Physics of Soft and Biological Matter II: Problem Set 1

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Problem 1 *Langevin Dynamics Using ESPResSo, 5 points*

Use the provided Espresso script to simulate a single particle undergoing Langevin dynamics. Fit the short time and long time limits of the mean square displacement using a power law. How do the coefficient and exponent relate to the parameters of the Langevin equation in these two limits? Fit the velocity-velocity autocorrelation function. Relate the parameters in this fit to the variable found in the Langevin equation.
Solution: For the mean square displacement at short times the motion is ballistic and the velocity can be found via the equipartition theorem:

$$\begin{aligned}\frac{1}{2}m < v^2 >= \frac{d}{2}kT \\ < x^2/t^2 >= \frac{d}{2}\frac{kT}{m} \\ < x^2 >= \frac{d}{2}\frac{kT}{m}t^2,\end{aligned} \tag{1}$$

where d is the number of dimensions. At long times we have diffusive behaviour and the slope can be related to the definition of the diffusion coefficient:

$$\begin{aligned}D = \frac{x^2}{2dt} \\ < x^2 >= 2dDt \\ D\zeta = D\gamma m = kT < x^2 >= 2d\frac{kT}{\gamma m}t.\end{aligned} \tag{2}$$

For the velocity autocorrelation function we again use the equipartition theorem to get the y-intercept:

$$\begin{aligned}\frac{1}{2}m < v^2 >= \frac{d}{2}kT \\ < v^2 >= d\frac{kT}{m},\end{aligned} \tag{3}$$

The decay can be understood by solving the Langevin eqnarray without noise:

$$\frac{d^2x}{dt^2} = -\gamma\frac{dx}{dt} \tag{4}$$
$$< v(t)v(0) >= d\frac{kT}{m}\exp\left(-\gamma t\right).$$

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Problem 2 *Diffusion of DNA, 5 points*

a) Calculate the radius of gyration of a double-stranded λ-DNA strand with $N_{\text{bases}} = 48490$ base pairs. The Kuhn length is $b \approx 50\text{nm}$ and the distance between bases is $l = 0.34\text{nm}$ such that the number of "steps" is $N_{\text{bases}}l/b$. Use the formula:

$$\left\langle R_{\text{G}}^2\right\rangle = \frac{1}{N^2}\int_0^N\int_u^N (r(u) - r(v))^2 \text{d}v\text{d}u, \tag{5}$$

recalling that each subsection of a polymer is a random walk and thus

$$(r(u) - r(v))^2 = (u - v)b^2. \tag{6}$$

Solution: First we must solve the integral

$$\begin{aligned}
\left\langle R_{\text{G}}^2\right\rangle &= \frac{1}{N^2}\int_0^N\int_u^N (r(u) - r(v))^2 \text{d}v\text{d}u \\
\left\langle R_{\text{G}}^2\right\rangle &= \frac{1}{N^2}\int_0^N\int_u^N (v - u)b^2 \text{d}v\text{d}u \\
\left\langle R_{\text{G}}^2\right\rangle &= \frac{b^2}{N^2}\int_0^N (N^2/2 - u^2/2 - Nu + u^2)\text{d}u \\
\left\langle R_{\text{G}}^2\right\rangle &= \frac{b^2}{N^2}\int_0^N (N^2/2 - Nu + u^2/2)\text{d}u \\
\left\langle R_{\text{G}}^2\right\rangle &= \frac{b^2}{N^2}(N^3/2 - N^3/2 + N^3/6) \\
\left\langle R_{\text{G}}^2\right\rangle &= \frac{1}{6}Nb^2,
\end{aligned} \tag{7}$$

Next the number of random "steps" needs to be expressed in terms of the number of bases:

$$\begin{aligned}
\left\langle R_{\text{G}}^2\right\rangle &= \frac{1}{6}Nb^2 \\
\left\langle R_{\text{G}}^2\right\rangle &= \frac{1}{6}\frac{N_{\text{bases}}l}{b}b^2 \\
\sqrt{\left\langle R_{\text{G}}^2\right\rangle} &= \sqrt{\frac{1}{6}N_{\text{bases}}lb} \\
\sqrt{\left\langle R_{\text{G}}^2\right\rangle} &= 371\text{nm}.
\end{aligned} \tag{8}$$

b) Calculate the hydrodynamic friction coefficient, $\zeta = 6\pi\eta R_{\mathrm{H}}$,assuming $R_{\mathrm{H}} = R_{\mathrm{G}}$ in water at 20^0

