mathbf{U} \equiv \mathbf{u}(t) - \mathbf{u}_0 e^{-\zeta t}$ formally in terms of $\mathbf{A}$, where $\zeta = \gamma/m$ and $\mathbf{A} = \mathbf{A}'/m$. From this deduce the variance $\langle U^2 \rangle$ and thereby determine τ from equipartition.

In order to evaluate higher moments of $\mathbf{U}$, assume that the random process $A(t)$ is Gaussian, so $\langle A(t_1)A(t_2)\cdots A(t_{2n+1})\rangle = 0$, and

$$\langle A(t_1)A(t_2)\cdots A(t_{2n})\rangle = \sum_{\text{all pairs}} \langle A(t_i)A(t_j)\rangle\langle A(t_k)A(t_l)\rangle\cdots$$

Considering carefully the number of pairs in the above sum, show that the moments satisfy

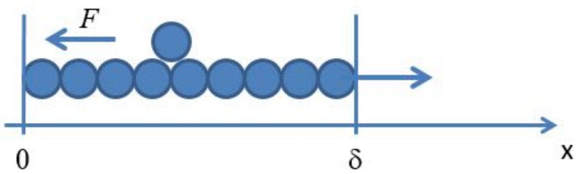
$$\langle U^{2n+1}\rangle = 0 \qquad \langle U^{2n}\rangle = (2n-1)!!\langle U^2\rangle^n$$

and hence that the probability distribution of $\mathbf{U}$ is Gaussian,

$$W(\mathbf{u}, t; \mathbf{u}_0) = \left[\frac{m}{2\pi k_B T(1-e^{-2\zeta t})}\right]^{3/2} \exp\left[-\frac{m|\mathbf{u} - \mathbf{u}_0 e^{-\zeta t}|^2}{2k_B T(1-e^{-2\zeta t})}\right] .$$

Integrate the equation for $\mathbf{u}$ to obtain the position vector $\mathbf{r}$. Find the mean and variance of $\mathbf{r}$. Examine the short and long-time behaviour and explain the distinction between the two.

2. *Polymerization.* Calculate how long it takes a linear polymer to polymerize to a length ℓ. Consider two cases, first without and second with a force $F > 0$ acting on the monomers.



To approach this problem, calculate first the *first passage time* τ_1 it takes a monomer to diffuse from $0 \to \ell$ for $F = 0$. You may assume that the particle reappears at the origin when it reaches position ℓ, thus ensuring that the probability p of finding the particle in the interval $(0, \ell)$ is unity . With this boundary condition one obtains a steady-state diffusion current $j = -D\partial p/\partial x$ with D the diffusion constant. Solve the steady-state diffusion equation $\partial^2 c/\partial x^2 = 0$ extracting j and the first passage time $\tau_1 = \ell^2/2D$. Now add a driving force F which acts on the monomer with friction coefficient ζ and solve the inhomogeneous equation

$$j = -D\frac{\partial p}{\partial x} - \frac{F}{\zeta}p \ .$$

Discuss your result for τ_1 in the case $F\ell \gg k_B T$.

3. *The wormlike chain.* As we saw in lecture, the wormlike chain is perhaps the simplest model of a polymer that accounts for its bending elasticity.
(a) A wormlike polymer of contour length L is subject to an external force f acting at its two ends, directed along the z axis. The effective energy is

$$\mathcal{E} = \frac{1}{2} A \int_0^L ds \kappa^2 - fz \ ,$$

where A is the bending modulus and z is the end-to-end extension. Consider the high-force limit, where the chain's configuration deviates only slightly from a straight line. Then the tangent vector $\hat{\mathbf{t}}$ fluctuates only slightly around $\hat{\mathbf{z}}$, the unit vector in the z direction. If we take t_x and t_y as independent fluctuating components, the constraint $|\hat{\mathbf{t}}| = 1$ shows that t_z deviates from unity quadratically in the vector $\mathbf{t}_\perp \equiv (t_x, t_y)$. Show that to quadratic order

$$\mathcal{E} \simeq \frac{1}{2} \int ds \left[A(\partial_s \mathbf{t}_\perp)^2 + f \mathbf{t}_\perp^2 \right] - fL \ .$$

Use equipartition to find the thermal average $\langle \mathbf{t}_\perp^2 \rangle$, being careful to account for the two independent components of $\mathbf{t}_\perp$. From this, show that in this high-force limit the force-extension relation takes the form

$$\frac{z}{L} = 1 - \frac{k_B T}{\sqrt{4fA}} \ . \qquad (1)$$

Compare this asymptotic result with that for the freely-jointed chain composed of N links, each of length b.

Calculate the correlation function $C(y) = \langle (1/L) \int_0^L ds \mathbf{t}_\perp(s) \cdot \mathbf{t}_\perp(s+r) \rangle$ of the tangent vector and thereby find the correlation length ξ, the length scale for decay of $C(y)$.

4. *Polymer chains.* (a) Consider a freely jointed chain (FJC) polymer consisting of two different types of monomers with length a and b with $a \neq b$. The polymer has a sequence *bababab*a... with $N/2$ monomers of each type. Calculate the room-mean-square end-to-end distance in the absence of any applied stretching force. Now apply a force f along the x-direction, with the origin of the chain fixed at $x = 0$. For very low forces, this is a harmonic spring with $f = \kappa \langle z \rangle$. Calculate the value of the spring constant κ of this chain.

