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.

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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 $b \approx 50$nm and the distance between bases is $l = 0.34$nm such that the number of "steps" is $N_{\text{bases}} l/b$. Use the formula:

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

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

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

b) Calculate the hydrodynamic friction coefficient, $\zeta = 6\pi\eta R_{\text{H}}$,assuming $R_{\text{H}} = R_{\text{G}}$ in water at 20^0
c) Use the relation $D = R_{\text{G}}^2/\tau$ to calculate the relaxation time of the DNA fragment.

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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.
b) Find the flux for a cell of radius $R = 1\mu$m in an oxygen concentration $c_0 = 0.2$mole m^{-3}.
c) Knowing that the metabolic rate of a cell is roughly 0.02mole kg^{-1} m^{-1} calculate the approximate maximum size of a cell.

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