Solution: Note that $\eta \approx 0.001$Pa·s:

$$\begin{aligned}\zeta &= 6\pi(0.001\mathrm{Pa}\cdot\mathrm{s})(371\mathrm{nm}) \\ \zeta &= 7.0\times10^{-9}\mathrm{kg/s}\end{aligned} \tag{9}$$

c) Use the relation $D = R_{\mathrm{G}}^2/\tau$ to calculate the relaxation time of the DNA fragment.

Solution: Use the Nernst-Einstein relation to get D from ζ and solve:

$$\begin{aligned}D &= \frac{R_{\mathrm{G}}^2}{\tau} \\ \frac{kT}{\zeta} &= \frac{R_{\mathrm{G}}^2}{\tau} \\ \tau &= \frac{R_{\mathrm{G}}^2\zeta}{kT} \\ \tau &= \frac{(371\mathrm{nm})^2 7.0\times10^{-9}\mathrm{kg/s}}{4.11\times10^{-21}\mathrm{J}} \\ \tau &= 0.23\mathrm{s}\end{aligned} \tag{10}$$

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Problem 3 *Metabolism of a Cell (Adopted from Biological Physics by Nelson), 5 points*

a) Calculate the flux of a substance with concentration c_0 at infinity into a spherical cell of radius R with concentration 0 at the surface. Hint: Use Fick's first law $j = -D\frac{dc}{dr}$ combined with the fact that the flux through all spherical shells at a distance r is constant to get an expression for the flux.

Solution: first create a formula from the fact that flux is constant at all r:

$$\begin{aligned}I = A(r)j(r) &= 4\pi r^2 j(r) \\ j(r) &= \frac{I}{4\pi r^2}\end{aligned} \tag{11}$$

Now sub into Fick's law and solve:

$$\begin{aligned}j &= -D\frac{dc}{dr} \\ \frac{I}{4\pi r^2} &= -D\frac{dc}{dr} \\ c &= A + \frac{B}{r}\end{aligned} \tag{12}$$

Using the boundary conditions $c = 0$ at $r = R$ and $c = c_0$ as r goes to infinity we get

$$c = c_0\left(1 - \frac{R}{r}\right) \tag{13}$$

Use Fick's law to get the flux and sub in $r = R$:

$$\begin{aligned} j(r) &= -D\frac{dc}{dr} \\ j(r) &= -Dc_0\frac{R}{r^2} \\ j(R) &= \frac{-Dc_0}{R} \end{aligned} \tag{14}$$

b) Find the flux for a cell of radius $R = 1\mu$m in an oxygen concentration $c_0 = 0.2$mole·m^{-3}.
Solution The problem is underspecified, lets take oxygen where $D \approx 2 \times 10^{-9}$m^2/s:

$$\begin{aligned} I &= A(R)j(R) \\ I &= 4\pi R^2\frac{Dc_0}{R} \\ I &= 4\pi RDc_0 \\ I &= 4\pi(1\mu\text{m})(2 \times 10^{-9}\text{m}^2/\text{s})0.2\text{mole} \cdot \text{m}^{-3} \\ I &= 5.0 \times 10^{-15}\text{mole} \end{aligned} \tag{15}$$

c) Knowing that the metabolic rate of a cell is roughly 0.02mole kg^{-1} s^{-1} calculate the approximate maximum size of a cell.
Solution: Equate the total consumption of oxygen with the total maximum flux from part a and set the density to that of water:

$$\begin{aligned} A(R)j(R) &= MV\rho \\ 4\pi R^2\frac{Dc_0}{R} &= M\frac{4}{3}\pi R^3\rho \\ R &= \sqrt{\frac{3Dc_0}{M\rho}} \\ R &= \sqrt{\frac{3(2 \times 10^{-9}\text{m}^2/\text{s})(0.2\text{mole} \cdot \text{m}^{-3})}{(0.02\text{mole} \cdot \text{kg}^{-1}\text{s}^{-1})(1000\text{kg}/\text{m}^3)}} \\ R &= 7.8\mu\text{m} \end{aligned} \tag{16}$$

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