

LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

## biophysikalische Chemie/molekulare Biophysik Wintersemester 2020/2021

## Solutions to Homework IV

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1. a) What is the Reynold's number of the bacterium?

$$R_e = \frac{\rho L v}{\eta} = \frac{1000 \frac{\text{kg}}{\text{m}^3} \cdot 2.8 \times 10^{-6} \,\text{m} \cdot 5.1 \times 10^{-6} \,\text{m/s}}{10^{-3} \,\text{Pa} \cdot \text{s}} = 1.428 \times 10^{-5}$$

b) What is the viscous drag on the bacterium?

$$\begin{split} F_{Drag} &= \gamma v = 6\pi \eta r v = 6\pi \; (10^{\text{-}3} \; \text{N} \cdot \text{s/m}^2) (1.4 \times 10^{\text{-}6} \, \text{m}) (5.1 \times 10^{\text{-}6} \; \text{m/s}) \\ &= 1.35 \times 10^{\text{-}13} \; \text{N} = 0.135 \; \text{pN} \end{split}$$

c) How far will the bacterium coast when it stops swimming?

$$d = \int_0^\infty \nu(t)dt = \nu(0) \cdot \tau$$

$$\tau = \frac{2r^2\rho}{9\eta} \approx \frac{2(1.4 \times 10^{-6}m)^2 (1000 \frac{kg}{m^3})}{9(0.001 Pa \cdot s)} = 4.36 \times 10^{-7} s$$

$$d = 5.1 \mu m/s \cdot 0.436 \mu s = 2.22 \times 10^{-12} m$$

2.

$$\begin{split} F_{Stall} &= \frac{\Delta G^0}{\delta} + \frac{k_B T}{\delta} \ln \left( \frac{[ADP][P_i]}{[ATP]} \right) \\ &= \frac{-54 \times 10^{-21} J}{3 \times 10^{-9} m} + \frac{1.38 \times 10^{-23} J/K \cdot 298 K}{3 \times 10^{-9} m} \ln \left( \frac{1 \times 10^{-5} M \cdot 1 \times 10^{-3} M}{1 \times 10^{-3} M} \right) \\ &= -3.4 \times 10^{-11} N = -34 \ pN \end{split}$$

3.  $1 \text{ cP} = 10^{-2} P = 10^{-2} g/(cm \cdot s) = 10^{-3} kg/(m \cdot s) = 10^{-3} Nsm^{-2}$ 

$$F_{\text{max}} = 6\pi \eta \text{rv}_{\text{max}} = 6\pi \cdot 1.002 \cdot 10^{-3} \text{ Nsm}^{-2} \cdot 0.5 \cdot 10^{-6} \text{ m} \cdot 180 \cdot 10^{-6} \text{ m/s} = 1.7 \text{ pN}$$

$$Q = \frac{F \cdot c}{n \cdot W} = \frac{1.7 \cdot 10^{-12} N \cdot 2.998 \cdot 10^8 \frac{m}{s}}{1.33 \cdot 30 \cdot 10^{-3} W} = 0.013$$

$$\left\langle r^{2} \right\rangle = \int_{0}^{\infty} r^{2}W(r)dr / \int_{0}^{\infty} W(r)dr$$

$$= \int_{0}^{\infty} 4\pi r^{4} \left(\frac{\beta}{\sqrt{\pi}}\right)^{3} e^{-\beta^{2}r^{2}}dr / \int_{0}^{\infty} 4\pi r^{2} \left(\frac{\beta}{\sqrt{\pi}}\right)^{3} e^{-\beta^{2}r^{2}}dr$$

$$= 4\pi \left(\frac{\beta}{\sqrt{\pi}}\right)^{3} \frac{3\sqrt{\pi}}{4} \frac{1}{2\beta^{5}} / 4\pi \left(\frac{\beta}{\sqrt{\pi}}\right)^{3} \frac{\sqrt{\pi}}{2} \frac{1}{2\beta^{3}}$$

= 1 (i.e. the distribution function was already normalized)

$$=\frac{3}{2\beta^2}$$

However,  $\beta = \left(\frac{3}{2nl^2}\right)^{\frac{1}{2}}$ , hence

$$\left\langle r^2 \right\rangle = \frac{3}{2\beta^2} = \frac{3}{2} \left( \frac{2nl^2}{3} \right) = nl^2$$

