PHY420 Problems Class 2: Biopolymers

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1. **Normalise 3D Gaussian distribution** The probability of an end to end vector $\boldsymbol{R}$ for a 3 dimensional random walk of $N \gg 1$ steps is given by the Gaussian distribution:

$$P(\boldsymbol{R}) \sim e^{-3\boldsymbol{R}^2/(2Na^2)}.$$

Normalise this. You may use the standard result for a Gaussian integral as given on your formula sheet ($I = \int_{-\infty}^{+\infty} \mathrm{d}x\ e^{-ax^2} = \sqrt{\frac{\pi}{a}}$).

2. **Force-extension curve of a flexible polymer**

   (a) From the distribution given in question 1, find the entropy and from this the free energy of stretching a Gaussian polymer to $\boldsymbol{R}$, which is the end to end distance under the influence of the force f. From the free energy find the force f required to stretch the polymer. NB you may assume the internal energy is constant and absorb this into the constant term denoted by a letter of your choice.

   (b) The partition function for a flexible, freely jointed, chain subjected to a constant stretching force f, is given by:

$$Z = \int \mathrm{d}^2 a_1 \int \mathrm{d}^2 a_2 \ldots \int \mathrm{d}^2 a_N e^{-\frac{E}{k_B T}}$$

   where

$$E = -\boldsymbol{f} \cdot \boldsymbol{R} = -\sum_{i=1}^{N} f a \cos\theta_i,$$

   N is the number of subunits in the polymer and $\int \mathrm{d}^2 a_i$ is the integral over the angular spherical coordinates for fixed radius $r = a = 1$. Keep f as f here (don't substitute in your answer to the previous part). Calculate this partition function and from it the extention given by:

$$\langle R \rangle = k_B T \frac{\partial}{\partial f} \ln Z.$$

   (c) Show that for small forces the answer in (b) gives the same as (a).

3. *Optional extra:* In question 1 you used the standard result for a Gaussian integral. This question derives that result.

   (a) The Gaussian integral (as given on your formula sheet) is:

   $$I = \int_{-\infty}^{+\infty} \mathrm{d}x \; e^{-x^2} = \sqrt{\pi}.$$

   Prove this by writing down I^2 and transforming to *polar coordinates*. You should now be able to integrate explicitly.

   (b) Calculate

   $$I(a) = \int_{-\infty}^{+\infty} \mathrm{d}x \;\; e^{-\frac{a}{2}x^2}$$

   by transforming the integration variable and using the result given in (a).

   (c) Use the trick of “completing the square” to calculate:

   $$I(a,b) = \int_{-\infty}^{+\infty} \mathrm{d}x \;\; e^{-\frac{a}{2}x^2 - bx}.$$

   (d) Finally, use the knowledge you have gained above to compute:

   $$K = \int_{-\infty}^{+\infty} \mathrm{d}x_1 \;\; \exp\left[-\frac{a}{2}(x_0 - x_1)^2 - \frac{b}{2}(x_1 - x_2)^2\right].$$