## Part III: Biological Physics and Fluid Dynamics (Michaelmas 2023)

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Example Sheet #1

- 1. Interaction of charged surfaces with nonuniform charge density. Two parallel charged, planar, laterally-infinite membranes are located at  $z = \pm d/2$ . The upper one has charge density  $\sigma_+ = \sigma \cos(kx)$ , while the lower has  $\sigma_- = \sigma \cos(kx + \theta)$ , where  $\theta$  is a constant phase shift. Within Debye-Hückel theory, find the total electrostatic energy of the pair as a function of  $\theta$ . Find the value of  $\theta$  that minimizes the energy, averaged over one wavelength of the charge modulation, and explain the physical content of this result.
- 2. Electrostatic contributions to elastic energy of surfaces.
- (a) Using Debye-Hückel theory, calculate the electrostatic potential inside and outside of an infinite cylindrical shell of radius R and infinitesimal thickness, and a spherical shell of radius R and negligible thickness, assuming that the charge densities inside and out are  $\sigma_{\rm in} = \sigma(1-\epsilon)$  and  $\sigma_{\rm out} = \sigma(1+\epsilon)$ , where  $\epsilon$  is a parameter that determines the charge asymmetry.
- (b) By comparing the energies from (a), along with that of a plane with the same charge densities  $\sigma_{\rm in}$  and  $\sigma_{\rm out}$ , in the regime such that  $\kappa R \gg 1$ , where R is the cylinder or sphere radius and  $\kappa$  is the inverse screening length, deduce the electrostatic contribution to the elastic modulus  $k_c$ , Gaussian curvature modulus  $\bar{k}_c$ , and spontaneous curvature  $H_0$  in the Helfrich elastic energy

$$\mathcal{E} = \frac{1}{2}k_c \int dS (H - H_0)^2 + \frac{1}{2}\bar{k}_c \int dS K,$$

where  $H = (1/R_1 + 1/R_2)/2$  is the mean curvature and  $K = 1/R_1R_2$  is the Gaussian curvature (with  $R_1$  and  $R_2$  the principal radii of curvature).

- (c) Estimate  $k_c$ ,  $\bar{k}_c$ , and the spontaneous radius  $R_0 = 1/H_0$  for typical values of  $\sigma$ .
- **3.** Brownian motion with inertia. Here we generalize the Langevin equation discussed in lecture to a particle with inertia.

Consider the Langevin equation for a single particle of mass m, drag coefficient  $\gamma$  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  $\langle \mathbf{A}'(t) \cdot \mathbf{A}'(t') \rangle$  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  $\tau$  from equipartition.

In order to evaluate higher moments of **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

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

and hence that the probability distribution of 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.

4. The wormlike chain. 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 configurational energy of the polymer is

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

where A is the bending modulus,  $\kappa$  is the curvature, and z is the end-to-end extension.

(a) 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

$$\mathcal{E} \simeq rac{1}{2} \int\! ds \left[ A (\partial_s \mathbf{t}_\perp)^2 + f \mathbf{t}_\perp^2 
ight] - f L.$$

(b) 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

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

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