QED

5. A) L = 47365 bp  $\cdot$  3.32 nm per turn / 10.4 bp per turn = 15120 nm = 15.12  $\mu$ m

as L is much larger than the persistence length,

$$\langle R^2 \rangle^{\frac{1}{2}} = (2PL)^{\frac{1}{2}}$$
  
=  $(2 \cdot 0.053 \ \mu \text{m} \cdot 15.12 \ \mu \text{m})^{1/2} = 1.266 \ \mu \text{m}$ 

$$\frac{\left[E_{2}\right]}{\left[E_{1}\right]} = \exp\left(-\frac{\Delta G}{kT}\right) = \exp\left(-\frac{\Delta G^{0} - F\Delta x}{kT}\right) = K_{eq}^{0} \exp\left(\frac{F\Delta x}{kT}\right)$$

Solving for F, we have:

$$F = \frac{kT}{\Delta x} ln \left( \frac{[E_2]}{[E_1 K_{eq}^0]} \right)$$

$$= \frac{(1.38 \times 10^{-23} J/K)(310K)}{2.8 \times 10^{-9} m} ln \left( \frac{0.9}{(0.1)(1)} \right)$$

$$= 3.36 pN$$

7. 
$$1 \text{ cP} = 10^{-2} P = 10^{-2} g/(cm \cdot s) = 10^{-3} kg/(m \cdot s) = 10^{-3} Nsm^{-2}$$

$$F_{\text{max}} = 6\pi \eta \text{rv}_{\text{max}} = 6\pi \cdot 1.002 \cdot 10^{-3} \text{ Nsm}^{-2} \cdot 0.5 \cdot 10^{-6} \text{ m} \cdot 200 \cdot 10^{-6} \text{ m/s} = 1.9 \text{ pN}$$

$$Q = \frac{F \cdot c}{c \cdot W} = \frac{1.9 \cdot 10^{-12} \, N \cdot 2.998 \cdot 10^8 \, \frac{m}{s}}{1.33 \cdot 20 \cdot 10^{-3} \, W} = 0.02$$

8.

$$\left\langle r^{2} \right\rangle = \int_{0}^{\infty} r^{2}W(r)dr / \int_{0}^{\infty} W(r)dr$$

$$= \int_{0}^{\infty} 4\pi r^{4} \left(\frac{\beta}{\sqrt{\pi}}\right)^{3} e^{-\beta^{2}r^{2}} dr / \int_{0}^{\infty} 4\pi r^{2} \left(\frac{\beta}{\sqrt{\pi}}\right)^{3} e^{-\beta^{2}r^{2}} dr$$

$$= 4\pi \left(\frac{\beta}{\sqrt{\pi}}\right)^{3} \frac{3\sqrt{\pi}}{4} \frac{1}{2\beta^{5}} / 4\pi \left(\frac{\beta}{\sqrt{\pi}}\right)^{3} \frac{\sqrt{\pi}}{2} \frac{1}{2\beta^{3}}$$

= 1 (i.e. the distribution function was already normalized)

$$=\frac{3}{2\beta^2}$$

However,  $\beta = \left(\frac{3}{2nl^2}\right)^{\frac{1}{2}}$ , hence

$$\left\langle r^2 \right\rangle = \frac{3}{2\beta^2} = \frac{3}{2} \left( \frac{2nl^2}{3} \right) = nl^2$$

**OED** 

9. A)  $L = 48,502 \text{ bp} \cdot 3.32 \text{ nm per turn} / 10.4 \text{ bp per turn} = 15,483 \text{ nm} = 15.483 \text{ } \mu\text{m}$ 

as L is much larger than the persistence length,

$$\langle R^2 \rangle^{\frac{1}{2}} = (2PL)^{\frac{1}{2}}$$
  
=  $(2 \cdot 0.053 \ \mu \text{m} \cdot 15.483 \ \mu \text{m})^{1/2} = 1.641 \ \mu \text{m}$ 

B) For the Freely Jointed Chain model:  $\langle R^2 \rangle_{EIC} = N_B \beta^2 = \beta L$ 

For L>>P (15.483 µm >> 53 nm): 
$$\langle R^2 \rangle = 2PL = \beta L$$

Hence, then Kuhn length is:  $\beta = 2P = 2 \cdot 53 \text{ nm} = 106 \text{ nm}$ 

and the number of segments is:  $N_{\beta}=L/\beta=(15,483 \text{ nm})/(106 \text{ nm})=146$ 

10. A) 
$$r = \frac{I_Z - I_Y}{I_T}$$

where  $I_T = I_X + I_Y + I_Z$  is the total intensity and the subscript represents the axis along with the intensity is measured. For a sample consisting of two species:

$$\begin{split} r &= \frac{I_{Z1} + I_{Z2} - I_{Y1} - I_{Y2}}{I_T} \\ &= \frac{I_{Z1} - I_{Y1}}{I_T} + \frac{I_{Z2} - I_{Y2}}{I_T} \\ &= \frac{I_{T1}}{I_T} \frac{I_{Z1} - I_{Y1}}{I_{T1}} + \frac{I_{T2}}{I_T} \frac{I_{Z2} - I_{Y2}}{I_{T2}} \\ &= f_1 r_1 + f_2 r_2 \end{split}$$

where  $f_i$  and  $r_i$  are the fractional intensity and anisotropy of the  $i^{th}$  species respectively.