(b) Now consider an almost ideal FJC with N monomers of type a. In this chain the maximum bending angle of the bonds between adjacent monomers is unconstrained between 0 and $\pi/2$ but is restricted from exceeding $\pi/2$. If $\boldsymbol{\zeta}_n$ represents the unit vector indicating the direction of monomer n, calculate $\langle \boldsymbol{\zeta}_n \cdot \boldsymbol{\zeta}_{n+1} \rangle$ where $\langle .. \rangle$ represents a thermal average.

5. *Stretching in electric fields.* Consider an ideal chain with $N = 1000$ segments of length $a = 0.5$ nm held at one end. Assume that in aqueous solution the chain carries $2e$ charges at the free end. What will be the average end-to-end distance $\langle z \rangle$ in a field $E = 30,000$ V/cm? At which field would $\langle z \rangle \approx 0.5(Na)$.

6. *A forced particle.* A microsphere of radius a and drag coefficient ζ is constrained to move along the x-axis, and is acted on by an optical trap which is moving in the positive x-direction at velocity v_T. When the trap is located at a point x_0 it exerts a force $F(x - x_0)$, so the overdamped dynamics of the particle is

$$\zeta \dot{x} = F(x - v_T t) \ .$$

Suppose that the trap has compact support, so that $F(x) = 0$ for $x < -X_L$ and for $x > X_R$. If the trap starts to the left of the particle, find the particle's net displacement Δx after the trap has passed it by, and the time Δt spent by the particle interacting with the trap. What is the condition that assures that the particle does not remain trapped as $t \to \infty$? Assuming this is the case, show that whatever the form of $F(y)$ the net displacement is always in the direction of the trap motion, and suggest a heuristic explanation for this result. Find the asymptotic behaviour of Δx for large trap velocities.

The trap is now moved around a circle of radius $R \gg a$. Derive the particle's net rotational frequency f_p as a function of the trap angular frequency $f_T = v_T/(2\pi R)$, the displacement Δx in each kick, the interaction time Δt and the potential width $2X_0 = X_R - X_L$. Confirm that in the regime of suitably large trap velocity, which you should define precisely, one obtains the intuitive result $f_p \simeq (\Delta x/2\pi R) f_T$. Specializing to the case of a triangular trapping potential, with $F(y) = F$ for $-X_0 < x < 0$ and $F(y) = -F$ for $0 < x < X_0$, obtain an explicit expression for f_p/f_c as a function of the two quantities $\alpha = X_0/(\pi R)$ and $\beta = f_T/f_c$, where $2\pi R f_c = F/\zeta$.

7. *Fluctuations of quasi-circular objects.* A long cylindrical vesicle of radius R_0, aligned along the z-axis, is subject to a tension $\sigma \gg \kappa/R_0^2$, where κ is the bending modulus. Thus, its energy is well-approximated by $\sigma\mathcal{S}$, where $\mathcal{S}$ is the total surface area of the vesicle. Assuming that fluctuations in the radius preserve axisymmetry, so the fluctuating radius $R(z)$ does not depend on the cylindrical polar angle, find the spectrum of thermal fluctuations as a function of the longitudinal wavevector q, at fixed enclosed volume of fluid. You may take $R(z) = \rho_0 + u_q \sin qz$, where ρ_0 is to be determined by volume conservation. Explain the significance of your result for $qR_0 < 1$.

A circular inclusion of radius R_0 in a lipid membrane consists of a distinct phase from the surrounding lipids, so there is a line tension γ between the two. Find the spectrum of thermal fluctuations in the radius, at fixed enclosed area, as above. Explain the significance of the result for the mode with $qR_0 = 1$.

8. *Fluctuations of elastic filaments.* An elastic filament with bending modulus A and length L has small-amplitude excursions $h(x)$ from the x-axis, and is characterized by the bending energy

$$\mathcal{E} = \frac{1}{2}\int_0^L dx A h_{xx}^2 \ .$$

a) Show that if the boundary conditions on the filament ends are taken to identical, then there are four distinct conditions that render the Euler-Lagrange operator self-adjoint. Explain how the terminology *free-free, clamped-clamped, hinged-hinged*, and *torqued-torqued* applies to these cases.

b) From general principles we know that the set of eigenfunctions of such an operator define a complete set of basis functions. Show that these can be written as

$$W^{(n)}(x) = A\cos(k^{(n)}x) + B\sin(k^{(n)}x) + D\cosh(k^{(n)}x) + E\sinh(k^{(n)}x) \ ,$$

and find the transcendental equation satisfied by $k^{(n)}$ for the case of *clamped-clamped* boundary conditions. By a graphical construction or otherwise give approximate values for the infinite sequence of wave vectors $k^{(n)}$.

c) Use the principle of equipartition to find the variance of $h(x)$, using the expansion $h(x) = \sum a_n W^{(n)}(x)$.

d) Suppose the filament is now subject to a spatially-varying tension $\sigma(x)$, with $\sigma(0) = \sigma(L) = 0$, so that the energy functional is now

$$\mathcal{E} = \frac{1}{2}\int_0^L dx \left\{ A h_{xx}^2 + \sigma(x) h_x^2 \right\} \ .$$

Find the Euler-Lagrange equation for this functional, and show how the modal decomposition necessary to apply equipartition can still be carried through formally (i.e. without solving explicitly for the modes).