B) Consider a single molecule whose emission dipole is at an angle  $\theta$  with respect to the z axis, which represents the polarization of the excitation laser (see figure). Assume to begin with that the absorption dipole and emission dipole are parallel. The fluorescence intensity parallel and perpendicular to the z axis is given by:

$$I_{\parallel} = \cos^2 \theta$$
$$I_{\perp} = \sin^2 \theta \sin^2 \phi$$

As the sample is isotropic, all  $\phi$  orientations are equally likely. Averaging over all  $\phi$  values yields:

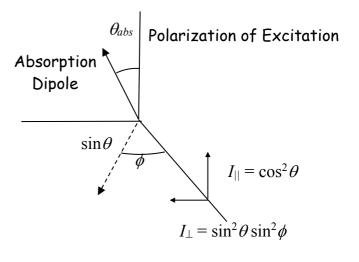
$$\left\langle \sin^2 \phi \right\rangle = \frac{\int_0^{2\pi} d\phi \sin^2 \phi}{\int_0^{2\pi} d\phi} = \frac{1}{2}$$

$$I_{\parallel} = \cos^2 \theta \qquad ; \qquad I_{\perp} = \frac{\sin^2 \theta}{2}$$

$$r = \frac{I_{\parallel} - I_{\perp}}{I_{\parallel} + 2I_{\perp}} = \frac{\cos^2 \theta - \sin^2 \theta / 2}{\cos^2 \theta + \sin^2 \theta}$$

$$= \frac{\cos^2 \theta - (1 - \cos^2 \theta) / 2}{1}$$

$$= \frac{3\cos^2 \theta - 1}{2}$$



As molecules are randomly orientated in the sample, we need to integrate over all possible orientations multiplied by the probability of excitation (a term known as photoselection). The probability of excitation is proportional to the angle between the absorption dipole and the polarization of the laser beam:

$$p(\theta) = \cos^2 \theta$$

Hence, the majority of excited molecules will have dipoles aligned along the z-axis and very few in the x-y plane. The number of molecules with an orientation between  $\theta$  and  $\theta$  + d $\theta$  is proportional to  $\sin \theta d\theta$ . Integrating over all orientations yields:

$$\left\langle \cos^2 \theta \right\rangle = \frac{\int_{0}^{\pi/2} \cos^2 \theta \ p(\theta) \sin \theta \ d\theta}{\int_{0}^{\pi/2} \int_{0}^{\pi/2} p(\theta) \sin \theta \ d\theta}$$

$$= \frac{\int_{0}^{\pi/2} \cos^4 \theta \sin \theta \ d\theta}{\int_{0}^{\pi/2} \cos^2 \theta \sin \theta \ d\theta}$$

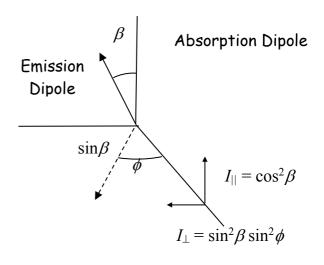
$$\left\langle \cos^2 \theta \right\rangle = \frac{3}{5}$$

$$r = \frac{3 \left\langle \cos^2 \theta \right\rangle - 1}{2}$$

$$= \frac{2}{5}$$

A molecule whose emission dipole is rotated by an angle  $\beta$  with respect to the absorption dipole will undergo an additional loss in anisotropy. The geometry between the absorption dipole and emission dipole is identical to the geometry we discussed above. Integrating over all possible values of  $\phi$ , the loss in anisotropy due to the rotation of the emission dipole with respect to the absorption dipole is given by:

$$r = \left(\frac{3\cos^2\beta - 1}{2}\right)$$



The total anisotropy is the product of the loss in anisotropy due to photoselection multiplied by the loss in anisotropy due to the non-parallel alignment of the absorption and emission dipoles:

$$r = \frac{2}{5} \left( \frac{3\cos^2 \beta - 1}{2} \right)$$

C) 
$$r = \frac{2}{5} \left( \frac{3\cos^2 \beta - 1}{2} \right) = 0.37$$